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SCDAP/RELAP5/MOD2 Code Manual

RELAP5 Code Structure, System
Models, and Solution Methods

Edited by C. M. Allison, E. C. Johnson

EG&G Idaho, Inc.

Prepared for
U.S. Nuclear Regulatory
Commission

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Models, and Solution Methods

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ABSTRACT

The SCDAP/RELAP5 code has been developed for best-estimate transient simulation of light water reactor coolant systems during a severe accident. The code models the coupled behavior of the reactor coolant system, the core, and the fission products and aerosols in the system during a severe accident transient as well as large and small break loss-of-coolant accidents, operational transients such as anticipated transient without SCRAM, loss of offsite power, loss of feedwater, and loss of flow. A generic modeling approach is used that permits as much of a particular system to be modeled as necessary. Control system and secondary system components are included to permit modeling of plant controls, turbines, condensers, and secondary feedwater conditioning systems.

The modeling theory and associated numerical schemes are documented in Volumes I and II to acquaint the user with the modeling base and thus aid in effective use of the code. Volume III contains detailed instructions for code application and input data preparation. In addition, Volume III contains user guidelines that have evolved over the past several years from application of the RELAP5 and SCDAP codes at the Idaho National Engineering Laboratory, at other national laboratories, and by users throughout the world.

EXECUTIVE SUMMARY

The light water reactor (LWR) severe accident transient analysis code, SCDAP/RELAP5, has been developed at the Idaho National Engineering Laboratory (INEL) for the U. S. Nuclear Regulatory Commission (NRC) to provide an advanced best-estimate predictive capability for use in severe accident applications in support of the regulatory process. Code uses include analysis required to support rulemaking, licensing audit calculations, evaluation of accident mitigation strategies, and experiment planning and analysis. Specific applications of this capability have included analytical support for the loss-of-fluid test (LOFT), Power Burst Facility (PBF), ACRR, MIST, ROSA IV, and NRU experimental programs, as well as simulations of transients that lead to severe accidents, such as loss of coolant, anticipated transients without scram (ATWS), and operational transients in LWR systems. SCDAP/RELAP5 is a highly generic code that, in addition to calculating the behavior of a reactor coolant system (RCS) during a severe accident transient, can be used for simulation of a wide variety of hydraulic and thermal transients in both nuclear and nonnuclear systems involving steam-water noncondensable solute fluid mixtures.

SCDAP/RELAP5 was developed by integrating three separate codes, RELAP5/MOD2, SCDAP, and TRAP-MELT. These codes were combined to model the coupled interactions that occur between the core, the RCS, and the fission products during a severe accident. For example, blockage in the core, caused by fuel rod ballooning and meltdown, can have a significant effect on RCS flows. Fission products released from the core can have a significant effect on the RCS because of the heat produced during decay. These and many other coupled effects can have a significant effect on the release of fission products from the RCS.

The RELAP5/MOD2 code is based on a nonhomogeneous and nonequilibrium model for the two-phase system that is solved by a fast, partially implicit numerical scheme to permit economical calculation of system transients. The objective of the RELAP5 development effort from the outset was to produce a code that includes important first-order effects necessary for

accurate prediction of system transients but is sufficiently simple and cost-effective such that parametric or sensitivity studies are possible. The development of SCDAP/RELAP5 has this same focus.

The SCDAP code models the core behavior during a severe accident. Treatment of the core includes fuel rod heatup, ballooning and rupture, fission product release, rapid oxidation, zircaloy melting, UO_2 dissolution, ZrO_2 breach, flow and freezing of molten fuel and cladding, and debris formation and behavior. The code also models control rod and flow shroud behavior.

The TRAP-MELT code models the behavior of fission products and aerosols within the RCS. This treatment includes aerosol agglomeration (including Brownian motion, gravitational settling, and turbulent eddy effects), aerosol deposition (including gravitational settling, thermophoresis, and diffusion from laminar or turbulent flow), fission product evaporation and condensation, and chemisorption of vapors by stainless steel.

The code includes many generic component models from which general systems can be simulated. The component models include fuel rods, control rods, pumps, valves, pipes, heat structures, reactor point kinetics, electric heaters, jet pumps, turbines, separators, accumulators, and control system components. In addition, special process models are included for effects such as form loss, flow at an abrupt area change, branching, choked flow, boron tracking, and noncondensable gas transport.

The system mathematical models are coupled into an efficient code structure. The code includes extensive input checking capability to help the user discover input errors and inconsistencies. Also included are free-format input, internal plot capability, restart, renodalization, and variable output edit features. These user conveniences were developed in recognition that generally the major cost associated with the use of a system transient code is in the engineering labor and time involved in accumulating system data and developing system models, while the computer cost associated with generation of the final result is usually small.

The development of the models and codes that constitute SCDAP/RELAP5 has spanned approximately 12 years from the early states of RELAP5 numerical scheme development to the present. SCDAP/RELAP5 represents the aggregate accumulation of experience in modeling core behavior during severe accidents, fission product and aerosol behavior, two-phase flow process, and LWR systems. The code development has benefited from extensive application and comparison to experimental data in the LOFT, PBF, Semiscale, ACRR, NRU, and other experimental programs.

Volumes I and II describe the basic theory and numerical methods used for the various system models. Volume III gives detailed descriptions of the input preparation and execution procedures and provides general guidelines on code application.

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NOMENCLATURE

A	Cross-sectional area (m^2), coefficient matrix in hydrodynamics, coefficient in pressure and velocity equations
A_l	Coefficient in heat conduction equation at boundaries
A_L	Surge line cross-sectional area (m^2)
A_t	Throat area (m^2)
a	Speed of sound (m/s), interfacial area per unit volume (m^{-1}), coefficient in gap conductance, coefficient in heat conduction equation, absorption coefficient
B	Coefficient matrix, drag coefficient, coefficient in pressure and velocity equations
B_l	Coefficient in heat conduction equation at boundaries
b	Coefficient in heat conduction equation, source vector in hydrodynamics
B_x	Body force in x coordinate direction (m/s^2)
B_y	Body force in y coordinate direction (m/s^2)
C	Coefficient of virtual mass, general vector function, coefficient in pressure, and velocity equations delay neutron precursors in reactor kinetics, concentration
C_0	Coefficient in noncondensable energy equation ($J/kg \cdot K$)
C_d	Drag coefficient
C_g	Dimensional constant in correlation for Γ_g
C_p	Specific heat at constant pressure ($J/kg \cdot K$)
C_v	Specific heat at constant volume ($J/kg \cdot K$)
c	Coefficient in heat conduction equation, coefficient in new time volume-average velocity equation
D	Coefficient of relative Mach number, diffusivity, diameter (m), heat conduction boundary condition matrix, coefficient in pressure and velocity equations
D_0	Coefficient in noncondensable energy equation ($J/kg \cdot K^2$)
D_l	Coefficient of heat conduction equation at boundaries

d	Coefficient in heat conduction equation, droplet diameter (m)
DISS	Energy dissipation function (W/m^3)
E	Total energy ($U + v^2/2$) (J/kg), emissivity, Young's modulus, term in iterative heat conduction algorithm, coefficient in pressure equation
e	Interfacial roughness
Eu	Euler number
F	Term in iterative heat conduction algorithm, gray-body factor with subscript, frictional loss coefficient, vertical stratification factor
FIF, FIG	Interphase drag coefficients (liquid, vapor) (s^{-1})
FI	Interphase drag coefficient ($\text{m}^3/\text{kg}\cdot\text{s}$)
FWF, FWG	Wall drag coefficients (liquid, vapor) (s^{-1})
f	Interphase friction factor, vector for liquid velocities in hydrodynamics
G _{head}	Pressure drop across valve due to gravity (Pa)
G	Mass velocity (kg/s), shear stress, gradient, coefficient in heat conduction, vector quantity, fraction of delayed neutrons in reactor kinetics
G _c	Dynamic pressure for valve (Pa)
Gr	Grashof number
g	Gravitational constant (m/s^2), temperature jump distance (m), vector for vapor velocities in hydrodynamics
g _Z , g	Acceleration due to gravity (m/s^2)
H	Elevation (m), volumetric heat transfer coefficient ($\text{W/K}\cdot\text{m}^3$), head (m)
HLOSSF, HLOSSG	Form or frictional losses (liquid, vapor) (m/s)
h	Specific enthalpy (J/kg), heat transfer coefficient ($\text{W/m}^2\cdot\text{K}$), energy transfer coefficient for Γ_g , head ratio
h _L	Dynamic head loss (m)

Subscripts

a	Average value
B	Boron, dissolved solid
b	Bubble
CHF	Value at critical heat flux
c	Vena contract, continuous phase, cladding, critical property, cross section
cm	Cladding midpoint
con	Condensation
cr	Critical property or condition
D	Drive line, vapor dome
d	Droplet, delay in control component
e	Thermodynamic equilibrium, equivalent quality in hydraulic volumes, value ring exit, elastic deformation
exp	Used to indicate explicit velocities in choking
F	Wall friction, fuel
FB, FBB	Film boiling, Bromley film boiling
f	Liquid phase
fg	Phasic difference (i.e., vapor term-liquid term)
fp	Onset of vapor pull-through
fr	Frictional
g	Vapor phase, gap
ge	Incipient liquid entrainment
H	Head
HE	Homogeneous equilibrium
HF	Homogeneous frozen
hy	Hydraulic
I	Interface

I	Identity matrix, moment of inertia (N-m-s^2)
J	Junction velocity (m/s)
K	Energy form loss coefficient
k	Thermal conductivity ($\text{W/m}\cdot\text{K}$)
k_B	Boltzmann constant
k_s	Spring constant
L	Length, limit function
L_L	Surge line length (m)
l_l	Liquid level (m)
M	Mach number, molecular weight, pump two-phase multiplier, mass transfer rate, mass (kg)
N	Number of system nodes, number density ($\#/\text{m}^3$), pump speed (rad/s)
Nu	Nusselt number
n	Unit vector, order of equation system
P_{Br}	Valve closing back pressure (Pa)
P	Pressure (Pa), reactor power (W), channel perimeter (m), turbine power (J/s)
P_D	Nitrogen pressure in dome (Pa)
P_f	Relates reactor power to heat generation rate in heat structures
P_0	Atmospheric pressure (Pa)
p	Wetted perimeter (m), particle probability function
PCV	Specified pressure required to close a valve (Pa)
Pr	Prandtl number
Q	Volumetric heat addition rate (W/m^3), space dependent function, volumetric flow rate (m^3/s)
Q_D	Total heat transfer to vapor dome (W)
q	Heat transfer rate (W), heat flux (W/m^2)

R_t	Specified time-dependent, space-dependent factor in the source term of heat conduction
R	Reynolds number, radius (m), surface roughness in gap conductance, radiation resistance term
Re	Reynolds number
Re_p	The particle Reynolds number
R_n, R_s	Universal gas constants (noncondensable, steam) ($N \cdot m/kg \cdot K$)
r	Reaction fraction for turbine
S	Chen's boiling suppression factor, stress gradient, specific entropy ($J/kg \cdot K$), shape factor, real constant, source term in heat conduction or reactor kinetics (W)
s	Surface, Laplace transform variable
T	Temperature (K), trip
T_c	Critical temperature (K)
T_R	Reduced temperature (K)
T_t	Specified time-dependent function in heat conduction
t	Time (s)
U	Specific internal energy (J/kg), vector of dependent variables
u	Radial displacement in gap conductance (m)
V	Volume (m^3), specific volume (m^3/kg), control quantity
V_v	Volume of noncondensable in accumulator dome (m^3)
$VFDP, VGDP$	Coefficient for pressure change in momentum equations (liquid, vapor) ($m/s-Pa$)
VIS	Numerical viscosity terms in momentum equations (m^2/s^2)
$VISF, VISG$	Numerical viscosity terms in momentum equations (liquid, vapor) (m^2/s^2)
$VUNDER, VOVER$	Separator model parameters (liquid, vapor)
v	Mixture velocity (m/s), phasic velocity (m/s), flow ratio, liquid surge line velocity (m/s)

v_c	Choking velocity (m/s)
W	Weight of valve disk, weighting function in reactor kinetics, relaxation parameter in heat conduction, shaft work per unit mass flow rate
W_{crit}	Critical Weber number
We	Weber number
w	Humidity ratio
X	Static quality, mass fraction, conversion from MeV/s to watts
x	Spatial coordinate (m), vector of hydrodynamic variables
Y	Control variable
Z	Two-phase friction correlation factor, function in reactor kinetics
z	Elevation change coordinate (m)

Symbols

α	Void fraction, subscripted volume fraction, angular acceleration (rad/s^2), coefficient for least-squares fit, speed ratio
β	Coefficient of isobaric thermal expansion (K^{-1}), effective delayed neutron fraction in reactor kinetics
Γ	Volumetric mass exchange rate ($\text{kg/m}^3\cdot\text{s}$)
ΔP_f	Dynamic pressure loss (Pa)
ΔP_s	Increment in steam pressure (Pa)
ΔV_s	Increment in specific volume of steam (m^3/kg)
Δt	Increment in time variable (s)
Δt_c	Courant time step (s)
Δx	Increment in spatial variable (m)
δ	Area ratio, truncation error measure, film thickness (m), impulse function, Deryagin number

ϵ	Coefficient, strain function, emissivity, tabular function of area ratio, surface roughness, wall vapor generation/condensation flag
ζ	Diffusion coefficient, multiplier, or horizontal stratification terms
η	Efficiency, bulk/saturation enthalpy flag
θ	Relaxation time in correlation for Γ , angular position (rad)
κ	Coefficient of isothermal compressibility (Pa^{-1})
Λ	Prompt neutron generation time, Baroczy dimensionless property index
λ	Eigenvalue, interface velocity parameter, friction factor, decay constant in reactor kinetics
μ	Viscosity ($\text{kg/m}\cdot\text{s}$)
ν	Kinematic viscosity (m^2/s), Poisson's ratio
ξ	Exponential function, RMS precision
π	3.141592654
ρ	Density (kg/m^3), reactivity in reactor kinetics (dollars)
Σ_f	Fission cross section
Σ'	Depressurization rate (Pa/s)
σ	Surface tension (J/m^2), stress, flag used in heat conduction equations to indicate transient or steady-state
τ	Shear stresses (N), torque (N-m)
ϕ	Donored property, Lockhart-Martinelli two-phase parameter, neutron flux in reactor kinetics, angle of inclination of valve assembly
Φ	Lockhart-Martinelli parameter
ψ	Coefficient, fission rate (number/s)
ω	Angular velocity (rad/s), function variable in reactor kinetics

Subscripts

a	Average value
B	Boron, dissolved solid
b	Bubble
CHF	Value at critical heat flux
c	Vena contract, continuous phase, cladding, critical property, cross section
cm	Cladding midpoint
con	Condensation
cr	Critical property or condition
D	Drive line, vapor dome
d	Droplet, delay in control component
e	Thermodynamic equilibrium, equivalent quality in hydraulic volumes, value ring exit, elastic deformation
exp	Used to indicate explicit velocities in choking
F	Wall friction, fuel
FB, FBB	Film boiling, Bromley film boiling
f	Liquid phase
fg	Phasic difference (i.e., vapor term-liquid term)
fp	Onset of vapor pull-through
fr	Frictional
g	Vapor phase, gap
ge	Incipient liquid entrainment
H	Head
HE	Homogeneous equilibrium
HF	Homogeneous frozen
hy	Hydraulic
I	Interface

IB	Incipience of boiling
i	Inlet, interface
j, j+1, j-1	Spatial noding indices, junctions
K	Spatial noding indices, volumes
L	Spatial noding index, volumes, laminar
l	Left boundary in heat conduction
M	Rightmost boundary in heat conduction
m	Mixture property, motor, mesh point
NB	Nucleate boiling
n	Noncondensable component of vapor phase
o	Reference value
R	Rated values
r	Relative Mach number, right boundary in heat conduction
S	Suction region
s	Steam component of vapor phase
sat	Saturated quantity
T	Point of minimum area, turbulent
TB	Transition film boiling
t	Turbulent, tangential
tt	Fully turbulent

up	Upstream quantity
v	Mass mean Mach number, vapor quantity, valve
w	Wall, water
wall	Wall of tank
wg, wf	Wall to vapor, wall to liquid
1	Upstream station, multiple junction index, vector index
1 ϕ	Single-phase value
2	Downstream station, multiple junction index, vector index
2 ϕ	Two-phase value
τ	Torque
$\sim$	Vector
$\approx$	Matrix

Superscripts

b	Boundary gradient weight factor in heat conduction, vector quantities
exp	Old time terms in velocity equation
i	Imaginary part of complex number
m-1, m, m+1	Mesh points in heat conduction finite difference equation or mean value
n, n+1	Time level index
n+1/2	An average of quantities with superscripts n and n+1
o	Initial value

R	Real part of complex number
γ	Right boundary in heat conduction
s	Saturation property, space gradient weight factor in heat conduction
v	Volume gradient weight factor in heat conduction
w	Wall
1	Vector index, coefficient in velocity equation
2	Vector index
*	Total derivative of a saturation property with respect to pressure, local variable, bulk/saturation property
'	Derivative
-	Vector, average quantity
.	Donored quantity
~	Unit momentum for mass exchange, intermediate time variable
	Linearized quantity, quality based on total mixture mass

SCDAP/RELAP5/MOD2 CODE MANUAL
VOLUME I: RELAP5 CODE STRUCTURE, SYSTEM MODELS, AND SOLUTION METHODS

1. INTRODUCTION

The SCDAP/RELAP5 computer code is designed to provide the overall reactor coolant system (RCS) thermal-hydraulic response, core damage progression, and fission product release and transport during severe accidents. The code is being developed at the Idaho National Engineering Laboratory (INEL) under the primary sponsorship of the Office of Nuclear Regulatory Research of the U.S. Nuclear Regulatory Commission (NRC). Secondary sponsors include the U. S. Department of Energy (DOE) and their contractors. The code is currently being used by the NRC, DOE, and associated organizations to support confirmatory experimental research, the TMI-2 accident evaluation, and the analyses of commercial light water reactors (LWRs) and DOE reactors.

1.1 General Code Capabilities

The code is the result of merging the RELAP5/MOD2,¹⁻¹ SCDAP,¹⁻² and TRAP-MELT^{1-3,4} models. The RELAP5 models calculate the overall RCS thermal-hydraulics, control system interactions, reactor kinetics, and the transport of noncondensable gases, fission products, and aerosols. The SCDAP models calculate the damage progression in the core structures and the formation, heatup, and melting of debris. The TRAP-MELT models calculate the deposition of fission products upon aerosols or structural surfaces; the formation, growth, or deposition of aerosols; and the evaporation of species from surfaces. These models are fully coupled at each time step. Their functional interaction is described in the bubble diagram shown in Figure 1-1.

The overall architecture of the code is described in more detail in Section 2.

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Figure 1-1. SCDAP/RELAP5 reactor coolant system interactions.

SCDAP/RELAP5 is capable of modeling a wide range of system configurations from single pipes to different experimental facilities to full-scale reactor systems. The configurations can be modeled using an arbitrary number of fluid control volumes and connecting junctions, heat structures, core components, and system components. Flow areas, volumes, and flow resistances can vary with time through either user control or models that describe the changes in geometry associated with damage in the core. System structures can be modeled with RELAP5 heat structures, SCDAP core components, or SCDAP debris models. The RELAP5 heat structures are one-dimensional models with slab, cylindrical, or spherical geometries. The SCDAP core components include representative LWR fuel rods, silver-indium-cadmium (Ag-In-Cd) and B_4C control rods or blades, electrically heated fuel rod simulators, non-LWR core structures, and general structures. The SCDAP debris models use a general, two-dimensional, finite-element, porous body subcode. The user defines the initial mesh for lower plenum structures and associated debris bed volumes. The debris bed is then created as the problem progresses. System components available to the user include pumps, valves, electric heaters, jet pumps, turbines, separators, and accumulators. Models to describe selected processes, such as fission product transport and deposition, reactor kinetics, control system response, and tracking noncondensable gases, can be invoked through user control. A detailed description of the configurations modeled by the code is presented in Volume III.

1.2 Relationship to Other NRC-Sponsored Software

The development of SCDAP/RELAP5 is closely related to the development of RELAP5/MOD3. Both codes share a common source deck. Separate codes are formed only prior to compilation, so changes made to the source deck are automatically reflected in both codes.

The development and application of the code is also related to several other NRC-sponsored software packages. Model improvements, led by theoretical work associated with the development of codes such as MELPROG¹⁻⁵ and FASTGRASS-VFP,¹⁻⁶ include melt ejection from the vessel,

steam explosions, and fission product release. Material properties are obtained through a standardized MATPRO¹⁻⁷ library. Animated plant response displays are possible through links to the Nuclear Plant Analyzer (NPA)¹⁻⁸ display software. Detailed plant simulations from accident initiation through release of fission products to the atmosphere are made available through links to the CONTAIN¹⁻⁹ containment response and CRAC2¹⁻¹⁰ or MACCS¹⁻¹¹ atmospheric dispersion codes.

1.3 Status and Future Development Plans

SCDAP/RELAP5/MOD2 designates the second major modification of SCDAP/RELAP5. MOD2 represents a major expansion in the capability of the code to treat the later phases of an accident. This expansion was driven by SCDAP/RELAP5's role in the analysis of the TMI-2 accident and includes new models that treat

- o the formation of debris beds either through the formation of a cohesive mass of molten or solidified material or through the accumulation of loose debris associated with the fragmentation or breakup of core materials;
- o heatup and melting of debris beds;
- o formation of a molten pool support by a crust of frozen material;
- o thinning and failure of the supporting crust;
- o penetration and potential fragmentation of a molten jet of material;
- o interaction of debris with the vessel wall; and
- o the failure of the vessel wall.

MOD2 also represents major modeling additions in four other areas. First, BWR-specific control blade or rod models have been added to treat the

unique features of B₄C. Second, electrically heated fuel rod simulator models have been added to treat fuel rod simulators with central, resistive heating elements. Third, models have been added that describe the thermal or mechanical failure of structures throughout the RCS to evaluate the potential for failure due to creep rupture. Third, models have been added to treat the decay heating associated with fission products either present in the coolant stream or on structures. Although transparent to the user, MOD2 also incorporates significant changes in the programming structure of SCDAP/RELAP5. All machine-dependent data structures have been removed, greatly reducing the effort necessary to install the code on a variety of computers. Improvements in organization of the code and changes in important algorithms have reduced the run time significantly.

Future releases of the code will be focused on (a) model development to support the application of the code to a wider range of plant designs and conditions, (b) generation of non-CRAY^a versions of the code, and (c) reductions in the cost of code analysis.

Five major SCDAP/RELAP5 model development activities are underway to support a wider range of code applications:

1. The two-dimensional debris models are being generalized to describe the thermal response of structures embedded in debris beds and debris beds or structures anywhere in the system modeled by the code. As an example, with these changes, a detailed two-dimensional analysis can be performed for instrument tubes surrounded by debris, structures anywhere in the system, or debris carried outside the core or lower plenum. The input for these models is also being expanded to allow the user to initialize the code with preexisting debris beds.

a. Mention of specific products and/or manufacturers in this document implies neither endorsement or preference nor disapproval by the U.S. Government, any of its agencies, or EG&G Idaho, Inc., of the use of a specific product for any purpose.

2. A third field is being added to the two-fluid, six-equation hydrodynamic models. This field will be used to track the movement of molten material or debris through the system. This model can then be used to track the radial movement of melt from the core to core barrel region, melt ejection, or the movement of debris through the RCS. The input for this model will also allow the user to initialize the code with a molten or debris field so that experiments starting with a melt can be directly analyzed.
3. The fission product transport models are also being generalized to allow additional species. In addition, the numerical algorithms used are being modified to reduce the cost of the calculations when this option is invoked.
4. Data interfaces are being developed that will allow SCDAP/RELAP5, other codes such as MELCOR¹⁻¹¹ and CONTAIN,¹⁻⁹ and graphics processors such as the NPA to run in parallel on CRAY (and potentially other) computers with UNIX operating systems. These data interfaces will allow the codes to be loosely coupled at user-specified time steps. Although this approach is machine- and operating-system-dependent, it will only require the addition of one or two subroutines to the existing codes.
5. Thermal-hydraulic and other system models are being improved through the RELAP5/MOD3 activities. These improvements include reflood heat transfer, inception of vertical and horizontal stratification, countercurrent flow limitations, metal-water reactions (for RELAP5 heat structures), condensation in horizontal pipes, downcomer penetration and emergency core cooling system (ECCS) bypass, and upper plenum deentrainment.

These improvements should be available in early 1990 at the current rate of development.

Creations of non-CRAY versions of the code will be built on the work started for SCDAP/RELAP5/MOD2. Through the RELAP5 activities, the RELAP5

portion of the code was converted and tested on CDC-NOS/VE, VAX, and IBM computers at the INEL. Consequently, MOD2 will execute RELAP5 input decks on the CRAY/XMP and CDC-NOS/VE, VAX, and IBM machines. Similar changes to the balance of SCDAP/RELAP5 will be available in future releases of the code (1990).

Other code improvements focused on the reduction in the cost of an analysis should be available over the longer term (1991 and beyond). These improvements concentrate on code input and output, addition of features that more fully automate control of transient calculations, and changes in coding structure and code numerics to further reduce run times. Proposed code improvements include:

- o Automatic time step repetition to allow the code to repeat time advancements if error tolerances are exceeded
- o Increased SCDAP component input error checking to reduce the time required to debug input decks
- o Merged RELAP5 and SCDAP input and output to reduce the cost of interpretation of code results.

Future model improvement will also be performed on an "as-needed" basis as a result of a parallel model assessment and validation effort. However, a number of areas have been identified where model changes are likely. These include ZrO_2 failure and rivulet flow, aerosol formation, fission product transport and deposition, and debris behavior.

1.4 Quality Assurance

SCDAP/RELAP5 is maintained under a strict code-configuration system that provides a historical record of the changes in the code. Changes are made using an update processor that allows separate identification of improvements made to each successive version of the code. Modifications and improvements to the coding are reviewed and checked as part of a formal

quality program for software. In addition, the theory and implementation of code improvements are validated through assessment calculations that compare the code-predicted results to idealized test cases or experimental results.

SCDAP/RELAP5 must meet the quality assurance (QA) requirements of the INEL.¹⁻¹² The QA requirements at INEL are summarized as follows: First, the QA policy must be administered for each software development activity through an established organization. Second, all significant software development must be thoroughly documented. Third, procedures must be in place to assure the traceability and retrievability of each version of software. Fourth, each version of software shall be clearly identified as to name, version, and date of last revision. All output must display this identification. Fifth, all software must be verified and validated for its intended application.

The group responsible for the development of SCDAP/RELAP5, the Energy and Systems Technology Group (E&ST) at INEL, has a team charged with the responsibility of administering the QA policy for the group. The leader of this team is the Quality Program Plan (QPP) manager. The QPP manager and Unit Managers have the responsibility for monitoring adherence to the QA policy.

A procedure with five basic stems has been established to implement the QA policy. In the first step, software is entered into the Software Index. Each entry must be approved by the QPP manager. In the second step, a quality level must be approved by the Unit Manager. For the third step, a Software Quality Assurance Plan (SQAP) will be written for each item in the Software Index. SQAPs will be maintained as controlled documents. The level of software verification and validation is specified in the SQAP. The fourth step is the review and approval of the SQAP by the Unit and QPP managers. The fifth step is the submittal of quality records as software development proceeds to the Quality Control Document Librarian. The SQAPs specify the quality records to be submitted.

The SQAP for SCDAP/RELAP5 addresses the thirteen categories specified by the ANSI/IEEE Standard 730-1984.¹⁻¹³ These include: (a) completion of forms that state the purpose of the software, identification of documents that reference the software, and management of the software; (b) documentation that explains the problem solved; (c) documentation of verification and validation of software; (d) documentation of software changes and the reverification of the software; and (e) documentation that keeps track of software problems and actions to correct the problems.

SCDAP/RELAP5 is being developed for critical applications and thus meets INEL quality standards associated with these applications. Critical applications implies that the calculations of the code could be used to determine the design of reactor safety systems. Failure of code calculations could involve undue risk to employees and the public health.

1.5 References

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2. CODE ARCHITECTURE

Modeling flexibility, user convenience, computer efficiency, and design for future growth were primary considerations in the selection of the basic architecture of the code. The architecture of SCDAP/RELAP5 is based upon that developed for RELAP5,²⁻¹ SCDAP,²⁻² and other large codes that have been developed at the INEL. The top level of the architecture, input and output processing and transient control, follows the architecture of RELAP5. The lower levels under transient control utilize a combination of structures based on RELAP5, SCDAP, and TRAP-MELT.²⁻³ RELAP5-based logic determines the overall transient time step, evaluates trip logic, and advances the calculations for the RELAP5 heat structures, hydrodynamics, reactor kinetics, and control systems. SCDAP-based logic advances the calculations for the representative core components, debris behavior, and radiation heat transfer. SCDAP logic also advances the convective heat transfer calculations for those structures or debris associated with the SCDAP models; however, the logic for convective heat transfer is derived from RELAP5. The fission product deposition solution logic was completely reorganized from that of TRAP-MELT and now follows the pattern established by RELAP5, although the logic of lower-level subroutines still has recognizable TRAP-MELT features.

2.1 Computer Adaptability

SCDAP/RELAP5 is written in FORTRAN 77. Compile time options are provided to allow operation on CRAY-1 and CRAY-XMP machines using either COS, CTSS, or UNIX operating systems. Compile time options are also being provided to allow operation on 64-bit machines (e.g., Cyber-NOS-VE, ETA) and 32-bit machines that have double-precision (64-bit), floating-point arithmetic (e.g., IBM, VAX, and many super-minis). A common source is maintained for all computer versions. Development is primarily on a CRAY computer, but compatibility checks are made on other computers. Reported errors are resolved on all computer versions derived from the common source.

2.2 Top Level Organization

SCDAP/RELAP5 is coded in a modular fashion using top-down structuring. The various models and procedures are isolated in separate subroutines. The top level structure is shown in Figure 2-1 and consists of input, transient/steady-state, plotting, and stripping blocks.

The input block processes input, checks input data, and prepares required data blocks for all program options and is discussed in more detail in Section 2.3.

The transient/steady-state block handles both the transient option and the steady-state option. The steady-state option determines the steady-state conditions if a properly posed steady-state problem is presented. Steady state is obtained by running an accelerated transient until the time derivatives approach zero. Thus, the steady-state option is very similar to the transient option but contains convergence testing algorithms to determine satisfactory steady state, divergence from steady state, or cyclic operation. If the transient technique alone were used, approach to steady state from an initial condition would be identical to a plant transient from that initial condition. Pressures, densities, and flow distributions would adjust quickly; but thermal effects would occur more slowly. To reduce the transient time required to reach steady state, the steady-state option artificially accelerates heat conduction by reducing the heat capacity of the conductors.

The plotting block produces time history plots of simulation results generated from the steady-state or transient blocks. This block can also produce plots from data saved on a restart plot file from an earlier simulation.

The strip block extracts simulation data from a restart plot file for convenient passing of SCDAP/RELAP5 simulation results to other computer programs.

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Figure 2-1. SCDAP/RELAP5 top level structure.

2.3 Input Processing Overview

SCDAP/RELAP5 provides detailed input checking for system thermal-hydraulic and fission product behavior/transport models. Three input processing phases are used in the code. The first phase reads all input data, checks for punctuation and typing errors (such as multiple decimal points and letters in numerical fields), and stores the data keyed by card number such that the data are easily retrieved. A listing of the input data is provided, and punctuation errors are noted.

During the second phase, restart data from a previous simulation are read if the problem is a RESTART type, and all input data are processed. Some processed input is stored in fixed common blocks, but the majority of the data is stored in dynamic data blocks that are created only if needed by a problem and sized to the particular problem. In a NEW-type problem, dynamic blocks must be created. In RESTART problems, dynamic blocks may be created, deleted, added to, partially deleted, or modified as modeling features and components within models are added, deleted, or modified. Extensive input checking is done, but at this level checking is limited to new data from the cards being processed. Relationships with other data cannot be checked because the latter may not yet be processed. As an illustration of this level of checking, junction data are checked to determine if they are within the appropriate range, such as positive, nonzero, or between zero and one; and volume connection codes are checked for proper format. However, no attempt is made at this point to check whether or not referenced volumes exist in the problem until all input data are processed.

The third phase of processing begins after all input data have been processed. Since all data have been placed in common or dynamic data blocks during the second phase, complete checking of interrelationships can proceed. Examples of cross-checking are: existence of hydrodynamic volumes referenced in junctions and heat structure boundary conditions; entry or existence of material property data specified in heat structures; and validity of variables selected for minor edits, plotting, or used in

trips and control systems. As the cross-checking proceeds, cross-linking of the data blocks is done so that it need not be repeated at every time step. The initialization required to prepare the model for start of transient advancement is done at this level.

Input data editing and diagnostic messages can be generated during the second and/or third phases. Input processing for most models generates output and diagnostic messages during both phases. Thus, input editing for these models appear in two sections.

As errors are detected, various recovery procedures are used so that input processing can be continued and a maximum amount of diagnostic information can be furnished. Recovery procedures include supplying default or benign replacement data, marking the data as erroneous so that other models do not attempt use of the data, or deleting the bad data. The recovery procedures sometimes generate additional diagnostic messages. Often after attempted correction of input, different diagnostic messages appear. These can be due to continued incorrect preparation of data, but the diagnostics may result from the more extensive testing permitted as previous errors are eliminated.

As a convenience to the user, a check plot option is provided that will produce plots of input data such as for time-dependent volumes and junctions, general tables, plot comparison data tables, valve area and flow coefficients, etc. This option can be utilized by the input of the check plot general plot request input card. The plots are constructed upon completion of the third phase of input data processing so that all information processed by the code will be included. Once the option is activated, it will remain in effect for all subsequent restart or plot only jobs, including restarts with renodalization, until cancelled by the user with appropriate input.

2.4 Transient Overview

Figure 2-2 shows the functional modular structure for the transient calculations, while Figure 2-3 shows the second-level structures for the transient/steady-state blocks or subroutines.

The subroutine TRNCTL shown in Figure 2-3 consists only of the logic to call the next lower level routines. Subroutine TRNSET brings dynamic blocks required for transient execution from disk into computer central memory, performs final cross-linking of information between data blocks, sets up arrays to control the sparse matrix solution, establishes scratch work space, and returns unneeded computer memory. Subroutine TRAN, the driver, controls the transient advancement of the solution. Nearly all the execution time is spent in this block, and this block is the most demanding of memory. Nearly all the dynamic data blocks must be in the central memory, and the memory required for instruction storage is high, since coding to advance all models resides in this block. The subroutine TRNFIN releases space for the dynamic data blocks that are no longer needed and prints the transient timing summary.

A description is next presented of the functions of all of the modules (subroutines) driven by TRAN.

The time step control module (named DTSTEP) determines the time step size, controls output editing, and determines whether transient advancements should be terminated. During program execution, this module displays such information as CPU time, problem time, and the maximum cladding temperature on a terminal screen.

The trip system module (named TRIP) evaluates logical statements. Each trip statement is a simple logical statement which has a true or false result. The decision of what action is needed resides within the components in other modules. For example, valve components are provided that open or close the valve based on trip values; pump components test trip status to determine whether a pump electrical breaker has tripped.

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Figure 2-2. Modular structures of transient calculations in SCDAP/RELAP5.

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Figure 2-3. Transient (steady-state) block structure.

The equation of state boundary volume model (named TSTATE) calculates the thermodynamic state of the fluid in each hydrodynamic boundary volume.

The heat structure model (named HTADV) advances heat conduction/transfer solutions using previous-time-step reactor kinetics power and previous-time-step hydrodynamic conditions for computing heat transfer coefficients. It calculates heat transferred across solid boundaries of hydrodynamic volumes.

The hydrodynamics module (named HYDRO) advances the hydrodynamic solution.

The reactor kinetics module (named RKIN) advances the reactor kinetics of the code. It computes the power behavior in a nuclear reactor using the space-independent or point kinetics approximation which assumes that power can be separated into space and time functions.

The control system module (named CONVAR) provides the capability of simulating control systems typically used in hydrodynamic systems. It consists of several types of control components. Each component defines a control variable as a specific function of time advanced quantities. The time advanced quantities include quantities from hydrodynamic volumes, junctions, pumps, valves, heat structures, reactor kinetics, trip quantities, and the control variables themselves. This permits control variables to be developed from components that perform simple, basic operations.

The SCDAP driver module drives the SCDAP discrete components, SCDAP heat transfer modules, and slumping of core material into the lower plenum. It advances all of the SCDAP calculations with the exception of those done in the SCDAP debris module. It is further divided into six submodules, as shown in Figure 2-4. The intact core module (named SBNTAC) is the main driver for the SCDAP discrete components. It drives the fuel pin, silver-indium-cadmium control rod, boron carbide control rod blade, electrically heated fuel rod simulator, and other core structure models.

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Figure 2-4. SCDAP modular structure.

The intact core heat transfer module (named HTRC1) computes the convective heat transfer between coolant and intact core. The debris heat transfer module (named HTRC3A) computes the convective heat transfer between coolant and core debris. The radiation module (named RADCC2) calculates the radiative heat transfer between elements in the intact core including the heat transfer between fuel pin and coolant, fuel pin and shroud, etc. The liquefied debris heatup module (named HEATLD) calculates the extent of core liquefaction and the heatup of the resulting molten pool of liquefied debris. The slumping of liquefied debris module (named SLUMP) models the slumping of liquefied debris into the lower plenum.

The fission product deposition and decay module (named FPRTR) performs fission product behavior and transport and radionuclide decay heating calculations.

The lower head debris module (named TCOUPL) calculates the heatup of debris that has slumped into the lower head of the reactor vessel. The module also calculates the heatup of the lower head and the amount of heat transfer from debris to coolant.

The creep rupture module (named TRUPT) calculates the creep damage of the reactor vessel and piping as a function of stress, temperature, and time.

2.5 References

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3. HYDRODYNAMIC MODEL

The SCDAP/RELAP5 hydrodynamic model is a one-dimensional, transient, two-fluid model for flow of a two-phase steam-water mixture that can contain noncondensable components in the steam phase and/or a nonvolatile component in the water phase.

The SCDAP/RELAP5 hydrodynamic model contains several options for invoking simpler hydrodynamic models. These include homogeneous flow, thermal equilibrium, and frictionless flow models. These options can be used independently or in combination. The homogeneous and equilibrium models were included primarily to be able to compare code results with calculations from the older codes based on the homogeneous equilibrium model (HEM).

The two-fluid equations of motion that are used as the basis for the SCDAP/RELAP5 hydrodynamic model are formulated in terms of area and time-averaged parameters of the flow. Phenomena that depend upon transverse gradients, such as friction and heat transfer, are formulated in terms of the bulk potentials using empirical transfer coefficient formulations. The system model is solved numerically using a semi-implicit finite-difference technique. The user can select an option for solving the system model using a nearly implicit finite-difference technique, which allows violation of the material Courant limit. This option is suitable for steady-state calculations and for slowly varying, quasi-steady transient calculations.

The basic two-fluid differential equations possess complex characteristic roots that give the system a partially elliptic character and thus constitutes an ill-posed initial boundary value problem. In SCDAP/RELAP5, the numerical problem is rendered well-posed by the introduction of artificial viscosity terms in the difference equation formulation that damp the high frequency spatial components of the solution. The ill-posed character of the two-fluid model is a result of the momentum formulation and is introduced as a result of the spatial averaging process and neglect of higher-order physical effects. Ransom and

Hicks³⁻¹ have studied several formulations in which two pressures (one for each fluid) are included in the model, and these models are totally hyperbolic and thus constitute well-posed problems. Limited numerical studies by Ransom and Scofield³⁻² have shown that solutions for the two-pressure model compare very well to that for the single-pressure model with damping. In general, the differences are significant only for short wavelength components of the solution where numerical truncation error is dominant. Thus, either approach provides a valid numerical simulation at solution component wavelengths of interest in most reactor safety problems. The simpler formulation of the single-pressure model favors using that approach.

The semi-implicit numerical solution scheme uses a direct sparse matrix solution technique for time step advancement. It is an efficient scheme and results in an overall grind time on the CDC Cyber 176 of ~0.0015 s. The method has a material Courant time step stability limit. However, this limit is implemented in such a way that single-node Courant violations are permitted without adverse stability effects. Thus, single small nodes embedded in a series of larger nodes will not adversely affect the time step and computing cost. The nearly implicit numerical solution scheme also uses a direct sparse matrix solution technique for time step advancement. This scheme has a grind time that is 25 to 60% greater than the semi-implicit scheme but allows violation of the material Courant limit for all nodes.

3.1 Field Equations

SCDAP/RELAP5 has six dependent variables (seven if a noncondensable component is present, i.e., P , U_g , U_f , α_g , X_n , v_g , and v_f). The noncondensable quality is defined as the ratio of the noncondensable gas mass to the total gaseous phase mass [i.e., $X_n = M_n / (M_n + M_s)$, where M_n = mass of noncondensable in the gaseous phase and M_s = mass of steam in the gaseous phase]. The other secondary dependent variables used in the equations are phasic densities (ρ_g , ρ_f), water vapor generation rate per unit volume due to condensation/evaporation process

(Γ_g) , n i-th noncondensable generation rate per unit volume due to metal-water reaction and inert fission product release, (Γ_{ni}) , total source rate for all the solutes $(\Gamma_{s,i})$, phasic interphase heat transfer rates per unit volume (Q_{ig}, Q_{if}) , phasic temperatures (T_g, T_f) , saturation temperature (T^s) , and noncondensable mass fraction in noncondensable gas phase (X_{ni}) for n i-th noncondensable species (i.e.,

$X_{ni} = M_{ni} / \sum_{n=1}^N M_{ni}$, where M_{ni} = mass of n i-th noncondensable in the gaseous phase).

The basic two-fluid differential equations that form the basis for the hydrodynamic model are next presented. This discussion will be followed by development of a convenient form of the differential equations that is used as the basis for the numerical solution scheme. The modifications necessary to model horizontal stratified flow and time-varying geometry are also discussed. Subsequently, the semi-implicit scheme difference equations, the volume-averaged velocity formulations, and the time advancement scheme are discussed. Finally, the nearly implicit scheme difference equations are presented.

3.1.1 Basic Differential Equations

The differential form of the one-dimensional transient field equations is first presented for a one-component system. The modifications necessary to consider noncondensibles as a component of the gaseous phase and boron as a nonvolatile solute component of the liquid phase are discussed separately.

3.1.1.1 Vapor/Liquid System. The basic field equations for the two-fluid nonequilibrium model consist of two-phasic continuity equations, two-phasic momentum equations, and two-phasic energy equations. The equations are recorded in differential stream tube form with time and one space dimension as independent variables and in terms of time and

volume-average dependent variables.^a The development of such equations for the two-phase process has been recorded in several references^{3-3,4} and is not repeated here. The equations are cast in the basic form with discussion of those terms that may differ from other developments. Manipulations required to obtain the form of the equations from which the numerical scheme was developed are described in Section 3.1.2.

The phasic continuity equations are

$$\frac{1}{V} \frac{\partial}{\partial t} (V \alpha_g \rho_g) + \frac{1}{A} \frac{\partial}{\partial x} (\alpha_g \rho_g v_g A) = \Gamma_g + \sum_{n=1}^N \Gamma_{ni} - \Gamma_h \quad (3-1)$$

where N is the total number of noncondensable species in the gas phase, and Γ_h is the hydrogen generation rate per unit volume due to metal/water reaction.

$$\frac{1}{V} \frac{\partial}{\partial t} (V \alpha_f \rho_f) + \frac{1}{A} \frac{\partial}{\partial x} (\alpha_f \rho_f v_f A) = -\Gamma_g + \Gamma_{si} \quad (3-2)$$

Generally, the flow does not include mass sources or sinks; and overall continuity consideration yields the requirement that the liquid generation term to be the negative of the vapor generation; that is,

$$\Gamma_f = -\Gamma_g \quad (3-3)$$

The interfacial mass transfer model assumes that total mass transfer consists of mass transfer in the bulk fluid (Γ_{ig}) and mass transfer at the wall (Γ_w); that is,

a. In all the field equations shown herein, the correlation coefficients are assumed to be unity so the average of a product of variables is equal to the product of the averaged variables.

$$\Gamma_g = \Gamma_{ig} + \Gamma_w \quad (3-4)$$

The phasic conservation of momentum equations are used, and recorded here, in the so-called nonconservative form. For the vapor phase, it is

$$\begin{aligned} \alpha_g \rho_g A \frac{\partial v_g}{\partial t} + \frac{1}{2} \alpha_g \rho_g A \frac{\partial v_g^2}{\partial x} = & -\alpha_g A \frac{\partial p}{\partial x} + \alpha_g \rho_g B_x A - (\alpha_g \rho_g A) FWG(v_g) \\ & + \Gamma_g A(v_{gI} - v_g) - (\alpha_g \rho_g A) FIG(v_g - v_f) \\ & - C\alpha_g \alpha_f \rho A \left[\frac{\partial(v_g - v_f)}{\partial t} + v_f \frac{\partial v_g}{\partial x} - v_g \frac{\partial v_f}{\partial x} \right] \\ & - \sum_{n=1}^N \Gamma_{ni} A v_g + g \Gamma_h A v_g, \end{aligned} \quad (3-5)$$

and for the liquid phase, it is,

$$\begin{aligned} \alpha_f \rho_f A \frac{\partial v_f}{\partial t} + \frac{1}{2} \alpha_f \rho_f A \frac{\partial v_f^2}{\partial x} = & -\alpha_f A \frac{\partial p}{\partial x} + \alpha_f \rho_f B_x A - (\alpha_f \rho_f A) FWF(v_f) \\ & - \Gamma_g A(v_{fI} - v_f) - (\alpha_f \rho_f A) FIF(v_f - v_g) \\ & - C\alpha_f \alpha_g \rho A \left[\frac{\partial(v_f - v_g)}{\partial t} + v_g \frac{\partial v_f}{\partial x} - v_f \frac{\partial v_g}{\partial x} \right] \\ & - \Gamma_{si} A v_f. \end{aligned} \quad (3-6)$$

The force terms on the right sides of Equations (3-5) and (3-6) are, respectively, the pressure gradient, the body force, wall friction, momenta due to interphase mass transfer, interphase frictional drag, and force due to virtual mass, noncondensable/solute source term. The terms FWG and FWF are part of the wall frictional drag, which is linear in velocity, and are

products of the friction coefficient, the frictional reference area per unit volume, and the magnitude of the fluid bulk velocity. The interfacial velocity in the interphase momentum transfer term is the unit momentum with which phase appearance or disappearance occurs. The coefficients FIG and FIF are parts of the interphase frictional drag, which is linear in relative velocity, and are products of the interphase friction coefficients, the frictional reference area per unit volume, and the magnitude of interphase relative velocity.

The coefficient of virtual mass is the same as that used by Anderson³⁻⁵ in the RISQUE code, where the value for C depends on the flow regime. A value of $C > 1/2$ has been shown to be appropriate for bubbly or dispersed flows,^{3-6,7} while $C = 0$ may be appropriate for a separated or stratified flow.

The virtual mass term listed in Equations (3-5) and (3-6) is the same objective formulation^{3-8,9} used in RELAP5/MOD1. In the SCDAP/RELAP5 coding, however, this term is simplified. In particular, the spatial derivative portion of the term is neglected. The reason for this change is that inaccuracies in approximating spatial derivatives for the relatively coarse nodalizations used in system representations can lead to nonphysical characteristics in the numerical solution. The primary effect of the virtual mass term is on the mixture sound speed; thus, the simplified form is adequate, since critical flows are calculated in SCDAP/RELAP5 using an integral model³⁻¹⁰ in which the sound speed is based on an objective formulation for the added mass terms.

Conservation of interphase momentum requires that the force terms associated with interphase mass and momentum exchange sum to zero, and is shown as

$$\begin{aligned} \Gamma_g v_{gI} - (\alpha_g \rho_g) FIG(v_g - v_f) - C\alpha_g \alpha_f \rho [\partial(v_g - v_f)/\partial t] \\ + \Gamma_f v_{fI} - (\alpha_f \rho_f) FIF(v_f - v_g) - C\alpha_f \alpha_g \rho [\partial(v_f - v_g)/\partial t] = 0 \end{aligned} \quad (3-7)$$

This particular form for interphase momentum balance results from consideration of the momentum equations in conservative form. The force terms associated with virtual mass acceleration in Equation (3-7) sum to zero identically as a result of the particular form chosen. In addition, it is usually assumed (although not required by any basic conservation principle) that the interphase momentum transfer due to friction and due to mass transfer independently sum to zero, that is,

$$v_{gI} = v_{fI} = v_I \quad (3-8)$$

and

$$\alpha_g \rho_g F_{IG} = \alpha_f \rho_f F_{IF} = \alpha_g \alpha_f \rho_g \rho_f F_I \quad (3-9)$$

These conditions are sufficient to ensure that Equation (3-7) is satisfied.

The phasic energy equations are

$$\begin{aligned} \frac{1}{V} \frac{\partial}{\partial t} (V \alpha_g \rho_g U_g) + \frac{1}{A} \frac{\partial}{\partial x} (\alpha_g \rho_g U_g v_g A) = -P \frac{\partial \alpha_g}{\partial t} - \frac{P}{A} \frac{\partial}{\partial x} (\alpha_g v_g A) \\ + Q_{wg} + Q_{ig} + \Gamma_{ig} h_g^* + \Gamma_w h_g^s + \text{DISS}_g + \sum_{n=1}^N \Gamma_{ni} h_{ni} - 9\Gamma_h h_g \end{aligned} \quad (3-10)$$

where

h_{ni} = enthalpy of ni -th noncondensable source.

$$\begin{aligned} \frac{1}{V} \frac{\partial}{\partial t} (V \alpha_f \rho_f U_f) + \frac{1}{A} \frac{\partial}{\partial x} (\alpha_f \rho_f U_f v_f A) = -P \frac{\partial \alpha_f}{\partial t} - \frac{P}{A} \frac{\partial}{\partial x} (\alpha_f v_f A) \\ + Q_{wf} + Q_{if} - \Gamma_{ig} h_f^* - \Gamma_w h_f^s + \text{DISS}_f + \Gamma_{si} h_{si} \end{aligned} \quad (3-11)$$

where

Γ_{si} = solute generation rate per unit volume

h_{si} = enthalpy of the solute source.

In the phasic energy equations, Q_{wg} and Q_{wf} are the phasic wall heat transfer rates per unit volume. These phasic wall heat transfer rates satisfy the equation

$$Q = Q_{wg} + Q_{wf} \quad (3-12)$$

where Q is the total wall heat transfer rate to the fluid per unit volume.

The phasic enthalpies (h_g^* , h_f^*) associated with interphase mass transfer in Equations (3-10) and (3-11) are defined in such a way that the interface energy jump conditions at the liquid-vapor interface are satisfied. In particular, the h_g^* and h_f^* are chosen to be h_g^s and h_f , respectively, for the case of vaporization and h_g and h_f^s , respectively, for the case of condensation. The logic for this choice will be further explained in the development of the mass transfer model.

The phasic energy dissipation terms, $DISS_g$ and $DISS_f$, are the sums of wall friction and pump effects. The wall friction dissipations are defined as

$$DISS_g = \alpha_g \rho_g F_{WG} v_g^2 \quad (3-13)$$

and

$$DISS_f = \alpha_f \rho_f F_{WF} v_f^2 \quad (3-14)$$

The phasic energy dissipation terms satisfy the relation

$$\text{DISS} = \text{DISS}_g + \text{DISS}_f , \quad (3-15)$$

where DISS is the energy dissipation. When a pump component is present the associated energy dissipation is also included in the dissipation terms (see Section 3.5.4).

The vapor generation (or condensation) consists of two parts, that which results from bulk energy exchange (Γ_{ig}) and that due to wall heat transfer effects (Γ_w). Each of the vapor generation (or condensation) processes involves interface heat transfer effects. The interface heat transfer terms appearing in Equations (3-10) and (3-11) include heat transfer from the bulk states to the interface, due to both interface energy exchange and wall heat transfer effects. The vapor generation (or condensation) rates are established from energy balance considerations at the interface.

The summation of Equations (3-10) and (3-11) produces the mixture energy equation, from which it is required that the interface transfer terms vanish, that is

$$Q_{ig} + Q_{if} + \Gamma_{ig}(h_g^* - h_f^*) + \Gamma_w(h_g^S - h_f^S) = 0 . \quad (3-16)$$

The interphase heat transfer terms consist of two parts, that is

$$Q_{ig} = H_{ig}(T^S - T_g) + Q_{ig}^w \quad (3-17)$$

and

$$Q_{if} = H_{if}(T^S - T_f) + Q_{if}^w . \quad (3-18)$$

H_{ig} and H_{if} are the interphase heat transfer coefficients per unit volume, and Q_{ig}^w and Q_{if}^w are the wall heat transfer terms.

The first term on the right side of Equations (3-17) and (3-18) is the thermal energy exchange between the fluid bulk states and the fluid interface, while the second term is that due to wall heat transfer effects and will be defined in terms of the wall vapor generation (or condensation) process.

Although it is not a fundamental requirement, it is assumed that Equation (3-16) will be satisfied by requiring that the wall heat transfer terms and the bulk exchange terms each sum to zero independently. Thus,

$$H_{ig}(T^S - T_g) + H_{if}(T^S - T_f) + \Gamma_{ig}(h_g^* - h_f^*) = 0 \quad (3-19)$$

and

$$Q_{ig}^W + Q_{if}^W + \Gamma_w(h_g^S - h_f^S) = 0 \quad (3-20)$$

In addition, since vapor appears at saturation, it is assumed that $Q_{ig}^W = 0$ for boiling processes where $\Gamma_w > 0$. Equation (3-20) can then be solved for the wall vaporization rate to give

$$\Gamma_w = \frac{-Q_{if}^W}{h_g^S - h_f^S}, \quad \Gamma_w > 0 \quad (3-21)$$

Similarly, since liquid appears at saturation, it is assumed that $Q_{if}^W = 0$ for condensation processes in which $\Gamma_w < 0$. Equation (3-21) can then be solved for the wall condensation rate to give

$$\Gamma_w = \frac{-Q_{ig}^W}{h_g^S - h_f^S}, \quad \Gamma_w < 0 \quad (3-22)$$

The interphase energy transfer terms, Q_{ig} and Q_{if} , can thus be expressed in a general way as

$$Q_{ig} = H_{ig}(T^S - T_g) - \left(\frac{1-\epsilon}{2}\right) \Gamma_w(h_g^S - h_f^S) \quad (3-23)$$

and

$$Q_{if} = H_{if}(T^S - T_f) - \left(\frac{1+\epsilon}{2}\right) \Gamma_w(h_g^S - h_f^S) , \quad (3-24)$$

where $\epsilon = 1$ for $\Gamma_w > 0$ and $\epsilon = -1$ for $\Gamma_w < 0$. Finally, Equation (3-16) can be used to define the interphase vaporization (or condensation) rate

$$\Gamma_{ig} = - \frac{Q_{ig} + Q_{if}}{h_g^* - h_f^*} - \Gamma_w \frac{(h_g^S - h_f^S)}{h_g^* - h_f^*} \quad (3-25)$$

which, upon substitution of Equations (3-23) and (3-24), becomes

$$\Gamma_{ig} = - \frac{H_{ig}(T^S - T_g) + H_{if}(T^S - T_f)}{h_g^* - h_f^*} . \quad (3-26)$$

The phase change process that occurs at the interface is envisioned as a process in which bulk fluid is heated or cooled to the saturation temperature and phase change occurs at the saturation state. The interphase energy exchange process from each phase must be such that at least the sensible energy change to reach the saturation state occurs. Otherwise, it can be shown that the phase change process implies energy transfer from a lower temperature to a higher temperature. Such conditions can be avoided by the proper choice of the variables h_g^* and h_f^* . In particular, it can be shown that they should be

$$h_g^* = \frac{1}{2} \left[(h_g^S + h_g) + \eta(h_g^S - h_g) \right] \quad (3-27)$$

and

$$h_f^* = \frac{1}{2} \left[(h_f^s + h_f) - \eta (h_f^s - h_f) \right] \quad (3-28)$$

where

$$\eta = 1 \text{ for } \Gamma_{ig} \geq 0$$

$$\eta = -1 \text{ for } \Gamma_{ig} < 0$$

Substituting Equation (3-26) into Equation (3-4) gives the final expression for the total interphase mass transfer as

$$\Gamma_g = - \frac{H_{ig}(T^s - T_g) + H_{if}(T^s - T_f)}{h_g^* - h_f^*} + \Gamma_w \quad (3-29)$$

3.1.1.2 Noncondensibles in the Gas Phase. The basic, two-phase, single-component model just discussed can be extended to include a noncondensable component in the gas phase. The noncondensable component is assumed to be in mechanical and thermal equilibrium with the vapor phase, so that

$$v_n = v_g \quad (3-30)$$

and

$$T_n = T_g \quad (3-31)$$

where the subscript, n, is used to designate the noncondensable component.

The general approach for inclusion of the noncondensable component consists of assuming that all properties of the gas phase (subscript g) are mixture properties of the steam/noncondensable mixture. The quality, X, is likewise defined as the mass fraction of the entire gas phase. Thus, the

two basic continuity equations [Equations (3-1) and (3-2)] are unchanged. However, it is necessary to add an additional mass conservation equation for the total noncondensable component.

$$\frac{1}{V} \frac{\partial}{\partial t} (V \alpha_g \rho_g X_n) + \frac{1}{A} \frac{\partial}{\partial x} (\alpha_g \rho_g X_n v_g A) = \sum_{n1=1}^N \Gamma_{n1} \quad (3-32)$$

where

X_n = total noncondensible mass fraction in the gas phase

$$= \frac{\sum_{n1=1}^N M_{n1}}{\sum_{n1=1}^N M_{n1} + M_s}$$

M_{n1} = mass of $n1$ -th noncondensible gas

M_s = mass of steam in the gas phase.

For each noncondensible specie, the mass conservation equation is

$$\frac{1}{V} \frac{\partial}{\partial t} (V d g \rho_g X_n X_{n1}) + \frac{1}{A} \frac{\partial}{\partial x} (\alpha_g \rho_g X_n X_{n1} v_g A) = \sum_{n1=1}^N \Gamma_{n1} \quad (3-33)$$

where

X_{n1} = mass fraction of $n1$ -th noncondensible gas in the total noncondensible gas phase

$$= \frac{M_{n1}}{\sum_{n1=1}^N M_{n1}} .$$

The remaining field equations for energy and phasic momentum are unchanged, but the vapor field properties are now evaluated for the steam/noncondensible mixture. The modifications appropriate to the state relationships are described in Section 3.2.3.

3.1.1.3 Boron Concentration in the Liquid Field. An Eulerian boron tracking model is used in SCDAP/RELAP5 that simulates the transport of a dissolved component in the liquid phase. The solution is assumed to be sufficiently dilute that the following assumptions are valid:

- o Liquid properties are not altered by the presence of the solute.
- o Solute is transported only in the liquid phase and at the velocity of the liquid phase.
- o Energy transported by the solute is negligible.
- o Inertia of the solute is negligible.
- o Solute is transported at the velocity of the vapor phase if no liquid is present.

Under these assumptions, only an additional field equation for the conservation of the solute is required. In differential form, the added equation is

$$\frac{\partial \rho_B}{\partial t} + \frac{1}{A} \frac{\partial (C_B \alpha_f \rho_f v_f A)}{\partial x} = \Gamma_s \quad (3-34)$$

where the concentration parameter, C_B , is defined as

$$C_B = \frac{\rho_B}{\rho(1 - X)} \quad (3-35)$$

C_B is the concentration of dissolved solid in mass units per mass unit of liquid phase.

3.1.2 Numerically Convenient Set of Differential Equations

A more convenient set of differential equations upon which to base the numerical scheme is obtained from the basic density and energy differential

equations by expanding the time derivative in each equation using the product rule. When the product rule is used to evaluate the time derivative, we will refer to this form as the expanded form.

A sum density equation is obtained by expanding the time derivative in the phasic density equations, Equations (3-1) and (3-2), adding these two new equations, and using the relation

$$\frac{\partial \alpha_f}{\partial t} = - \frac{\partial \alpha_g}{\partial t} \quad (3-36)$$

This gives

$$\begin{aligned} & \frac{(\alpha_g \rho_g + \alpha_f \rho_f)}{V} \frac{\partial V}{\partial t} + \alpha_g \left(\frac{\partial \rho_g}{\partial t} + \alpha_f \frac{\partial \rho_f}{\partial t} \right) + (\rho_g - \rho_f) \frac{\partial \alpha_g}{\partial t} \\ & + \frac{1}{A} \frac{\partial}{\partial x} (\alpha_g \rho_g v_g A + \alpha_f \rho_f v_f A) = \sum_{n=1}^N \Gamma_{ni} + \Gamma_{si} - g \Gamma_h \quad (3-37) \end{aligned}$$

A difference density equation is obtained by expanding the time derivative in the phasic density equations, Equations (3-1) and (3-2), subtracting these two new equations, again using the relation

$$\frac{\partial \alpha_f}{\partial t} = - \frac{\partial \alpha_g}{\partial t} \quad (3-38)$$

and substituting Equation (3-39) for Γ_g . This gives

$$\begin{aligned} & \frac{(\alpha_g \rho_g - \alpha_f \rho_f)}{V} \frac{\partial V}{\partial t} + \alpha_g \left(\frac{\partial \rho_g}{\partial t} - \alpha_f \frac{\partial \rho_f}{\partial t} \right) + (\rho_g + \rho_f) \frac{\partial \alpha_g}{\partial t} \\ & + \frac{1}{A} \frac{\partial}{\partial x} (\alpha_g \rho_g v_g A + \alpha_f \rho_f v_f A) \end{aligned}$$

$$= - \frac{2[H_{ig}(T^S - T_g) + H_{if}(T^S - T_f)]}{h_g^* - h_f^*} + 2\Gamma_w + \sum_{n=1}^N \Gamma_{ni} - \Gamma_{si} - 9\Gamma_n. \quad (3-39)$$

The time derivative of the total noncondensable density equation, Equation (3-32), is expanded to give

$$\begin{aligned} \frac{1}{V} \left(\rho_g X_n V \frac{\partial \alpha_g}{\partial t} + \alpha_g X_n V \frac{\partial \rho_g}{\partial t} + \alpha_g \rho_g \frac{\partial X_n}{\partial t} V + \alpha_g \rho_g X_n \frac{\partial V}{\partial t} \right) \\ + \frac{1}{A} \frac{\partial}{\partial x} (\alpha_g \rho_g X_n v_g A) = \sum_{n=1}^N \Gamma_{ni} . \end{aligned} \quad (3-40)$$

The momentum equations are also rearranged into a sum and difference form. The sum momentum equation is obtained by direct summation of Equations (3-5) and (3-6) with the interface conditions [Equations (3-7), (3-8), and (3-9)] substituted where appropriate and the cross-sectional area canceled throughout. The resulting sum equation is

$$\begin{aligned} \alpha_g \rho_g \frac{\partial v_g}{\partial t} + \alpha_f \rho_f \frac{\partial v_f}{\partial t} + \frac{1}{2} \alpha_g \rho_g \frac{\partial v_g^2}{\partial x} + \frac{1}{2} \alpha_f \rho_f \frac{\partial v_f^2}{\partial x} = - \frac{\partial p}{\partial x} + \rho B_x \\ - \alpha_g \rho_g v_g F_{WG} - \alpha_f \rho_f v_f F_{WF} - \Gamma_g (v_g - v_f) - \sum_{n=1}^N \Gamma_{ni} v_g - \Gamma_{si} v_f \\ + 9\Gamma_h v_g . \end{aligned} \quad (3-41)$$

The difference of the phasic momentum equations is obtained by first dividing the vapor and liquid phasic momentum equations by $\alpha_g \rho_g$ and $\alpha_f \rho_f$, respectively, and subsequently subtracting. Here again, the interface conditions are used, and the common area is divided out. As previously discussed, the virtual mass term is simplified by neglecting the spatial derivative portion. The resulting equation is

$$\begin{aligned}
\frac{\partial v_g}{\partial t} - \frac{\partial v_f}{\partial t} + \frac{1}{2} \frac{\partial v_g^2}{\partial x} - \frac{1}{2} \frac{\partial v_f^2}{\partial x} = & - \left(\frac{1}{\rho_g} - \frac{1}{\rho_f} \right) \frac{MP}{\partial x} - v_g \text{FWG} + v_f \text{FWF} \\
& + \Gamma_g [\rho v_I - (\alpha_f \rho_f v_g + \alpha_g \rho_g v_f)] / (\alpha_g \rho_g \alpha_f \rho_f) - \rho^F I (v_g - v_f) \\
& - C[\rho^2 / (\rho_g \rho_f)] \frac{\partial (v_g - v_f)}{\partial t} - \sum_{n=1}^N \Gamma_{n1} \frac{v_g}{\alpha_g \rho_g} + \frac{\Gamma_{s1} v_f}{\alpha_f \rho_f} \\
& + \frac{9\Gamma_h v_g}{\alpha_g \rho_g}
\end{aligned} \tag{3-42}$$

where the interfacial velocity, v_I , is defined as

$$v_I = \lambda v_g + (1 - \lambda) v_f \quad . \tag{3-43}$$

This definition for v_I has the property that if $\lambda = 1/2$, the interphase momentum transfer process associated with mass transfer is reversible. This value leads to either an entropy sink or source, depending on the sign of Γ_g . However if λ is chosen to be 0 for positive values of Γ_g and +1 for negative values of Γ_g (that is, a donor formulation), the mass exchange process is always dissipative. The latter model for v_I is the most realistic for the momentum exchange process and is used for the numerical scheme development.

To develop an expanded form of the vapor energy, the time derivative of the vapor energy Equation (3-10) is expanded, the Q_{ig} Equation (3-23) and the Γ_{ig} Equation (3-26) are substituted, and the H_{ig} , H_{if} , $\partial \alpha_g / \partial t$, and convective terms are collected. This gives the desired form for the vapor energy equation

$$\frac{1}{v} (\alpha_g \rho_g u_g) \frac{\partial v}{\partial t} + (\rho_g u_g + \rho) \frac{\partial \alpha_g}{\partial t}$$

$$\begin{aligned}
& + \alpha_g U_g \frac{\partial \rho_g}{\partial t} + \alpha_g \rho_g \frac{\partial U_g}{\partial t} + \frac{1}{A} \left[\frac{\partial}{\partial x} (\alpha_g \rho_g U_g v_g A) + \rho \frac{\partial}{\partial x} (\alpha_g v_g A) \right] \\
& = - \left(\frac{h_f^*}{h_g^* - h_f^*} \right) H_{ig} (T^S - T_g) - \left(\frac{h_g^*}{h_g^* - h_f^*} \right) H_{if} (T^S - T_f) + \left[\left(\frac{1+\epsilon}{2} \right) h_g^S \right. \\
& \quad \left. + \left(\frac{1-\epsilon}{2} \right) h_f^S \right] \Gamma_w + \Gamma_{wg} + \text{DISS}_g + \sum_{n=1}^N \Gamma_{ni} h_{ni} - 9 \Gamma_h h_g . \quad (3-44)
\end{aligned}$$

To develop an expanded form of the liquid energy Equation (3-25), the time derivative is expanded, the Q_{if} Equation (3-24) and the Γ_{ig} Equation (3-26) are substituted, and

$$\frac{\partial \alpha_f}{\partial t} = - \frac{\partial \alpha_g}{\partial t} \quad (3-45)$$

is used. Then, the H_{ig} , H_{if} , $\partial \alpha_g / \partial t$, and convective terms are collected. This gives the desired form for the liquid energy equation

$$\begin{aligned}
& \frac{1}{V} (\alpha_f \rho_f U_f) \frac{\partial V}{\partial t} - (\rho_f U_f + \rho) \frac{\partial \alpha_g}{\partial t} \\
& + \alpha_f U_f \frac{\partial \rho_f}{\partial t} + \alpha_f \rho_f \frac{\partial U_f}{\partial t} + \frac{1}{A} \left[\frac{\partial}{\partial x} (\alpha_f \rho_f U_f v_f A) + \rho \frac{\partial}{\partial x} (\alpha_f v_f A) \right] \\
& = \left(\frac{h_f^*}{h_g^* - h_f^*} \right) H_{ig} (T^S - T_g) + \left(\frac{h_g^*}{h_g^* - h_f^*} \right) H_{if} (T^S - T_f) - \left[\left(\frac{1+\epsilon}{2} \right) h_g^S \right. \\
& \quad \left. + \left(\frac{1-\epsilon}{2} \right) h_f^S \right] \Gamma_w + Q_{wf} + \text{DISS}_f + \Gamma_{si} h_{si} . \quad (3-46)
\end{aligned}$$

The basic density and energy differential equations are used in nonexpanded form in the back substitution part of the numerical scheme. When the product rule is not used to evaluate the time derivative, we will refer to this form as the nonexpanded form.

The vapor, liquid, and noncondensable density equations, Equations (3-1), (3-2), and (3-32), are in nonexpanded form. The Γ_g , Equation (3-29), is not substituted into the vapor and liquid density equations. (The reason will be apparent in the Time Step Solution Scheme, Section 3.1.6.) The vapor energy equation, Equation (3-10), is altered by substituting Equation (3-23) for Q_{ig} , substituting Equation (3-26) for Γ_{ig} , and collecting the H_{ig} , H_{if} , and convective terms. This gives

$$\begin{aligned} \frac{1}{V} \frac{\partial}{\partial t} (V \alpha_g \rho_g U_g) + \frac{1}{A} \left[\frac{\partial}{\partial x} (\alpha_g \rho_g U_g v_g A) + P \frac{\partial}{\partial x} (\alpha_g v_g A) \right] \\ = - P \frac{\partial \alpha_g}{\partial t} - \left(\frac{h_f^*}{h_g^* - h_f^*} \right) H_{ig} (T^S - T_g) - \left(\frac{h_g^*}{h_g^* - h_f^*} \right) H_{if} (T^S - T_f) + \left[\left(\frac{1+\epsilon}{2} \right) h_g^S \right. \\ \left. + \left(\frac{1-\epsilon}{2} \right) h_f^S \right] \Gamma_w + Q_{wg} + \text{DISS}_g + \sum_{n1=1}^N \Gamma_{n1} h_{n1} - 9 \Gamma_h h_g \quad (3-47) \end{aligned}$$

The liquid energy equation, Equation (3-11), is also altered by substituting Equation (3-23) for Q_{if} , substituting Equation (3-26) for Γ_{ig} , using

$$\frac{\partial \alpha_f}{\partial t} = - \frac{\partial \alpha_g}{\partial t} \quad (3-48)$$

and collecting the H_{ig} , H_{if} , and convective terms. This gives

$$\frac{1}{V} \frac{\partial}{\partial t} (V \alpha_f \rho_f U_f) + \frac{1}{A} \left[\frac{\partial}{\partial x} (\alpha_f \rho_f U_f v_f A) + P \frac{\partial}{\partial x} (\alpha_f v_f A) \right]$$

$$\begin{aligned}
&= P \frac{\partial \alpha_g}{\partial t} + \left(\frac{h_f^*}{h_g^* - h_f^*} \right) H_{ig} (T^S - T_g) + \left(\frac{h_g^*}{h_g^* - h_f^*} \right) H_{if} (T^S - T_f) \\
&- \left[\left(\frac{1+\epsilon}{2} \right) h_g^S + \left(\frac{1-\epsilon}{2} \right) h_f^S \right] \Gamma_w + Q_{wf} + \text{DISS}_f + \Gamma_{si} h_{si}. \quad (3-49)
\end{aligned}$$

3.1.3 Horizontal Stratified Flow

Flow at low velocity in a horizontal passage can be stratified as a result of buoyancy forces caused by density differences between vapor and liquid. When the flow is stratified, the area average pressures are affected by nonuniform transverse distribution of the phases. Appropriate modifications to the basic field equations when stratified flow exists are obtained by considering separate area average pressures for the vapor and liquid phases and the interfacial pressure between them. Using this model, the pressure gradient force terms of Equations (3-5) and (3-6) become

$$- \alpha_g A \left(\frac{\partial P}{\partial x} \right) \rightarrow - \alpha_g A \left(\frac{\partial P_g}{\partial x} \right) + (P_I - P_g) A \left(\frac{\partial \alpha_g}{\partial x} \right) \quad (3-50)$$

and

$$- \alpha_f A \left(\frac{\partial P}{\partial x} \right) \rightarrow - \alpha_f A \left(\frac{\partial P_f}{\partial x} \right) + (P_I - P_f) A \left(\frac{\partial \alpha_f}{\partial x} \right). \quad (3-51)$$

The area average pressure for the entire cross section of the flow is expressed in terms of the phasic area average pressures by

$$P = \alpha_g P_g + \alpha_f P_f. \quad (3-52)$$

With these definitions, the sum of the phasic momentum equations, written in terms of the cross-section average pressure [Equation (3-26)] remains unchanged. However, the difference of the phasic momentum equations [Equation (3-27)], contains the following additional terms on the right side

$$[\rho/(\alpha_g \alpha_f \rho_g \rho_f)] [-\alpha_f \partial(\alpha_g P_g)/\partial x + \alpha_g \partial(\alpha_f P_f)/\partial x + P_I(\partial\alpha_g/\partial x)] . \quad (3-53)$$

The interface and phasic cross-sectional average pressures, P_I , P_g , and P_f , can be found by means of the assumption of a transverse hydrostatic pressure in a round pipe. For a pipe having diameter D , pressures P_I , P_g , and P_f are given by

$$P_g = P_I - \rho_g B_y D \left[\sin^3 \theta / (3 \pi \alpha_g) - \cos \theta / 2 \right] \quad (3-54)$$

$$P_f = P_I + \rho_f B_y D \left[\sin^3 \theta / (3 \pi \alpha_f) + \cos \theta / 2 \right] . \quad (3-55)$$

The angle, θ , is defined by the void fraction, as illustrated in Figure 3-1. The algebraic relationship between α_g and θ is

$$\alpha_g \pi = (\theta - \sin \theta \cos \theta) . \quad (3-56)$$

The additional term in the momentum difference equation [Equation (3-53)] can be simplified using Equations (3-54), (3-55), and (3-56) to obtain

$$- [\rho/(\rho_g \rho_f)] (\rho_f - \rho_g) \pi D B_y / (4 \sin \theta) (\partial\alpha_g/\partial x) \quad (3-57)$$

where θ is related to the void fraction using Equation (3-56).

The additional force term that arises for a stratified flow geometry in horizontal pipes is added to the basic equation when the flow is established to be stratified from flow regime considerations. It should be noted that the additional force term was derived assuming a round pipe. If the cross section is rectangular, this assumption is not valid. A similar term is added when the flow is vertically stratified. In order to provide for a smooth transition between stratified and non-stratified flow situations, this term is activated in all flow regimes. Since this term is small compared to other terms in the momentum equation when the flow is non-stratified, this was felt to be a reasonable assumption.

Figure 3-1. Relation of central angle θ to void fraction α_g .

3.1.4 Semi-Implicit Scheme Difference Equations

The semi-implicit numerical solution scheme is based on replacing the system of differential equations with a system of finite-difference equations partially implicit in time. The terms evaluated implicitly are identified as the scheme is developed. In all cases, the implicit terms are formulated to be linear in the dependent variables at new time. This results in a linear time-advancement matrix that is solved by direct inversion using a sparse matrix routine.³⁻¹¹ An additional feature of the scheme is that implicitness is selected such that the field equations can be reduced to a single difference equation per fluid control volume or mesh cell, which is in terms of the hydrodynamic pressure. Thus, only an $N \times N$ system of the difference equations must be solved simultaneously at each time step. (N is the total number of control volumes used to simulate the fluid system.)

It is well known^{3-5,12} that the system of differential equations constitutes an ill-posed, initial-value problem. This fact is of little concern physically, since the addition of any second-order differential effect (regardless of how small), such as viscosity or surface tension, results in a well-posed problem.³⁻¹³ However, the ill-posedness is of some concern numerically, since it is necessary that the numerical problem be well-posed. The approximations inherent in any numerical scheme modify the solution somewhat (truncation error); these effects can be either stabilizing or destabilizing. The resulting numerical scheme must be stable for mesh sizes of practical interest.

A well-posed and stable numerical algorithm is obtained by several means. These include the selective implicit evaluation of spatial gradient terms at the new time, donor formulations for the mass and energy flux terms, and use of a donor-like formulation for the momentum flux terms. Donor formulations for these flux terms are used because of the well-known instability of a centered finite difference scheme. The term donor-like is used because the momentum flux formulation consists of a centered formulation for the spatial velocity gradient plus a numerical viscosity

term similar to the form obtained when the momentum flux terms are donored with the conservative form of the momentum equations. The well-posedness of the final numerical scheme (as well as its accuracy) has been demonstrated by extensive numerical testing during development.

The difference equations are based on the concept of a control volume (or mesh cell) in which mass and energy are conserved by equating accumulation to rate of influx through the cell boundaries. This model results in defining mass and energy volume average properties and requiring knowledge of velocities at the volume boundaries. The velocities at boundaries are most conveniently defined through use of momentum control volumes (cells) centered on the mass and energy cell boundaries. This approach results in a numerical scheme having a staggered spatial mesh. The scalar properties (pressure, energies, and void fraction) of the flow are defined at cell centers, and vector quantities (velocities) are defined on the cell boundaries. The resulting one-dimensional spatial noding is illustrated in Figure 3-2. The term cell means an increment in the spatial variable, x , corresponding to the mass and energy control volume.

The difference equations for each cell are obtained by integrating the mass and energy equations [Equations (3-37), (3-39), (3-40), (3-44), and (3-46)] with respect to the spatial variable, x , from the junction at x_j to x_{j+1} . The momentum equations [Equations (3-41) and (3-42)] are integrated with respect to the spatial variable from cell center to adjoining cell center (x_k to x_l , Figure 3-2). The equations are listed for the case of a pipe with no branching.

When the mass and energy equations [Equations (3-37), (3-39), (3-40), (3-44), and (3-46)] are integrated with respect to the spatial variable from junction j to $j+1$, differential equations in terms of cell-average properties and cell boundary fluxes are obtained. The subscripts and superscripts within the parentheses indicate integration limits for the enclosed quantity. The quantities not enclosed in parentheses are volume averages.

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Figure 3-2. Difference equation nodalization schematic.

The sum density Equation (3-37) becomes

$$\begin{aligned}
 (\alpha_g \rho_g + \alpha_f \rho_f) \frac{\partial v}{\partial t} + v \left[\alpha_g \frac{\partial \rho_g}{\partial t} + \alpha_f \frac{\partial \rho_f}{\partial t} + (\rho_g - \rho_f) \frac{\partial \alpha_g}{\partial t} \right] \\
 + (\alpha_g \rho_g v_g A)_{x_j}^{x_{j+1}} + (\alpha_f \rho_f v_f A)_{x_j}^{x_{j+1}} = v (\Gamma_{n1} - \Gamma_{s1} - 9\Gamma_h) \quad (3-58)
 \end{aligned}$$

The difference density Equation (3-39) becomes

$$\begin{aligned}
 (\alpha_g \rho_g - \alpha_f \rho_f) \frac{\partial v}{\partial t} + v \left[\alpha_g \frac{\partial \rho_g}{\partial t} - \alpha_f \frac{\partial \rho_f}{\partial t} + (\rho_g + \rho_f) \frac{\partial \alpha_g}{\partial t} \right] + (\alpha_g \rho_g v_g A)_{x_j}^{x_{j+1}} - (\alpha_f \rho_f v_f A)_{x_j}^{x_{j+1}} \\
 = -v \left\{ \frac{2[H_{1g}(T^S - T_g) + H_{1f}(T^S - T_f)]}{h_g^* - h_f^*} + 2\Gamma_w \right\} \\
 + v \sum_{n1=1}^N \Gamma_{n1} - \Gamma_{s1} - 9\Gamma_h \quad (3-59)
 \end{aligned}$$

The total noncondensable density Equation (3-40) becomes

$$\begin{aligned}
 \alpha_g \rho_g X_n \frac{\partial v}{\partial t} + v \left(\rho_g X_n \frac{\partial \alpha_g}{\partial t} + \alpha_g X_n \frac{\partial \rho_g}{\partial t} + \alpha_g \rho_g \frac{\partial X_n}{\partial t} \right) + [(\alpha_g \rho_g X_n v_g A)]_{x_j}^{x_{j+1}} \\
 = v \sum_{n1=1}^N \Gamma_{n1} \quad (3-60)
 \end{aligned}$$

The vapor energy Equation (3-44) becomes

$$\begin{aligned}
 \alpha_g \rho_g U_g \frac{\partial v}{\partial t} + v \left[(\rho_g U_g + P) \frac{\partial \alpha_g}{\partial t} + \alpha_g U_g \frac{\partial \rho_g}{\partial t} + \alpha_g \rho_g \frac{\partial U_g}{\partial t} \right] + [(\alpha_g \rho_g U_g v_g A) + P(\alpha_g v_g A)]_{x_j}^{x_{j+1}} \\
 = v \left\{ - \left(\frac{h_f^*}{h_g^* - h_f^*} \right) H_{1g} (T^S - T_g) - \left(\frac{h_g^*}{h_g^* - h_f^*} \right) H_{1f} (T^S - T_f) \right\}
 \end{aligned}$$

$$+ \left[\left(\frac{1+\epsilon}{2} \right) h_g^s + \left(\frac{1-\epsilon}{2} \right) h_f^s \right] \Gamma_w + \Gamma_{wg} + \text{DISS}_g + \sum_{n1+1}^N \Gamma_{ni} h_{ni} - 9\Gamma_h h_g \left\} (3-61)$$

The liquid energy Equation (3-46) becomes

$$\begin{aligned} & \alpha_f \rho_f U_f \frac{\partial v}{\partial t} + V \left[- (\rho_f U_f + P) \frac{\partial \alpha_g}{\partial t} + \alpha_f U_f \frac{\partial \rho_f}{\partial t} + \alpha_f \rho_f \frac{\partial U_f}{\partial t} \right] \\ & + [(\alpha_f \rho_f U_f v_f A) + P(\alpha_f v_f A)]_{x_j}^{x_{j+1}} \\ & = V \left\{ \left(\frac{h_f^*}{h_g^* - h_f^*} \right) H_{ig} (T^s - T_g) + \left(\frac{h_g^*}{h_g^* - h_f^*} \right) H_{if} (T^s - T_f) \right. \\ & \quad \left. - \left[\left(\frac{1+\epsilon}{2} \right) h_g^s + \left(\frac{1-\epsilon}{2} \right) h_f^s \right] \Gamma_w + Q_{wf} + \text{DISS}_f + \Gamma_{si} h_{si} \right\} \end{aligned} \quad (3-62)$$

The sum and difference momentum equations [Equations (3-41) and (3-42)] are integrated from cell center to cell center to obtain

$$\begin{aligned} & \frac{V}{A} \left[(\alpha_g \rho_g) \frac{\partial v_g}{\partial t} + (\alpha_f \rho_f) \frac{\partial v_f}{\partial t} \right] + \frac{1}{2} \alpha_g \rho_g (v_g^2)_{x_K}^{x_L} + \frac{1}{2} \alpha_f \rho_f (v_f^2)_{x_K}^{x_L} \\ & = - (P)_{x_K}^{x_L} + \rho B_x (x_L - x_K) - (\alpha_g \rho_g v_g^{\text{FWG}} + \alpha_f \rho_f v_f^{\text{FWF}}) (x_L - x_K) \\ & \quad - \Gamma_g (v_g - v_f) (x_L - x_K) - \sum_{n1+1}^N \Gamma_{ni} v_g (x_L - x_K) - \Gamma_{si} v_f (x_L - x_K) \\ & \quad + 9\Gamma_h v_g (x_L - x_K) \end{aligned} \quad (3-63)$$

and

$$\begin{aligned}
& \left(\frac{V}{A} \right) \left[1 + C \rho^2 / (\rho_g \rho_f) \right] \left(\frac{\partial v_g}{\partial t} - \frac{\partial v_f}{\partial t} \right) + \frac{1}{2} \left(v_g^2 \right)_{x_K}^L - \frac{1}{2} \left(v_f^2 \right)_{x_K}^L \\
& = - \left(\frac{1}{\rho_g} - \frac{1}{\rho_f} \right) (P)_{x_K}^L - (v_g^{FWG} - v_f^{FWF}) (x_L - x_K) + \left\{ \Gamma_g [\rho v_I \right. \\
& \quad \left. - (\alpha_f \rho_f v_g + \alpha_g \rho_g v_f)] / (\alpha_g \rho_g \alpha_f \rho_f) \right\} (x_L - x_K) - \rho F I (v_g - v_f) (x_L - x_K) \\
& \quad - S_{ni=1}^N \Gamma_{ni} - \frac{V_g}{\alpha_g \rho_g} (x_L - x_K) + \frac{\Gamma_{si} V_f}{\alpha_f \rho_f} (x_L - x_K) + \frac{9 \Gamma_h V_g}{\alpha_g \rho_g} (x_L - x_K) .
\end{aligned}
\tag{3-64}$$

Here, the common area term, A, has been factored from most terms. The quantities shown in brackets with limits are evaluated at the indicated limits, while the coefficients are averaged over the cell or integration interval. The indicated derivatives are now derivatives of cell average quantities. Since the integration interval is centered on the junction, the coefficient averages are approximated by the junction values. In all cases, the correlation coefficients for averaged products are taken as unity, so averaged products are replaced directly with products of averages.

Several general guidelines were followed in developing numerical approximations for Equations (3-58) through (3-64). These guidelines are summarized below.

- o Mass and energy inventories are very important quantities in water reactor safety analysis. The numerical scheme should be consistent and conservative in these quantities. (A greater degree of approximation for momentum effects is considered acceptable.) Both mass and energy are convected from the same cell, and each is evaluated at the same time level; that is, mass density is evaluated at old time level, so energy density is also evaluated at old time.

- o To achieve fast execution speed, implicit evaluation is used only for those terms responsible for the sonic wave propagation time step limit and those phenomena known to have small time constants. Thus, implicit evaluation is used for the velocity in the mass and energy transport terms, the pressure gradient in the momentum equations, and the interphase mass and momentum exchange terms.
- o To further increase computing speed, time-level evaluations are selected so the resulting implicit terms are linear in the new time variables. Where it is necessary to retain nonlinearities, Taylor series expansions about old time values are used to obtain a formulation linear in the new time variables. (Higher-order terms are neglected.) Linearity results in high computing speed by eliminating the need to iteratively solve systems of nonlinear equations.
- o To allow easy degeneration to homogeneous, or single-phase, formulations, the momentum equations are used as a sum and a difference equation. The particular difference equation used is obtained by first dividing each of the phasic momentum equations by $\alpha_g \rho_g$ and $\alpha_f \rho_f$, for the vapor and liquid phase equations, respectively, and then subtracting.

Using the above guidelines, the finite-difference equations for the mass and energy balances, corresponding to Equations (3-58) through (3-62), are listed below. Some of the terms are intermediate time variables, which are written with a tilde ($\sim$). The reason for their use will be explained in the Time Advancement Scheme, Section 3.1.6.

The sum density equation is

$$V_L^n [\alpha_{g,L}^n (\tilde{\rho}_{g,L}^{n+1} - \rho_{g,L}^n) + \alpha_{f,L}^n (\tilde{\rho}_{f,L}^{n+1} - \rho_{f,L}^n) + (\rho_{g,L}^n - \rho_{f,L}^n) (\tilde{\alpha}_{g,L}^{n+1} - \alpha_{g,L}^n)]$$

$$\begin{aligned}
& + (\dot{\alpha}_{g,j+1}^n \dot{\rho}_{g,j+1}^n v_{g,j+1}^{n+1} A_{j+1}^n - \dot{\alpha}_{g,j}^n \dot{\rho}_{g,j}^n v_{g,j}^{n+1} A_j^n) \Delta t \\
& + (\dot{\alpha}_{f,j+1}^n \dot{\rho}_{f,j+1}^n v_{f,j+1}^{n+1} A_{j+1}^n - \dot{\alpha}_{f,j}^n \dot{\rho}_{f,j}^n v_{f,j}^{n+1} A_j^n) \Delta t \\
& = \left(\sum_{n=1}^N \Gamma_{ni,L}^N + \Gamma_{si,L}^N - 9\Gamma_{hi,L}^N \right) V_L^n \Delta t - (\alpha_{g,L}^n \rho_{g,L}^n + \alpha_{f,L}^n \rho_{f,L}^n) (V_L^{n+1} - V_L^n). \quad (3-65)
\end{aligned}$$

The difference density equation is

$$\begin{aligned}
& V_L^n [\alpha_{g,L}^n (\tilde{\rho}_{g,L}^{n+1} - \rho_{g,L}^n) - \alpha_{f,L}^n (\tilde{\rho}_{f,L}^{n+1} - \rho_{f,L}^n) + (\rho_{g,L}^n + \rho_{f,L}^n) (\tilde{\alpha}_{g,L}^{n+1} - \alpha_{g,L}^n)] \\
& + (\dot{\alpha}_{g,j+1}^n \dot{\rho}_{g,j+1}^n v_{g,j+1}^{n+1} A_{j+1}^n - \dot{\alpha}_{g,j}^n \dot{\rho}_{g,j}^n v_{g,j}^{n+1} A_j^n) \Delta t \\
& - (\dot{\alpha}_{f,j+1}^n \dot{\rho}_{f,j+1}^n v_{f,j+1}^{n+1} A_{j+1}^n - \dot{\alpha}_{f,j}^n \dot{\rho}_{f,j}^n v_{f,j}^{n+1} A_j^n) \Delta t \\
& = - \left(\frac{2}{h_g^* - h_f^*} \right)_L^n V_L \Delta t [H_{ig,L}^n (\tilde{T}_L^{s,n+1} - \tilde{T}_{g,L}^{n+1}) \\
& + H_{if,L}^n (\tilde{T}_L^{s,n+1} - \tilde{T}_{f,L}^{n+1})] + 2V_L \Delta t \Gamma_{w,L}^n + \left(\sum_{n=1}^N \Gamma_{ni,L}^N - \Gamma_{si,L}^N - 9\Gamma_{hi,L}^N \right) V_L^n \Delta t \\
& - (\alpha_{g,L}^n \rho_{g,L}^n - \alpha_{f,L}^n \rho_{f,L}^n) (V_L^{n+1} - V_L^n). \quad (3-66)
\end{aligned}$$

The total noncondensable density equation is

$$V_L^n [\rho_{g,L}^n \chi_{n,L}^n (\tilde{\alpha}_{g,L}^{n+1} - \alpha_{g,L}^n) + \alpha_{g,L}^n \chi_{n,L}^n (\tilde{\rho}_{g,L}^{n+1} - \rho_{g,L}^n)]$$

$$\begin{aligned}
& + \alpha_{g,L}^n \rho_{g,L}^n (\tilde{x}_{n,L}^{n+1} - x_{n,L}^n) + (\dot{\alpha}_{g,j+1}^n \dot{\rho}_{g,j+1}^n \dot{x}_{n,j+1}^n v_{g,j+1}^{n+1} A_{j+1}^n \\
& - \dot{\alpha}_{g,j}^n \dot{\rho}_{g,j}^n \dot{x}_{n,j}^n v_{g,j}^{n+1} A_j^n) \Delta t = \sum_{n \neq 1}^n \Gamma_{n1}^n v_L^n \Delta t - \alpha_{g,L}^n \rho_{g,L}^n x_{n,L}^n (v_L^{n+1} - v_L^n) \quad .
\end{aligned}
\tag{3-67}$$

The vapor energy equation is

$$\begin{aligned}
v_L^n & \left[(\rho_{g,L}^n U_{g,L}^n + p_L^n) (\tilde{\alpha}_{g,L}^{n+1} - \alpha_{g,L}^n) + \alpha_{g,L}^n U_{g,L}^n (\tilde{\rho}_{g,L}^{n+1} - \rho_{g,L}^n) \right. \\
& + \alpha_{g,L}^n \rho_{g,L}^n (\tilde{U}_{g,L}^{n+1} - U_{g,L}^n) + \dot{\alpha}_{g,j+1}^n (\dot{\rho}_{g,j+1}^n \dot{U}_{g,j+1}^n + p_L^n) v_{g,j+1}^{n+1} A_{j+1}^n \\
& \left. - \dot{\alpha}_{g,j}^n (\dot{\rho}_{g,j}^n \dot{U}_{g,j}^n + p_L^n) v_{g,j}^{n+1} A_j^n \right] \Delta t = \left\{ - \left(\frac{h_f^*}{h_g^* - h_f^*} \right)_L^n H_{ig,L}^n (\tilde{T}_L^{s,n+1} - \tilde{T}_{g,L}^{n+1}) \right. \\
& - \left(\frac{h_g^*}{h_g^* - h_f^*} \right)_L^n H_{if,L}^n (\tilde{T}_L^{s,n+1} - \tilde{T}_{f,L}^{n+1}) + \left[\left(\frac{1+\epsilon}{2} \right) h_{g,L}^{s,n} + \left(\frac{1-\epsilon}{2} \right) h_{f,L}^{s,n} \right] \Gamma_{w,L}^n \\
& + Q_{wg,L}^n + \text{DISS}_{g,L}^n \left\{ v_L^n \Delta t + \left(\sum_{n \neq 1}^n \Gamma_{n1,L}^n h_{n1,L}^n - 9 \Gamma_{h,L}^n h_{g,L}^n \right) v_L^n \Delta t \right. \\
& \left. - \alpha_{g,L}^n \rho_{g,L}^n U_{g,L}^n (v_L^{n+1} - v_L^n) \right\} \quad .
\end{aligned}
\tag{3-68}$$

The liquid energy equation is

$$v_L^n [- (\rho_{f,L}^n U_{f,L}^n + p_L^n) (\tilde{\alpha}_{g,L}^{n+1} - \alpha_{g,L}^n) + \alpha_{f,L}^n U_{f,L}^n (\tilde{\rho}_{f,L}^{n+1} - \rho_{f,L}^n)]$$

$$\begin{aligned}
& + \alpha_{f,L}^n \rho_{f,L}^n (\dot{U}_{f,L}^{n+1} U_{f,L}^n) + [\dot{\alpha}_{f,j+1}^n (\dot{\rho}_{f,j+1}^n U_{f,j+1}^n + p_L^n) v_{f,j+1}^{n+1} A_{j+1}^n \\
& - \dot{\alpha}_{f,j}^n (\dot{\rho}_{f,j}^n \dot{U}_{f,j}^n + p_L^n) v_{f,j}^{n+1} A_j^n] \Delta t = \left\{ \left(\frac{h_f^*}{h_g^* - h_f^*} \right)_L^n H_{ig,L}^n (\tilde{T}_L^{s,n+1} - \tilde{T}_{g,L}^{n+1}) \right. \\
& + \left(\frac{h_g^*}{h_g^* - h_f^*} \right)_L^n H_{if,L}^n (\tilde{T}_L^{s,n+1} - \tilde{T}_{f,L}^{n+1}) - [(\frac{1+\epsilon}{2}) h_{g,L}^{s,n} + (\frac{1-\epsilon}{2}) h_{f,L}^{s,n}] \Gamma_{w,L}^n \\
& \left. + Q_{wf,L}^n + DISS_{f,L}^n \right\} v_L^n \Delta t + \Gamma_{si,L}^n h_{si,L}^n v_L^n \Delta t - \alpha_{f,L}^n \rho_{f,L}^n U_{f,L}^n (v_L^{n+1} - v_L^n) .
\end{aligned} \tag{3-69}$$

The quantities having a dot overscore are donored quantities based on the junction velocities, v_g and v_f . The donored quantities are volume average scalar quantities defined analytically as

$$\dot{\phi} = \frac{1}{2} (\phi_K + \phi_L) + \frac{1}{2} \frac{|v|}{v} (\phi_K - \phi_L), \quad v \neq 0 \tag{3-70}$$

where ϕ is any of the donored properties and v is the appropriate velocity (that is, vapor or liquid). For the degenerate case of $v = 0$, the quantity in the K volume is used, that is

$$\dot{\phi} = \phi_K, \quad v = 0 . \tag{3-71}$$

Where donored values are not used at junctions, linear interpolations between neighboring cell values are used.

The intermediate time phasic densities used in Equations (3-65) through (3-69) are obtained by linearizing the phasic state relations about the old time values (see State Relationships, Section 3.2).

$$\begin{aligned}\tilde{\rho}_{g,L}^{n+1} = & \rho_{g,L}^n + \left(\frac{\partial \rho_g}{\partial p}\right)_L^n (p_L^{n+1} - p_L^n) + \left(\frac{\partial \rho_g}{\partial x_n}\right)_L^n (\tilde{x}_{n,L}^{n+1} - x_{n,L}^n) \\ & + \left(\frac{\partial \rho_g}{\partial u_g}\right)_L^n (\tilde{u}_{g,L}^{n+1} - u_{g,L}^n)\end{aligned}\quad (3-72)$$

$$\tilde{\rho}_{f,L}^{n+1} = \rho_{f,L}^n + \left(\frac{\partial \rho_f}{\partial p}\right)_L^n (p_L^{n+1} - p_L^n) + \left(\frac{\partial \rho_f}{\partial u_f}\right)_L^n (\tilde{u}_{f,L}^{n+1} - u_{f,L}^n) \quad (3-73)$$

The method of obtaining the state derivatives used in Equations (3-72) and (3-73) is also indicated in the State Relationships, Section 3.2.

Intermediate time interphase heat transfer rates can be written using the finite difference form of Equations (3-23) and (3-24).

$$\tilde{Q}_{ig,L}^{n+1} = H_{ig,L}^n (\tilde{T}_L^{s,n+1} - \tilde{T}_{g,L}^{n+1}) - \left(\frac{1-\epsilon}{2}\right) \Gamma_{w,L}^n (h_{g,L}^{s,n} - h_{f,L}^{s,n}) \quad (3-74)$$

$$\tilde{Q}_{if,L}^{n+1} = H_{if,L}^n (\tilde{T}_L^{s,n+1} - \tilde{T}_{f,L}^{n+1}) - \left(\frac{1+\epsilon}{2}\right) \Gamma_{w,L}^n (h_{g,L}^{s,n} - h_{f,L}^{s,n}) \quad (3-75)$$

The intermediate time temperatures are obtained by linearizing the temperature relations about the old time values (see State Relationships, Section 3.2).

$$\tilde{T}_L^{s,n+1} = T_L^{s,n} + \left(\frac{\partial T^s}{\partial p}\right)_L^n (p_L^{n+1} - p_L^n) + \left(\frac{\partial T^s}{\partial x_n}\right)_L^n (\tilde{x}_{n,L}^{n+1} - x_{n,L}^n)$$

$$+ \left(\frac{\partial T^s}{\partial U_g} \right)_L^n (\tilde{U}_{g,L}^{n+1} - U_{g,L}^n) \quad (3-76)$$

$$\begin{aligned} \tilde{T}_{g,L}^{n+1} = & T_{g,L}^n + \left(\frac{\partial T_g}{\partial P} \right)_L^n (P_L^{n+1} - P_L^n) + \left(\frac{\partial T_g}{\partial X_n} \right)_L^n (\tilde{X}_{n,L}^{n+1} - X_{n,L}^n) \\ & + \left(\frac{\partial T_g}{\partial U_g} \right)_L^n (\tilde{U}_{g,L}^{n+1} - U_{g,L}^n) \end{aligned} \quad (3-77)$$

$$\tilde{T}_{f,L}^{n+1} = T_{f,L}^n + \left(\frac{\partial T_f}{\partial P} \right)_L^n (P_L^{n+1} - P_L^n) + \left(\frac{\partial T_f}{\partial U_f} \right)_L^n (\tilde{U}_{f,L}^{n+1} - U_{f,L}^n) \quad (3-78)$$

The method of obtaining the temperature derivatives used in Equations (3-76) through (3-78) is also indicated in the State Relationships, Section 3.2.

A similar approach is used to obtain the finite-difference form for the phasic momentum equations. In this case, volume-average properties for the momentum control volume are taken as junction properties (that is, linear interpolations between mass and energy control volume centers). The momentum flux terms are approximated using a donor-like formulation that results in a centered velocity gradient term and a viscous-like term. The difference equations for the sum and difference momentum equations, Equations (3-41) and (3-42), are

$$\begin{aligned} & (\alpha_g \rho_g)_j^n (v_g^{n+1} - v_g^n)_j \Delta x_j + (\alpha_f \rho_f)_j^n (v_f^{n+1} - v_f^n)_j \Delta x_j \\ & + \frac{1}{2} (\dot{\alpha}_g \dot{\rho}_g)_j^n \left[(v_g^2)_L^n - (v_g^2)_K^n \right] \Delta t + \frac{1}{2} (\dot{\alpha}_f \dot{\rho}_f)_j^n \left[(v_f^2)_L^n - (v_f^2)_K^n \right] \Delta t \end{aligned}$$

$$\begin{aligned}
& - \frac{1}{2} \left[(\dot{\alpha}_g \dot{\rho}_g)_j^n \text{VISG}_j^n + (\dot{\alpha}_f \dot{\rho}_f)_j^n \text{VISF}_j^n \right] \Delta t \\
& = - (P_L - P_K)^{n+1} \Delta t + \left[\rho_j^n B_x - (\alpha_g \rho_g)_j^n (v_g)_j^{n+1} \text{FWG}_j^n \right. \\
& \quad \left. - (\alpha_f \rho_f)_j^n (v_f)_j^{n+1} \text{FWF}_j^n - (\Gamma_g)_j^n (v_g - v_f)_j^{n+1} \right] \Delta x_j \Delta t \\
& \quad - [(\dot{\alpha}_g \dot{\rho}_g)_j^n \text{HLOSSG}_j^n v_{g,j}^{n+1} + (\dot{\alpha}_f \dot{\rho}_f)_j^n \text{HLOSSF}_j^n v_{f,j}^{n+1}] \Delta t \\
& \quad - \left(\sum_{n=1}^N \rho_{ni,j}^n - g \Gamma_{n,j}^n \right) v_{g,j}^{n+1} \Delta x_j \Delta t - \Gamma_{s,j}^n v_{f,j}^{n+1} \Delta x_j \Delta t \tag{3-79}
\end{aligned}$$

and

$$\begin{aligned}
& \left[1 + c \rho^2 / (\rho_g \rho_f) \right]_j^n \left[(v_g^{n+1} - v_g^n) - (v_f^{n+1} - v_f^n) \right]_j \Delta x_j \\
& \quad + \frac{1}{2} \left[(\dot{\alpha}_g \dot{\rho}_g) / (\alpha_g \rho_g) \right]_j^n \left[(v_g^2)_L^n - (v_g^2)_K^n \right] \Delta t - \frac{1}{2} \left[(\dot{\alpha}_g \dot{\rho}_g) / (\alpha_g \rho_g) \right]_j^n \text{VISG}_j^n \Delta t \\
& \quad - \frac{1}{2} \left[(\dot{\alpha}_f \dot{\rho}_f) / (\alpha_f \rho_f) \right]_j^n \left[(v_f^2)_L^n - (v_f^2)_K^n \right] \Delta t + \frac{1}{2} \left[(\dot{\alpha}_f \dot{\rho}_f) / (\alpha_f \rho_f) \right]_j^n \text{VISF}_j^n \Delta t \\
& = - [(\rho_f - \rho_g) / (\rho_g \rho_f)]_j^n (P_L - P_K)^{n+1} \Delta t - \left\{ \text{FWG}_j^n (v_g)_j^{n+1} - \text{FWF}_j^n (v_f)_j^{n+1} \right. \\
& \quad \left. - \left[\Gamma_g^n \left(\rho^n v_I^{n+1} - \alpha_f \rho_f^n v_g^{n+1} - \alpha_g \rho_g^n v_f^{n+1} \right) / (\alpha_g \rho_g \alpha_f \rho_f) \right]_j^n \right. \\
& \quad \left. + \left(\sum_{n=1}^N \Gamma_{ni,j}^n - g \Gamma_{h,j}^n \right) v_{g,j}^{n+1} / \alpha_{g,j}^n \rho_{g,j}^n \right. \\
& \quad \left. - \Gamma_{si,j}^n v_{f,j}^{n+1} / \alpha_{f,j}^n \rho_{f,j}^n \right.
\end{aligned}$$

$$\begin{aligned}
& + (pFI)_j^n (v_g - v_f)_{j,j}^{n+1} \left\{ \Delta x_j \Delta t - \left\{ [\dot{\alpha}_g \dot{\rho}_g] / (\alpha_g \rho_g) \right\}_j^n HLOSSG_j^n v_{g,j}^{n+1} \right. \\
& \left. - [\dot{\alpha}_g \dot{\rho}_g] / (\alpha_g \rho_g) \right\}_j^n HLOSSF_j^n v_{f,j}^{n+1} \Delta t
\end{aligned} \quad (3-80)$$

where the viscous terms are defined as

$$\begin{aligned}
VISG_j^n = \frac{1}{2} \left\{ \left| v_{g,L}^n \right| \left[(v_g)_{j+1}^n (A_{j+1}^n / A_j^n) - (v_g)_j^n \right] \right. \\
\left. - \left| v_{g,K}^n \right| \left[(v_g)_j^n - (v_g)_{j-1}^n (A_{j-1}^n / A_j^n) \right] \right\}
\end{aligned} \quad (3-81)$$

and

$$\begin{aligned}
VISF_j^n = \frac{1}{2} \left\{ \left| v_{f,L}^n \right| \left[(v_f)_{j+1}^n (A_{j+1}^n / A_j^n) - (v_f)_j^n \right] \right. \\
\left. - \left| v_{f,K}^n \right| \left[(v_f)_j^n - (v_f)_{j-1}^n (A_{j-1}^n / A_j^n) \right] \right\} .
\end{aligned} \quad (3-82)$$

In Equations (3-79) and (3-80), the scalar or thermodynamic variables needed at the junctions are either linear interpolations between the neighboring cell values or donored quantities. The $HLOSSG_j$ and $HLOSSF_j$ terms contain both code-calculated abrupt area change loss terms and user-specified loss terms. The energy change associated with these terms is not included in the energy dissipation terms ($DISS_g$ and $DISS_f$) at this time due to temperature problems (i.e., overheating).

Using the same averaging techniques, the nonexpanded form of the mass and energy equations [Equations (3-1), (3-2), (3-32), (3-33), (3-47), and (3-49)] are next presented in their final finite difference form.

The nonexpanded vapor density Equation (3-1) becomes

$$(v \alpha_g \rho_g)_L^{n+1} - (v \alpha_g \rho_g)^n + (\dot{\alpha}_{g,j+1} \dot{\rho}_{g,j+1} v_{g,j+1}^{n+1} A_{j+1}^n - \dot{\alpha}_{g,j} \dot{\rho}_{g,j} v_{g,j}^{n+1} A_j^n) \Delta t$$

$$= \tilde{\Gamma}_{g,L}^{n+1} V_L^n \Delta t + \sum_{ni=1}^N \Gamma_{ni,L}^n V_L^n \Delta t - 9 \Gamma_{h,L}^n V_L^n \Delta t \quad (3-83)$$

The intermediate time variable, $\tilde{\Gamma}_{g,L}^{n+1}$, is obtained using the finite difference form of Equation (3-29) and is written

$$\tilde{\Gamma}_{g,L}^{n+1} = - \frac{H_{ig,L}^n (\tilde{T}_L^{S,n+1} - \tilde{T}_{g,L}^{n+1}) + H_{if,L}^n (\tilde{T}_L^{S,n+1} - \tilde{T}_{f,L}^{n+1})}{h_{g,L}^{*,n} - h_{f,L}^{*,n}} + \Gamma_{w,L}^n \quad (3-84)$$

The nonexpanded liquid density Equation (3-2) becomes

$$\begin{aligned} (\alpha_f \rho_f V)_L^{n+1} - (\alpha_f \rho_f V)_L^n + (\dot{\alpha}_{f,j+1}^n \dot{\rho}_{f,j+1}^n v_{f,j+1}^{n+1} A_{j+1}^n \\ - \dot{\alpha}_{f,j}^n \dot{\rho}_{f,j}^n v_{f,j}^{n+1} A_j^n) \Delta t = - \tilde{\Gamma}_{g,L}^{n+1} V_L \Delta t + \Gamma_{Si,L}^n V_L^n \Delta t \quad (3-85) \end{aligned}$$

The nonexpanded total noncondensable density Equation (3-32) becomes

$$\begin{aligned} (\alpha_g \rho_g X_n V)_L^{n+1} - (\alpha_g \rho_g X_n V)_L^n + (\dot{\alpha}_{g,j+1}^n \dot{\rho}_{g,j+1}^n \dot{X}_{n,j+1}^n v_{g,j+1}^{n+1} A_{j+1}^n \\ - \dot{\alpha}_{g,j}^n \dot{\rho}_{g,j}^n \dot{X}_{n,j}^n v_{g,j}^{n+1} A_j^n) \Delta t + \sum_{ni=1}^N \Gamma_{ni,L}^n V_L^n \Delta t \quad (3-86) \end{aligned}$$

The nonexpanded individual noncondensable density Equation (3-33) becomes

$$\begin{aligned} (\alpha_g \rho_g X_n X_{ni} V)_L^{n+1} - (\alpha_g \rho_g X_n X_{ni} V)_L^n + (\dot{\alpha}_{g,j+1}^n \dot{\rho}_{g,j+1}^n \dot{X}_{n,j+1}^n \dot{X}_{ni,j+1}^n \\ v_{g,j+1}^{n+1} A_{j+1}^n - \dot{\alpha}_{g,j}^n \dot{\rho}_{g,j}^n \dot{X}_{n,j}^n \dot{X}_{ni,j}^n v_{gi,j}^{n+1} A_j^n) \Delta t = \Gamma_{ni,L}^n V_L^n \Delta t \quad (3-87) \end{aligned}$$

The nonexpanded vapor energy Equation (3-47) becomes

$$\begin{aligned}
& (\alpha_g \rho_g U_g V)_L^{n+1} - (\alpha_g \rho_g U_g V)_L^n + [\dot{\alpha}_{g,j+1}^n (\dot{\rho}_{g,j+1}^n \dot{U}_{g,j+1}^n + p_L^n) v_{g,j+1}^{n+1} A_{j+1}^n \\
& - \dot{\alpha}_{g,j}^n (\dot{\rho}_{g,j}^n \dot{U}_{g,j}^n + p_L^n) v_{g,j}^{n+1} A_j^n] \Delta t = -v_L^n p_L^n (\tilde{\alpha}_{g,L}^{n+1} - \alpha_{g,L}^n) \\
& + \left\{ - \left(\frac{h_f^*}{h_g^* - h_f^*} \right)_L^n H_{ig,L}^n (\tilde{T}_L^{s,n+1} - \tilde{T}_{g,L}^{n+1}) - \left(\frac{h_g^*}{h_g^* - h_f^*} \right)_L^n H_{if,L}^n (\tilde{T}_L^{s,n+1} - \tilde{T}_{f,L}^{n+1}) \right. \\
& + \left. \left[\left(\frac{1+\epsilon}{2} \right) h_{g,L}^{s,n} + \left(\frac{1-\epsilon}{2} \right) h_{f,L}^{s,n} \right] \Gamma_{w,L}^n + Q_{wg,L}^n + DISS_{g,L}^n \right\} v_L^n \Delta t \\
& + \left(\sum_{n1=1}^N \Gamma_{n1,L}^n h_{n1,L}^n - g \Gamma_{n,L}^n h_{g,L}^n \right) v_L^n \Delta t \quad . \quad (3-88)
\end{aligned}$$

The variables $\tilde{\alpha}_{g,L}^{n+1}$, $\tilde{T}_L^{s,n+1}$, $\tilde{T}_{g,L}^{n+1}$, and $\tilde{T}_{f,L}^{n+1}$ are written with a tilde (~) to indicate they are intermediate time variables. The nonexpanded liquid energy Equation (3-49) becomes

$$\begin{aligned}
& (\alpha_f \rho_f U_f V)_L^{n+1} - (\alpha_f \rho_f U_f V)_L^n + [\dot{\alpha}_{f,j+1}^n (\dot{\rho}_{f,j+1}^n \dot{U}_{f,j+1}^n + p_L^n) v_{f,j+1}^{n+1} A_{j+1}^n \\
& - \dot{\alpha}_{f,j}^n (\dot{\rho}_{f,j}^n \dot{U}_{f,j}^n + p_L^n) v_{f,j}^{n+1} A_j^n] \Delta t = v_L^n p_L^n (\tilde{\alpha}_{g,L}^{n+1} - \alpha_{g,L}^n) \\
& + \left\{ \left(\frac{h_f^*}{h_g^* - h_f^*} \right)_L^n H_{ig,L}^n (\tilde{T}_L^{s,n+1} - \tilde{T}_{g,L}^{n+1}) + \left(\frac{h_g^*}{h_g^* - h_f^*} \right)_L^n H_{if,L}^n (\tilde{T}_L^{s,n+1} - \tilde{T}_{f,L}^{n+1}) \right. \\
& - \left. \left[\left(\frac{1+\epsilon}{2} \right) h_{g,L}^{s,n} + \left(\frac{1-\epsilon}{2} \right) h_{f,L}^{s,n} \right] \Gamma_{w,L}^n + Q_{wf,L}^n + DISS_{f,L}^n \right\} v_L^n \Delta t
\end{aligned}$$

$$+ i_{Si,L}^n h_{Si,L}^n v_L^n \Delta t \quad (3-89)$$

3.1.5 Volume-Average Velocities

Volume-average velocities are required for the momentum flux calculation, evaluation of the frictional forces, and the Courant time step limit. In a simple constant area passage, the arithmetic average between the inlet and outlet is a satisfactory approximation. However, at branch volumes with multiple inlets and/or outlets or for volumes with abrupt area change, use of the arithmetic average results in nonphysical behavior.

The volume-average velocity formulas have the form

$$\begin{aligned} (v_f)_L^n = & \frac{\left\{ \sum_j (\dot{\alpha}_f \dot{\rho}_f v_f)_j^n A_j^n \cdot \sum_j A_j^n \right\}_{\text{inlets}}}{\left\{ \sum_j (\dot{\alpha}_f \dot{\rho}_f)_j^n A_j^n \cdot A_L^n \right\}_{\text{inlets and outlets}}} \\ & + \frac{\left\{ \sum_j (\dot{\alpha}_f \dot{\rho}_f v_f)_j^n A_j^n \cdot \sum_j A_j^n \right\}_{\text{outlets}}}{\left\{ \sum_j (\dot{\alpha}_f \dot{\rho}_f)_j^n A_j^n \cdot A_L^n \right\}_{\text{inlets and outlets}}} \end{aligned} \quad (3-90)$$

and

$$\begin{aligned} (v_g)_L^n = & \frac{\left\{ \sum_j (\dot{\alpha}_g \dot{\rho}_g v_g)_j^n A_j^n \cdot \sum_j A_j^n \right\}_{\text{inlets}}}{\left\{ \sum_j (\dot{\alpha}_g \dot{\rho}_g)_j^n A_j^n \cdot A_L^n \right\}_{\text{inlets and outlets}}} \\ & + \frac{\left\{ \sum_j (\dot{\alpha}_g \dot{\rho}_g v_g)_j^n A_j^n \cdot \sum_j A_j^n \right\}_{\text{outlets}}}{\left\{ \sum_j (\dot{\alpha}_g \dot{\rho}_g)_j^n A_j^n \cdot A_L^n \right\}_{\text{inlets and outlets}}} \end{aligned} \quad (3-91)$$

3.1.6 Semi-Implicit Scheme Time Advancement

The solution scheme will be discussed with regard to the state of the fluid in a control volume for two successive time steps. There are four possible transition cases. They are:

1. Two-phase to two-phase, where two-phase conditions exist at both old time (n) and new time (n+1).
2. One-phase to one-phase, where one-phase conditions (either pure gas or pure liquid) exist at both old time (n) and new time (n+1).
3. Two-phase to one-phase (disappearance), where two-phase conditions exist at old time (n) and one-phase conditions exist at new time (n+1).
4. One-phase to two-phase (appearance), where one-phase conditions exist at old time (n) and two-phase conditions exist at new time (n+1).

The solution scheme will first be presented for the two-phase to two-phase case, because it is the most general. Then, the solution scheme for the other three cases will be presented.

3.1.6.1 Two-Phase To Two-Phase. First, the state and temperature Equations (3-72), (3-73), (3-76), (3-77) and (3-78) are substituted into the five expanded density and energy difference Equations (3-61) through (3-69). The equations then are ordered so that the noncondensable density equation is first, the vapor energy equation is second, the liquid energy equation is third, the difference density equation is fourth, and the sum density equation is fifth. The five density and energy variables are expressed as differences, and the order is

$$(\tilde{x}_{n,L}^{n+1} - x_{n,L}^n) , (\tilde{U}_{g,L}^{n+1} - U_{g,L}^n) , (\tilde{U}_{f,L}^{n+1} - U_{f,L}^n) , (\tilde{\alpha}_{g,L}^{n+1} - \alpha_{g,L}^n) ,$$

and

$$(p_L^{n+1} - p_L^n) \quad .$$

The tilde ($\sim$) is used for X_n , U_g , U_f , and α_g to indicate that these are intermediate new time variables and do not represent the final new time variables for the two-phase to two-phase case. The ordering of the variables and equations was selected so that a given equation is dominated by its corresponding variable (e.g., the vapor energy equation is second and the vapor energy variable U_g is also second). The noncondensable equation is placed first for ease of degeneration when a noncondensable component is not specified in the problem, and the pressure variable is placed last for numerical convenience in the pressure solution. The system of equations has the following form, where 0 indicates a zero entry in the matrix A and the vectors

$$\underline{b}, \underline{g}^1, \underline{g}^2, \underline{f}^1, \underline{f}^2$$

contain only old-time level variables:

$$\underline{\tilde{A}} \underline{\tilde{x}} = \underline{\tilde{b}} + \underline{\tilde{g}}^1 v_{g,j+1}^{n+1} + \underline{\tilde{g}}^2 v_{g,j}^{n+1} + \underline{\tilde{f}}^1 v_{f,j+1}^{n+1} + \underline{\tilde{f}}^2 v_{f,j}^{n+1} \quad (3-92)$$

where

$$\underline{\tilde{A}} = \begin{bmatrix} A_{11} & A_{12} & 0 & A_{14} & A_{15} \\ A_{21} & A_{22} & A_{23} & A_{24} & A_{25} \\ A_{31} & A_{32} & A_{33} & A_{34} & A_{35} \\ A_{41} & A_{42} & A_{43} & A_{44} & A_{45} \\ A_{51} & A_{52} & A_{53} & A_{54} & A_{55} \end{bmatrix} \quad \underline{\tilde{x}} = \begin{bmatrix} \tilde{x}_{n,L}^{n+1} - x_{n,L}^n \\ \tilde{U}_{g,L}^{n+1} - U_{g,L}^n \\ \tilde{U}_{f,L}^{n+1} - U_{f,L}^n \\ \tilde{\alpha}_{g,L}^{n+1} - \alpha_{g,L}^n \\ p_L^{n+1} - p_L^n \end{bmatrix}$$

$$\underset{\sim}{b} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \end{bmatrix} \quad \underset{\sim}{g}^1 = \begin{bmatrix} g_1^1 \\ g_2^1 \\ 0 \\ g_4^1 \\ g_5^1 \end{bmatrix} \quad \underset{\sim}{g}^2 = \begin{bmatrix} g_1^2 \\ g_2^2 \\ 0 \\ g_4^2 \\ g_5^2 \end{bmatrix} \quad \underset{\sim}{f}^1 = \begin{bmatrix} 0 \\ 0 \\ f_3^1 \\ f_4^1 \\ f_5^1 \end{bmatrix} \quad \underset{\sim}{f}^2 = \begin{bmatrix} 0 \\ 0 \\ f_3^2 \\ f_4^2 \\ f_5^2 \end{bmatrix}$$

A Gaussian elimination system solver³⁻¹⁴ is used to obtain the bottom row of A^{-1} . Multiplying Equation (3-54) by A^{-1} , one can verify that just the bottom row of A^{-1} is needed to obtain an equation that involves only the unknown variables $(p_L^{n+1} - p_L^n)$, $v_{g,j+1}^{n+1}$, $v_{g,j}^{n+1}$, $v_{f,j+1}^{n+1}$, and $v_{f,j}^{n+1}$. Substituting the velocity equations [solving Equations (3-79) and (3-80) for $v_{f,j}^{n+1}$ and $v_{g,j}^{n+1}$] into this equation results in a single equation involving only pressures. This is done for each volume, giving rise to an $N \times N$ system of linear equations for the new time pressure. Next, a sparse matrix solver³⁻¹¹ is used to obtain $(p_L^{n+1} - p_L^n)$ for each volume. Then, the pressure differences $(p_L^{n+1} - p_L^n)$ are substituted into the velocity Equations (3-79) and (3-80) to obtain the new time velocities.

Now, the new time velocities are substituted back into Equation (3-46) to obtain a single vector on the right side. The Gaussian elimination system solver^{a,3-14} is called again to obtain the intermediate time

variables $\tilde{x}_{n,L}^{n+1}$, $\tilde{u}_{g,L}^{n+1}$, $\tilde{u}_{f,L}^{n+1}$, and $\tilde{\alpha}_{g,L}^{n+1}$.

A mixture density, $\rho_{m,L}^{n+1}$, is then calculated from a numerically mass-preserving mixture density equation and compared with the mixture

a. Private communication, E. S. Marwill and J. A. Trapp, EG&G Idaho, Inc., January 1983.

density, ρ_L^{n+1} , which is calculated from the state relations. The difference between these two mixture densities is used to provide a time step control based on mass error. The quantity $\rho_{m,L}^{n+1}$ is calculated as follows: Adding the phasic density Equations (3-1) and (3-2) and letting $\rho_m = \alpha_g \rho_g + \alpha_f \rho_f$ gives the differential equation

$$\frac{1}{V} \frac{\partial(\rho_m V)}{\partial t} + \frac{1}{A} \frac{\partial}{\partial x}(\alpha_g \rho_g v_g A + \alpha_f \rho_f v_f A) = \left(\sum_{n1=1}^N \Gamma_{n1} - 9\Gamma_h + \Gamma_{s1} \right) . \quad (3-93)$$

The numerically mass-preserving finite difference equation corresponding to Equation (3-96) is

$$\begin{aligned} V_L^n [\rho_{m,L}^{n+1} - \rho_L^n] + \rho_L^n (V_L^{n+1} - V_L^n) + (\dot{\alpha}_{g,j+1}^n \dot{\rho}_{g,j+1}^n v_{g,j+1}^{n+1} A_{j+1}^n \\ - \dot{\alpha}_{g,j}^n \dot{\rho}_{g,j}^n v_{g,j}^{n+1} A_j^n) \Delta t + (\dot{\alpha}_{f,j+1}^n \dot{\rho}_{f,j+1}^n v_{f,j+1}^{n+1} A_{j+1}^n \\ - \dot{\alpha}_{f,j}^n \dot{\rho}_{f,j}^n v_{f,j}^{n+1} A_j^n) \Delta t = \left(\sum_{n1=1}^N \Gamma_{n1,L} - 9\Gamma_{h,L}^n + \Gamma_{s1,L}^n \right) V_L^n \end{aligned} \quad (3-94)$$

from which $\rho_{m,L}^{n+1}$ is obtained. Next, $\tilde{\Gamma}_{g,L}^{n+1}$ is calculated using Equation (3-84), where $\tilde{T}_L^{s,n+1}$, $\tilde{T}_{g,L}^{n+1}$ and $\tilde{T}_{f,L}^{n+1}$ are obtained from Equations (3-76) through (3-78) using the newly calculated variables p_L^{n+1} , $\tilde{U}_{g,L}^{n+1}$, $\tilde{U}_{f,L}^{n+1}$, and $\tilde{x}_{n,L}^{n+1}$.

To obtain the new time variables $x_{n,L}^{n+1}$, $U_{g,L}^{n+1}$, $U_{f,L}^{n+1}$, and $\alpha_{g,L}^{n+1}$

the nonexpanded difference equations, Equations (3-83), (3-85), (3-86), (3-88), and (3-89) are used. Using the phasic convective terms along with

$\tilde{\Gamma}_{g,L}^{n+1}$ from Equation (3-84), the nonexpanded phasic density Equations (3-83) and (3-47) are used to obtain $(\alpha_g \rho_g V)_L^{n+1}$ and $(\alpha_f \rho_f V)_L^{n+1}$.

Next, the nonexpanded noncondensable density Equation (3-86) is used to calculate $(\alpha_g \rho_g X_n V)_L^{n+1}$, which is then divided by $(\alpha_g \rho_g V)_L^{n+1}$ to obtain $X_{n,L}^{n+1}$, and each nonexpanded noncondensable density. Equation (3-87) is used to calculate $(\alpha_g \rho_g X_n X_{ni} V)_L^{n+1}$, which is then divided by $(\alpha_g \rho_g X_n V)_L^{n+1}$ to obtain $X_{ni,L}^{n+1}$.

Following this, the nonexpanded vapor energy Equation (3-88) is used with the old time vapor energy source and convective terms as well as the intermediate time variables for T^S , T_g , and T_f to obtain $(\alpha_g \rho_g U_g V)_L^{n+1}$, which is divided by $(\alpha_g \rho_g V)_L^{n+1}$ to give $U_{g,L}^{n+1}$.

Analogously, the nonexpanded liquid energy Equation (3-89) is used to obtain $(\alpha_f \rho_f U_f V)_L^{n+1}$, which is divided by $(\alpha_f \rho_f V)_L^{n+1}$ to give $U_{f,L}^{n+1}$.

Finally, $\alpha_{g,L}^{n+1}$ is calculated from $(\alpha_f \rho_f)_L^{n+1}$ using the equation

$$\alpha_{g,L}^{n+1} = 1 - \alpha_{f,L}^{n+1} = 1 - \frac{(\alpha_f \rho_f V)_L^{n+1}}{\rho_f^{n+1} V^{n+1}} \quad (3-95)$$

where ρ_f^{n+1} is obtained using the linearized state Equation (3-73) and the new time variables P_L^{n+1} and $U_{f,L}^{n+1}$.

3.1.6.2 One-Phase to One-Phase. For this case, the pressure calculation remains the same as in the two-phase to two-phase case. For the densities and energies, however, the nonexpanded equations are not used and the intermediate time variables obtained from the expanded equations are taken to be the new time variables. For the phase that is not present, a large interfacial heat transfer coefficient (10^7) is used, resulting in the internal energy of that phase being very close to saturation conditions. Slight numerical variations from saturation occur due to linearization; and the phasic energy, temperature, and density of the missing phase are reset to the saturation values in the state subroutine. This ensures agreement with saturation conditions. For the phase that is present, a value of 0.0 for the interfacial heat transfer coefficient is used, since there is no mass transfer occurring.

3.1.6.3 Two-Phase to One-Phase (Disappearance). For this case, the calculation is carried out in the same way as in the two-phase to two-phase case, where expanded calculations followed by nonexpanded calculations are used. Then, for the phase that disappears, the phasic energy, temperature, and density are reset to saturation values in the state subroutine, as is done with the one-phase to one-phase case.

3.1.6.4 One-Phase to Two-Phase (Appearance). Here, the calculation proceeds in the same way as in the one-phase to one-phase case. A large interfacial heat transfer coefficient (10^7) is used for the appearing phase, resulting in the energy and temperature of that phase being very close to saturation. Because the phase that is appearing is assumed to appear at saturation conditions, an error can be made if, in reality, the phase appeared by convection from a neighboring volume that was at a temperature different from saturation. The magnitude of the potential error is controlled by letting the phase appear at saturation but restricting the amount that can appear by time step control (corresponds to a typical thermal boundary layer thickness). If more than the limiting amount appears, an error is assumed to have occurred; and the time step is reduced and repeated. This approach is modified when a noncondensable component is present. For the case when vapor appears with noncondensable present, the old time saturation temperature ($T_L^{S,n}$) is set to the old time liquid temperature ($T_{f,L}^n$) if it is smaller. This is then used to recalculate the old time vapor energy ($U_{g,L}^n$).

3.1.7 Nearly Implicit Scheme Difference Equations and Time Advancement

For problems where the flow is expected to change very slowly with time, it is possible to obtain adequate information from an approximate solution based on very large time steps. This would be advantageous if a reliable and efficient means could be found for solving difference equations treating all terms--phase exchanges, pressure propagation, and convection--by implicit differences. Unfortunately, the state of the art is less satisfactory here than in the case of semi-implicit (convection-explicit) schemes. A fully implicit scheme for the

six-equation model of a 100-cell problem would require the solution of 600 coupled algebraic equations. If these equations were linearized for a straight pipe, inversion of a block tri-diagonal, 600 x 600 matrix with 6 x 6 blocks would be required. This would yield a matrix of bandwidth 23 containing ~13,800 nonzero elements, resulting in an extremely costly time advancement scheme.

To reduce the number of calculations required for solving fully implicit difference schemes, fractional step (sometimes called multiple step) methods have been tried. The equations can be split into fractional steps based upon physical phenomena. This is the basic idea in the nearly implicit scheme. Fractional step methods for two-phase flow problems have been developed in References 3-15 and 3-16. These earlier efforts have been used to guide the development of the nearly implicit scheme. The fractional step method described here³⁻¹⁷ differs significantly from prior efforts in the reduced number of steps used to evaluate the momentum equations.

The nearly implicit scheme consists of a first step that solves all seven conservation equations, treating all interphase exchange processes, the pressure propagation process, and the momentum convection process implicitly. These finite difference equations are exactly the expanded ones [Equations (3-65) through (3-69), (3-79), and (3-80)] solved in the semi-implicit scheme with one major change. The convective terms in the momentum Equations (3-79) and (3-80) are evaluated implicitly (in a linearized form) instead of in an explicit donored fashion as is done in the semi-implicit scheme.

The linearized implicit technique used for the convective terms can be seen by examining the convective terms in the vapor part of the sum momentum Equation (3-63). An analogous result occurs for the liquid part as well as for the difference momentum Equation (3-64). The convective term is

$$\frac{1}{2} \alpha_g \rho_g (v_g^2)_{x_K}^L \quad (3-96)$$

In the nearly implicit formulation, the VISF and VISG terms that result from the donor cell formulation are not used. Evaluating the velocities at new time gives the finite difference form as

$$\frac{1}{2} (\dot{\alpha}_g \dot{\rho}_g)_j^n \left[(v_{g,L}^{n+1})^2 - (v_{g,K}^{n+1})^2 \right] \quad (3-97)$$

This term can be rewritten as

$$\begin{aligned} \frac{1}{2} (\dot{\alpha}_g \dot{\rho}_g)_j^n & \left[(v_{g,L}^{n+1} - v_{g,L}^n)^2 + 2v_{g,L}^n (v_{g,L}^{n+1} - v_{g,L}^n) + (v_{g,L}^n)^2 \right. \\ & \left. - (v_{g,K}^{n+1} - v_{g,K}^n)^2 - 2v_{g,K}^n (v_{g,K}^{n+1} - v_{g,K}^n) - (v_{g,K}^n)^2 \right] \quad (3-98) \end{aligned}$$

Assuming that the leading quadratic term for L and K is small compared to the others results in the following form

$$\frac{1}{2} (\dot{\alpha}_g \dot{\rho}_g)_j^n \left[2v_{g,L}^n (v_{g,L}^{n+1} - v_{g,L}^n) + (v_{g,L}^n)^2 - 2v_{g,K}^n (v_{g,K}^{n+1} - v_{g,K}^n) - (v_{g,K}^n)^2 \right] \quad (3-99)$$

Using this linearized implicit form, the explicit convective and viscous terms in the sum momentum finite difference Equation (3-79) are replaced by

$$\begin{aligned} \frac{1}{2} (\dot{\alpha}_g \dot{\rho}_g)_j^n & \left[2v_{g,L}^n (v_{g,L}^{n+1} - v_{g,L}^n) + (v_{g,L}^n)^2 - 2v_{g,K}^n (v_{g,K}^{n+1} - v_{g,K}^n) - (v_{g,K}^n)^2 \right] \Delta t \\ & + \frac{1}{2} (\dot{\alpha}_f \dot{\rho}_f)_j^n \left[2v_{f,L}^n (v_{f,L}^{n+1} - v_{f,L}^n) + (v_{f,L}^n)^2 \right] \end{aligned}$$

$$- 2v_{f,K}^n (v_{f,K}^{n+1} - v_{f,K}^n) - (v_{f,K}^n)^2 \Delta t \quad . \quad (3-100)$$

Similarly, for the difference momentum finite difference Equation (3-80), the convective terms become

$$\begin{aligned} & \frac{1}{2} \left[(\dot{\alpha}_g \dot{\rho}_g) / (\alpha_g \rho_g) \right]_j^n \left[2v_{g,L}^n (v_{g,L}^{n+1} - v_{g,L}^n) + (v_{g,L}^n)^2 \right. \\ & \quad \left. - 2v_{g,K}^n (v_{g,K}^{n+1} - v_{g,K}^n) - (v_{g,K}^n)^2 \right] \Delta t \\ & - \frac{1}{2} \left[(\dot{\alpha}_f \dot{\rho}_f) / (\alpha_f \rho_f) \right]_j^n \left[2v_{f,L}^n (v_{f,L}^{n+1} - v_{f,L}^n) + (v_{f,L}^n)^2 \right. \\ & \quad \left. - 2v_{f,K}^n (v_{f,K}^{n+1} - v_{f,K}^n) - (v_{f,K}^n)^2 \right] \Delta t \quad . \quad (3-101) \end{aligned}$$

The new time volume-averaged velocities ($v_{f,L}^{n+1}$ and $v_{g,L}^{n+1}$) in Equations (3-100) and (3-101) use the same equations as the old time volume-averaged velocities [Equations (3-90) and (3-91)], except that the junction velocities are at new time. Thus, the new time volume-averaged velocities have the form

$$v_{f,L}^{n+1} = \left(\sum_j c_{f,j}^n v_{f,j}^{n+1} \right)_{\text{inlets}} + \left(\sum_j c_{f,j}^n v_{f,j}^{n+1} \right)_{\text{outlets}} \quad (3-102)$$

and

$$v_{g,L}^{n+1} = \left(\sum_j c_{g,j}^n v_{g,j}^{n+1} \right)_{\text{inlets}} + \left(\sum_j c_{g,j}^n v_{g,j}^{n+1} \right)_{\text{outlets}} \quad (3-103)$$

where $c_{f,j}^n$ and $c_{g,j}^n$ contain all old time quantities.

Although this additional implicitness involves only the momentum convective terms, it has a large impact on the algebraic solution algorithm in the first step. In the semi-implicit scheme, Equations (3-65) through (3-69) are solved locally to give a single equation of the form

$$p_L^{n+1} = A v_{g,j+1}^{n+1} + B v_{g,j}^{n+1} + C v_{f,j+1}^{n+1} + D v_{f,j}^{n+1} + E \quad (3-104)$$

for pressure, where A, B, C, D, and E contain old time variables only (see Figure 3-2 for cell indexes).

In the semi-implicit scheme, the momentum equations are also solved locally to obtain

$$v_{g,j}^{n+1} = A^1 \left(p_L^{n+1} - p_K^{n+1} \right) + C^1 \quad (3-105)$$

$$v_{f,j}^{n+1} = B^1 \left(p_L^{n+1} - p_K^{n+1} \right) + D^1 \quad (3-106)$$

where A^1 , B^1 , C^1 , and D^1 again contain only n time level variables. If the momentum Equations (3-105) and (3-106) are used to eliminate the $n+1$ level velocities from Equation (3-104), we get the normal pressure equation used in the semi-implicit scheme to obtain all the $n+1$ pressures. For a 100-cell straight pipe problem, this results in a 100 x 100 tri-diagonal matrix system to solve for all the p^{n+1} .

In the nearly implicit scheme, because the momentum flux terms are implicit, the momentum Equations (3-79) and (3-80) [using the convective terms from Equations (3-100) and (3-101)] cannot be locally solved to get Equations (3-105) and (3-106). The new time convective terms bring in $n+1$ level upstream and downstream velocities. Equations (3-65) through (3-69) are still used to obtain Equation (3-104). In the nearly implicit scheme, Equation (3-104) is used to eliminate the $n+1$ level

pressure terms from Equations (3-79) and (3-80), [using the convective terms from Equations (3-100) and (3-101)], and a coupled pair of momentum equations involving only $n+1$ level velocities is obtained. Because of the $n+1$ level flux terms, this is a globally coupled system. For a straight pipe of 100 junctions, a block tri-diagonal 200×200 matrix system with 2×2 blocks is obtained. This system of equations is solved using a sparse matrix solution algorithm.³⁻¹¹ Once the v_f^{n+1} and v_g^{n+1} solution is obtained, p^{n+1} is obtained by back substitution into Equation (3-104). Using Equations (3-65) through (3-69), intermediate/provisional $n+1$ values for α_g , U_g , U_f , and X_n , denoted by $\tilde{\alpha}_g^{n+1}$, $\tilde{U}_g^{n+1}$, $\tilde{U}_f^{n+1}$, and $\tilde{X}_n^{n+1}$, can also be obtained.

The second step in the nearly implicit scheme is used to stabilize the convective terms in the mass and energy balance equations. This step uses the final $n+1$ level velocities from the first step along with the interphase exchange terms resulting from the first step, i.e., the interphase heat and mass exchanges for step two are calculated using p^{n+1} , $\tilde{U}_g^{n+1}$, $\tilde{U}_f^{n+1}$, $\tilde{X}_n^{n+1}$ from step one. The phasic continuity and energy equations in this second step have the fluxed variables evaluated at the $n+1$ time level, i.e., implicitly as compared to their explicit evaluation in the first step.

The vapor density equation is

$$V_L [(\alpha_g \rho_g)_L^{n+1} - (\alpha_g \rho_g)_L^n] + [(\dot{\alpha} \rho)_{g,j+1}^{n+1} v_{g,j+1}^{n+1} A_{j+1} - (\dot{\alpha} \rho)_{g,j}^{n+1} v_{g,j}^{n+1} A_j] \Delta t \\ = \tilde{r}_{g,L}^{n+1} V_L \Delta t \quad (3-107)$$

The liquid density equation is

$$V_L [(\alpha_f \rho_f)_L^{n+1} - (\alpha_f \rho_f)_L^n] + [(\dot{\alpha} \rho)_{f,j+1}^{n+1} v_{f,j+1}^{n+1} A_{j+1} - (\dot{\alpha} \rho)_{f,j}^{n+1} v_{f,j}^{n+1} A_j] \Delta t$$

$$= -\tilde{\Gamma}_{g,L}^{n+1} v_L \Delta t \quad (3-108)$$

In Equations (3-107) and (3-108), the mass exchange $\tilde{\Gamma}_g^{n+1}$ is evaluated using the provisional values from the first step and is written

$$\tilde{\Gamma}_{g,L}^{n+1} = - \frac{H_{ig,L}^n (\tilde{T}_L^{s,n+1} - \tilde{T}_{g,L}^{n+1}) + H_{if,L}^n (\tilde{T}_L^{s,n+1} - \tilde{T}_{f,L}^{n+1})}{h_{g,L}^{*,n} - h_{f,L}^{*,n}} + \Gamma_{w,L}^n \quad (3-109)$$

where the provisional temperatures from the linearized state relationship are known as functions of U_g^{n+1} , U_f^{n+1} , X_n^{n+1} , and P^{n+1} .

The total noncondensable density equation is

$$v_L \left[(\alpha_g \rho_g X_n)_L^{n+1} - (\alpha_g \rho_g X_n)_L^n \right] + \left[(\alpha_g \rho_g X_n)_{j+1}^{n+1} v_{g,j+1}^{n+1} A_{j+1} - (\alpha_g \rho_g X_n)_j^{n+1} v_{g,j}^{n+1} A_j \right] \Delta t = 0 \quad (3-110)$$

The vapor energy equation is given by

$$\begin{aligned} & v_L \left[(\alpha_g \rho_g U_g)_L^{n+1} - (\alpha_g \rho_g U_g)_L^n \right] + \left[(\alpha \dot{\rho} U)_{g,j+1}^{n+1} v_{g,j+1}^{n+1} A_{j+1} - (\alpha \dot{\rho} U)_{g,j}^{n+1} v_{g,j}^{n+1} A_j \right] \Delta t \\ &= - v_L P_L^n (\tilde{\alpha}_{g,L}^{n+1} - \alpha_{g,L}^n) - P_L^n \left(\dot{\alpha}_{g,j+1}^n v_{g,j+1}^{n+1} A_{j+1} - \dot{\alpha}_{g,j}^n v_{g,j}^{n+1} A_j \right) \Delta t \\ &+ \left\{ - \left(\frac{h_f^*}{h_g^* - h_f^*} \right)_L^n H_{ig,L}^n (\tilde{T}_L^{s,n+1} - \tilde{T}_{g,L}^{n+1}) - \left(\frac{h_g^*}{h_g^* - h_f^*} \right) H_{if,L}^n (\tilde{T}_L^{s,n+1} - \tilde{T}_{f,L}^{n+1}) \right. \\ &\left. + \left[\left(\frac{1+\epsilon}{2} \right) h_{g,L}^{s,n} + \left(\frac{1-\epsilon}{2} \right) h_{f,L}^{s,n} \right] \Gamma_{w,L}^n + Q_{wg,L}^n + \text{DISS}_{g,L}^n \right\} v_L \Delta t \quad (3-111) \end{aligned}$$

The liquid energy equation is given by

$$\begin{aligned}
 & V_L \left[(\alpha_f \rho_f U_f)_L^{n+1} - (\alpha_f \rho_f U_f)_L^n \right] + \left[(\alpha \dot{\rho} U)_{f,j+1}^{n+1} v_{f,j+1}^{n+1} A_{j+1} - (\alpha \dot{\rho} U)_{f,j}^{n+1} v_{f,j}^{n+1} A_j \right] \Delta t \\
 & = V_L P_L^n \left(\tilde{\alpha}_{g,j}^{n+1} - \alpha_{g,L}^n \right) - P_L^n \left(\dot{\alpha}_{f,j+1}^n v_{f,j+1}^{n+1} A_{j+1} - \dot{\alpha}_{f,j}^n v_{f,j}^{n+1} A_j \right) \Delta t \\
 & + \left\{ \left(\frac{h_f^*}{h_g^* - h_f^*} \right)_L^n H_{ig,L}^n \left(\tilde{T}_L^{s,n+1} - \tilde{T}_{g,L}^{n+1} \right) + \left(\frac{h_g^*}{h_g^* - h_f^*} \right)_L^n H_{if,L}^n \left(\tilde{T}_L^{s,n+1} - \tilde{T}_{f,L}^{n+1} \right) \right. \\
 & \left. - \left[\left(\frac{1+\epsilon}{2} \right) h_{g,L}^{s,n} + \left(\frac{1-\epsilon}{2} \right) h_{f,L}^{s,n} \right] \Gamma_{w,L}^n + Q_{wf,L}^n + DISS_{f,L}^n \right\} V_L \Delta t \quad (3-112)
 \end{aligned}$$

This second step uses the mass and energy balance equations only. If the structure of Equations (3-107) through (3-112) is examined, it is seen that each equation only involves one unknown variable:

Equation (3-107) - $(\alpha \rho)_g^{n+1}$; Equation (3-162) - $(\alpha \rho)_f^{n+1}$;
 Equation (3-164) - $(\alpha_g \rho_g X_g)_g^{n+1}$; Equation (3-165) - $(\alpha \rho U)_g^{n+1}$; and
 Equation (3-166) - $(\alpha \rho U)_f^{n+1}$.

This is because the new time velocities, v_g^{n+1} , v_f^{n+1} , are known from step one, and provisional $n+1$ values from step one are used in the exchange terms. Hence, each equation is uncoupled from the others and can be solved independently. In addition, the three equations involving the gas phase, Equations (3-107), (3-110), and (3-111), have the same structural form for the convective terms, i.e., each equation convects with velocity v_g^{n+1} . Equation (3-107) is inverted once, and then this inverse may be used with different right sides to solve Equations (3-110) and (3-111). Hence, for a straight pipe problem of 100 cells, only one 100 x 100 tri-diagonal system is inverted to obtain $(\alpha \rho)_g^{n+1}$, $(\alpha_g \rho_g X_g)_g^{n+1}$, and $(\alpha \rho U)_g^{n+1}$. In like manner, the liquid phase Equations (3-108) and (3-112) have the same structure and require only one inversion to be carried out to solve both equation sets, giving $(\alpha \rho)_f^{n+1}$ and $(\alpha \rho U)_f^{n+1}$.

With the above five new time variables known, we obtain x_n^{n+1} , U_g^{n+1} , and U_f^{n+1} from

$$x_n^{n+1} = (\alpha_g \rho_g x_n)^{n+1} / (\alpha \rho)_g^{n+1} \quad (3-113)$$

$$U_g^{n+1} = (\alpha \rho U)_g^{n+1} / (\alpha \rho)_g^{n+1} \quad (3-114)$$

$$U_f^{n+1} = (\alpha \rho U)_f^{n+1} / (\alpha \rho)_f^{n+1} \quad (3-115)$$

The void fraction, α_g^{n+1} , is obtained from

$$\alpha_g^{n+1} = \frac{\rho_m^{n+1} - \rho_f^{n+1}}{\rho_g^{n+1} - \rho_f^{n+1}} = \frac{(\alpha \rho)_g^{n+1} + (\alpha \rho)_f^{n+1} - \rho_f^{n+1}}{\rho_g^{n+1} - \rho_f^{n+1}} \quad (3-116)$$

where ρ_m^{n+1} is the mixture density, ρ_f^{n+1} is the liquid density calculated from the linearized state relationship [Equation(3-73)] using U_f^{n+1} and p^{n+1} , and ρ_g^{n+1} is the vapor density calculated from the linearized state relationship [Equation(3-72)] using U_g^{n+1} and p^{n+1} .

Up to this point of this section on the nearly implicit scheme, the difference equations have been recorded along with the time advancement for the case of two-phase to two-phase only. As indicated in the Semi-Implicit Scheme Time Advancement Section 3.1.6, there are three other possible transaction cases (one-phase to one-phase, two-phase to one-phase, and one-phase to two-phase). These three cases will now be presented for the nearly implicit scheme.

For the one-phase to one-phase case, both the first step and the second step are carried out as in the two-phase to two-phase case. For the phase that is not present, α is zero, and thus $(\alpha \rho)^{n+1}$ equals zero for that phase. The provisional $n+1$ value of the corresponding variable is

used in order to avoid the zero divide in Equations (3-113) through (3-115). For the phase that is not present, a large interfacial heat transfer coefficient (10^7) is used; and for the phase that is present, a value of 0.0 is used for the interfacial heat transfer coefficient. The first step quantities are used for the appearing phase. As with the semi-implicit time advancement, phasic energy, temperature, and density of the missing phase are reset to the saturation values in the state subroutine.

For the two-phase to one-phase case (disappearance), the calculation is carried out the same as in the two-phase to two-phase case. Then, for the phase that is missing, the phasic energy, temperature, and density of the missing phase are reset to saturation values in the state subroutine as is done with the one-phase to one-phase case. This is the same approach used in the semi-implicit scheme time advancement.

For the one-phase to two-phase case (appearance), the first step quantities are used for the appearing phase. A large interfacial heat transfer coefficient (10^7) is used for the appearing phase, resulting in the energy and temperature of that phase being very close to saturation. Because the phase that is appearing is assumed to appear at saturation conditions, an error can be made if, in reality, the phase appeared by convection from a neighboring volume that was at a temperature different from saturation. The magnitude of the potential error is controlled by letting the phase appear at saturation but restricting the amount that can appear by time step control (corresponds to a typical thermal boundary layer thickness). If more than the limiting amount appears, an error is assumed to have occurred; and the time step is reduced and repeated. This is the same approach used in the semi-implicit scheme time advancement.

In summary, the second step stabilizes the convective terms in the mass and energy equations, and it does so with very little computational effort due to the fractional step nature of the scheme. If the nearly implicit method is compared with the fully implicit method for a straight pipe problem of 100 cells, we have the following efficiency estimates. The

fully implicit method requires the inversion of a banded block tri-diagonal 600×600 matrix of bandwidth 23 containing 13,800 nonzero elements. The nearly implicit method requires the inversion of one block tri-diagonal 200×200 matrix with 2×2 blocks and bandwidth 7 containing 1,400 nonzero elements plus two 100×100 tri-diagonal matrices with 300 nonzero elements. The nearly implicit method thus requires about 1/10 the number of storage locations required by the fully implicit method. If the computational efficiency is estimated by counting the number of multiplications in the forward part of a Gaussian elimination algorithm, then the fully implicit method for this problem requires about 450,000 multiplications, whereas the nearly implicit method requires about 2,000 multiplications. Thus, the nearly implicit method requires about 1/200 of the computational time needed for a fully implicit scheme.

3.2 State Relationships

The six-equation model with an additional equation for the noncondensable gas component has five independent state variables. The independent variables are chosen to be P , α_g , U_g , U_f , and X_n . All the remaining thermodynamic variables (temperatures, densities, partial pressures, qualities, etc.) are expressed as functions of these five independent properties. In addition to these properties, several state derivatives are needed because of the linearization used in the numerical scheme. This section contains three parts. The first discusses the state property derivatives needed in the numerical scheme. The second section develops the appropriate derivative formulas for the single component case, and the third section does the same for the two-phase, two-component case.

3.2.1 State Equations

To expand the time derivatives of the phasic densities in terms of these dependent variables using two-term Taylor series expansions, the following derivatives of the phasic densities are needed:

$$\left(\frac{\partial \rho_g}{\partial P}\right)_{U_g, X_n} \cdot \left(\frac{\partial \rho_g}{\partial U_g}\right)_{P, X_n} \cdot \left(\frac{\partial \rho_g}{\partial X_n}\right)_{P, U_g} \cdot \left(\frac{\partial \rho_f}{\partial P}\right)_{U_f} \cdot \left(\frac{\partial \rho_f}{\partial U_f}\right)_P \cdot$$

The interphase mass and heat transfer requires an implicit (linearized) evaluation of the interphase temperature potentials $T_f - T_I$ and $T_g - T_I$. T_I is the temperature that exists at the phase interface. For a single-component mixture, we have

$$T_I = T^s(P) \quad (3-117)$$

where the superscript s denotes a saturation value. In the presence of a noncondensable mixed with the steam, we have

$$T_I = T^s(P_s) \quad (3-118)$$

where P_s is the partial pressure of the steam in the gaseous phase. The gaseous phase properties for a two-component mixture can be described with three independent properties. In particular, the steam partial pressure, P_s , can be expressed as

$$P_s = P_s(P, X_n, U_g) \quad (3-119)$$

Substituting Equation (3-119) into Equation (3-118) gives the interface temperature, T_I , as the desired function of P , X_n , and U_g .^a The implicit evaluation of the temperature potential in the numerical scheme requires the following derivatives of the phasic and interface temperatures:

$$\left(\frac{\partial T_g}{\partial P}\right)_{U_g, X_n} \cdot \left(\frac{\partial T_g}{\partial U_g}\right)_{P, X_n} \cdot \left(\frac{\partial T_g}{\partial X_n}\right)_{P, U_g} \cdot$$

a. ρ_g and T_g could have initially been written with P_s , X_n , U_g as the independent arguments. Equation (3-119) would then be used to write ρ_g and T_g , with P , X_n , and U_g as the independent variables.

$$\left(\frac{\partial T_f}{\partial P}\right)_{U_f}, \left(\frac{\partial T_f}{\partial U_f}\right)_P, \left(\frac{\partial T^S}{\partial P}\right)_{U_g, X_n}, \left(\frac{\partial T^S}{\partial U_g}\right)_{P, X_n}, \left(\frac{\partial T^S}{\partial X_n}\right)_{P, U_g}.$$

If we have a single-component mixture, the X_n derivatives are zero and

$$\left(\frac{\partial T^S}{\partial U_g}\right)_P = 0 \quad (3-120)$$

since T^S is only a function of P for this case.

In addition to these derivatives, the basic phasic properties as a function of P , α_g , U_g , U_f , and X_n are needed, along with the homogeneous equilibrium sound speed for the critical flow model.

The basic properties are obtained from steam tables that tabulate for each phase the phasic properties and three phasic derivatives; the isobaric thermal expansion coefficient (β), the isothermal compressibility (κ), and the specific heat at constant pressure (C_p).

3.2.2 Single-Component, Two-Phase Mixture

For the purposes of this report, a single-component, two-phase mixture will be referred to as Case 1. Case 1 is straightforward. Liquid properties are obtained from the steam tables, given P and U_f . All the desired density and temperature derivatives can then be obtained from κ_f , β_f , and C_{pf} . The desired derivatives are given as

$$\left(\frac{\partial \rho_f}{\partial U_f}\right)_P = - \left(\frac{V_f \beta_f}{C_{pf} - V_f \beta_f P} \right) / V_f^2 \quad (3-121)$$

$$\left(\frac{\partial T_f}{\partial U_f}\right)_P = \left(\frac{1}{C_{pf} - V_f \beta_f P} \right) \quad (3-122)$$

$$\left(\frac{\partial \rho_f}{\partial P}\right)_{U_f} = \left[\frac{C_{pf} V_f \kappa_f - T_f (V_f \beta_f)^2}{C_{pf} - V_f \beta_f P} \right] / V_f^2 \quad (3-123)$$

$$\left(\frac{\partial T_f}{\partial P}\right)_{U_f} = - \left(\frac{P V_f \kappa_f - T_f V_f \beta_f}{C_{pf} - V_f \beta_f P} \right) \quad (3-124)$$

Parallel formulas hold for the vapor phase, with P and U_g as the independent variables.

The only nonstandard feature involved in the evaluation of the formulas in Equation (3-124) is the calculation of V , T , κ , β , and C_p if the steam is subcooled or the liquid is superheated, i.e., metastable states. The extrapolation used for these cases is a constant pressure extrapolation from the saturation state for the temperature and specific volume. Using the first two terms of a Taylor series, this gives

$$T = T(P) + \frac{1}{C_p(P) - P V(P) \beta(P)} [U - U(P)] \quad (3-125)$$

$$V = V(P) + V(P) \beta(P) [T - T(P)] \quad (3-126)$$

In Equations (3-125) and (3-126), the argument P indicates a saturation value.

To obtain the β , κ , and C_p corresponding to the extrapolated V and T , the extrapolation formulas are differentiated. Taking the appropriate derivatives of Equation (3-125) and (3-126) gives

$$C_p(P, T) \triangleq \left(\frac{\partial h}{\partial T}\right)_P = \left(\frac{\partial U}{\partial T}\right)_P + P \left(\frac{\partial V}{\partial T}\right)_P = C_p(P) \quad (3-127)$$

$$\beta(P, T) \triangleq \frac{1}{V} \left(\frac{\partial V}{\partial T}\right)_P = \frac{V(P) \beta(P)}{V(P, T)} \quad (3-128)$$

$$\kappa(P,T) \stackrel{\Delta}{=} - \frac{1}{V} \left(\frac{\partial V}{\partial P} \right)_T = [V(P) + [T - T(P)]V(P)\beta(P)] \frac{\kappa(P)}{V(P,T)} \\ - [T - T(P)] V(P) \left[\frac{d\beta(P)}{dP} + \beta^2(P) \right] \frac{dT}{dP}(P)/V(P,T) \quad . \quad (3-129)$$

Equation (3-127) shows that a consistently extrapolated C_p is just the saturation value $C_p(P)$. Equation (3-128) gives the extrapolated β as a function of the saturation properties and the extrapolated V . Equation (3-129) gives the consistently extrapolated κ as a function of the extrapolated and saturation properties. The extrapolated κ in Equation (3-129) involves a change of saturation properties along the saturation line. In particular, $\frac{d\beta}{dP}(P)$ involves a second derivative of specific volume. Since no second-order derivatives are available from the steam property tables, this term was approximated for the vapor phase by assuming that the fluid behaves as an ideal gas. With this assumption, the appropriate formula for the vapor phase κ is

$$\kappa_g(P,T) = \{V_g(P) + [T_g - T(P)] V_g(P)\beta_g(P)\} \kappa_g(P)/V_g(P,T) \quad . \quad (3-130)$$

For the liquid phase extrapolation (superheated liquid), only the specific volume correction factor in Equation (3-129) was retained, i.e.,

$$\kappa_f(P,T) = \frac{V_f(P)\kappa_f(P)}{V_f(P,T)} \quad . \quad (3-131)$$

The homogeneous equilibrium sound speed is calculated from standard formulas using the saturation κ 's, β 's, and C_p 's. The sound speed formula

$$a^2 = V^2 \left(\frac{dP^S}{dT} \right)^2 \left\{ x \left[\frac{C_{pg}}{T_g} + V_g \frac{dP^S}{dT} \kappa_g \left(\frac{dP^S}{dT} - 2\beta_g \right) \right] \right. \\ \left. + (1-x) \left[\frac{C_{pf}}{T_f} + V_f \frac{dP^S}{dT} \kappa_f \left(\frac{dP^S}{dT} - 2\beta_f \right) \right] \right\} \quad (3-132)$$

is used, where from Clapeyron's equation

$$\frac{dp^s}{dT} = \frac{h_g^s - h_f^s}{T^s(v_g^s - v_f^s)} \quad (3-133)$$

and X is the steam quality based on the mixture mass.

3.2.3 Two-Component, Two-Phase Mixture

This case is referred to as Case 2. The liquid phase properties and derivatives are calculated in exactly the same manner as described in Case 1 (see Section 3.2.2); we assume that the noncondensable component is present only in the gaseous phase.

The properties for the gaseous phase are calculated assuming a Gibbs-Dalton mixture of steam and an ideal noncondensable gas. A Gibbs-Dalton mixture is based upon the following assumptions:

$$1. \quad P = \sum_{n=1}^N P_{ni} + P_s \quad (3-134)$$

$$2. \quad U_g = X_n U_n + (1 - X_n) U_s \quad (3-135)$$

$$3. \quad V_g = X_n V_n + (1 - X_n) V_s \quad (3-136)$$

where P_s and P_{ni} are the partial pressures of the steam and the individual noncondensable components, respectively. The internal energies, U_s , U_n , and the specific volumes, V_s , V_n , are evaluated at the gas

temperature and the respective partial pressures. The vapor properties are obtained from the steam tables, and the noncondensable state equations are^a

$$P_n V_n = R_n T_g \quad (3-137)$$

$$U_n = \begin{cases} C_o T_g + U_o & T_g < T_o \\ C_o T_g + \frac{1}{2} D_o (T_g - T_o)^2 + U_o & T_g \geq T_o \end{cases} \quad (3-138)$$

Given P , U_g , and X_n , we must solve Equations (3-134) through (3-136) implicitly to find the state of the gaseous phase. If Equation (3-134) is used to eliminate P_n and Equation (3-137) is used for V_n , Equations (3-135) and (3-136) can be written as

$$(1 - X_n)U_s + X_n U_n [T_g(U_s, P_s)] - U_g = 0 \quad (3-139)$$

$$(1 - X_n) \left[\frac{V_s(U_s, P_s) P_s}{T_g(U_s, P_s)} \right] (P - P_s) - X_n R_n P_s = 0 \quad (3-140)$$

Given P , U_g , and X_n , Equations (3-139) and (3-140) implicitly determine U_s and P_s . [Equation (3-136) was divided by the temperature and multiplied by the partial pressures to obtain Equation (3-140).]

To obtain the derivatives needed in the numerical scheme, we must evaluate the derivatives of U_s and P_s with respect to P , U_g , and X_n . These derivatives can be obtained from Equations (3-139) and (3-140) by the use of the chain rule and implicit differentiation. For example, taking the derivative of Equations (3-139) and (3-140) with respect to P [recall that $P_s = P_s(P, U_g, X_n)$ and $U_s = U_s(P, U_g, X_n)$], we obtain

a. The code input permits selection of any one of six noncondensable gases. The constants used to represent air are in SI units; $T_o = 250.0$ K, $C_o = 715.0$ J/(kg·K), $U_o = 158990.52$ J/kg, $D_o = 0.10329$ J/(kg·K²), and $R_n = 287.066$ N m/(kg·K).

$$\begin{bmatrix}
 X_n \left(\frac{dU_n}{dT_g} \right) \left(\frac{\partial T_g}{\partial P_s} \right) & 1 - X_n + X_n \left(\frac{dU_n}{dT_g} \right) \left(\frac{\partial T_g}{\partial U_s} \right) \\
 -X_n R_n - (1 - X_n) R_s & 0 + \text{TERM2} \\
 + R_s + \text{TERM1} &
 \end{bmatrix} \times \begin{bmatrix}
 \left(\frac{\partial P_s}{\partial P} \right)_{U_g, X_n} \\
 \left(\frac{\partial U_s}{\partial P} \right)_{U_g, X_n}
 \end{bmatrix}$$

$$= \begin{bmatrix}
 0 \\
 (1 - X_n) R_s
 \end{bmatrix} \quad (3-141)$$

as a linear system of two equations determining

$$\left(\frac{\partial P_s}{\partial P} \right)_{U_g, X_n} \text{ and } \left(\frac{\partial U_s}{\partial P} \right)_{U_g, X_n} .$$

In Equation (3-141),

$$R_s = \frac{P_s V_s}{T_g} \quad (3-142)$$

is the equivalent gas constant for the steam vapor,

$$\text{TERM1} = (1 - X_n) P_n R_s \left[\frac{1}{P_s} + \frac{1}{V_s} \left(\frac{\partial V_s}{\partial P_s} \right)_{U_s} - \frac{1}{T_g} \left(\frac{\partial T_g}{\partial P_s} \right)_{U_s} \right] \quad (3-143)$$

and

$$\text{TERM2} = (1 - X_n) P_n R_s \left[\frac{1}{V_s} \left(\frac{\partial V_s}{\partial U_s} \right)_{P_s} - \frac{1}{T_g} \left(\frac{\partial T_g}{\partial U_s} \right)_{P_s} \right] . \quad (3-144)$$

The TERM factors have been singled out, as they are treated in a special manner in the numerical scheme. To obtain the derivatives of P_s and U_s with respect to U_g and X_n , we repeat the above development taking derivatives of Equations (3-139) and (3-140) with respect to U_g and X_n . In each case, linear equations parallel to those in Equation (3-141) are obtained. In fact, the left side matrix is exactly the same, only the right side vector changes.

Having obtained all the derivatives of P_s and U_s , it is relatively easy to obtain the derivatives needed for the gaseous phase. From the chain rule, we have

$$\left(\frac{\partial T_g}{\partial P}\right)_{U_g, X_n} = \left(\frac{\partial T_g}{\partial P_s}\right)_{U_s} \left(\frac{\partial P_s}{\partial P}\right)_{U_g, X_n} + \left(\frac{\partial T_g}{\partial U_s}\right)_{P_s} \left(\frac{\partial U_s}{\partial P}\right)_{U_g, X_n} \quad (3-145)$$

$$\left(\frac{\partial T_g}{\partial U_g}\right)_{P, X_n} = \left(\frac{\partial T_g}{\partial P_s}\right)_{U_s} \left(\frac{\partial P_s}{\partial U_g}\right)_{P, X_n} + \left(\frac{\partial T_g}{\partial U_s}\right)_{P_s} \left(\frac{\partial U_s}{\partial U_g}\right)_{P, X_n} \quad (3-146)$$

$$\left(\frac{\partial T_g}{\partial X_n}\right)_{P, U_g} = \left(\frac{\partial T_g}{\partial P_s}\right)_{U_s} \left(\frac{\partial P_s}{\partial X_n}\right)_{P, U_g} + \left(\frac{\partial T_g}{\partial U_s}\right)_{P_s} \left(\frac{\partial U_s}{\partial X_n}\right)_{P, U_g} \quad (3-147)$$

where

$$\left(\frac{\partial T_g}{\partial P_s}\right)_{U_s} \quad \text{and} \quad \left(\frac{\partial T_g}{\partial U_s}\right)_{P_s}$$

are the standard phasic derivatives for the vapor phase. Equations (3-145) through (3-147) give all the desired gaseous temperature derivatives. The interface temperature derivatives are obtained from Clapeyron's equation and the known P_s derivatives, i.e.,

$$\left(\frac{\partial T_I}{\partial P}\right)_{U_g, X_n} = \frac{dT_I}{dP_s} \left(\frac{\partial P_s}{\partial P}\right)_{U_s, X_n} \quad (3-148)$$

$$\left(\frac{\partial T_I}{\partial U_g}\right)_{P, X_n} = \frac{dT_I}{dP_s} \left(\frac{\partial P_s}{\partial U_g}\right)_{P, X_n} \quad (3-149)$$

$$\left(\frac{\partial T_I}{\partial X_n}\right)_{P, U_g} = \frac{dT_I}{dP_s} \left(\frac{\partial P_s}{\partial X_n}\right)_{P, U_g}, \quad (3-150)$$

where dT_I/dP_s is given by the reciprocal of Equation (3-133).

The density derivatives can be obtained from $V_g = X_n V_n$ or $V_g = (1 - X_n)V_s$, as these two formulas for the gaseous specific volume are equivalent [see Equation (3-136)]. A symmetric formula can be obtained by eliminating X_n from the above two formulas, giving

$$V_g = \frac{V_s V_n}{V_s + V_n} \quad (3-151)$$

Using Equation (3-151), we have for the ρ_g derivatives with respect to P

$$\left(\frac{\partial \rho_g}{\partial P}\right)_{U_g, X_n} = -\frac{1}{V_n^2} \left(\frac{\partial V_n}{\partial P}\right)_{U_g, X_n} - \frac{1}{V_s^2} \left(\frac{\partial V_s}{\partial P}\right)_{U_g, X_n} \quad (3-152)$$

Parallel formulas are obtained when either U_g or X_n is the independent variable. The partial derivatives on the right side of Equation (3-152) are obtained from formulas exactly parallel to those in Equations (3-145) through (3-147) with U_g replaced by V_s or V_n . When taking the derivatives of V_n , remember that

$$V_n = \frac{R T_g (P_s, V_s)}{P - P_s} \quad (3-153)$$

Hence, an additional term appears in Equation (3-145) due to the direct dependence of V_n on P .

The homogeneous equilibrium sound speed for a noncondensable steam-water mixture is derived in Reference 3-18.

The sound speed formula in Reference 3-18 is

$$a^2 = V^2 (P'_s)^2 / \left\{ \begin{aligned} & \left[-X_n V_n P'_s \beta_n - X_f V_f P'_s (\beta_f - P'_s \kappa_f) \right] \\ & + \left\{ \hat{X}_s P'_s \left[\frac{C_{ps}}{T^s} + P'_s V_s (-2\beta_s + \kappa_s P'_s) \right] + \hat{X}_n P'_s \left(\frac{C_{pn}}{T^s} + P'_s V_n \beta_n \right) \right. \\ & \left. + \hat{X}_f P'_s \left(\frac{C_{pf}}{T^s} - P'_s V_s \beta_s \right) \right\} \left(\frac{\partial T}{\partial P} \right)_{S, X_n} \end{aligned} \right\}, \quad (3-154)$$

where

$$P'_s = \frac{dP^s}{dT} = \frac{h_s^s - h_f^s}{T^s (V_s^s - V_f^s)} \quad (3-155)$$

and

$$\begin{aligned} \left(\frac{\partial T}{\partial P} \right)_{S, X_n} = & 1 + \left[\hat{X}_n V_n \beta_n + X_f V_f \beta_f \right] / \left[\hat{X}_s \kappa_n (S_s - S_f) \right] / \\ & \left[P'_s + \left(\frac{\kappa_s}{\kappa_n} \right) \left\{ P'_s + \left(\frac{\beta_n - \beta_s}{\kappa_s} \right) + \left[(\hat{X}_n V_n \beta_n - \hat{X}_s V_s \beta_s) P'_s + (\hat{X}_n C_{pn} + \hat{X}_s C_{ps} \right. \right. \right. \\ & \left. \left. + \hat{X}_f C_{pf}) / T^s \right] / [\hat{X}_s \kappa_s (S_s - S_f)] \right\} \right]. \end{aligned} \quad (3-156)$$

In the above formulas, $\hat{X}_s$, $\hat{X}_n$, and $\hat{X}_f$ are mass qualities based on the total mixture mass.

Evaluation of the sound speed formulas at the saturated equilibrium state requires a second iteration. To avoid this extra iteration, the sound speed formulas were evaluated using the nonequilibrium state properties.

The liquid properties and derivatives are obtained as above for Case 1. To obtain the gaseous properties, Equations (3-139) and (3-140) must be solved iteratively. A standard Newton iteration in two variables is used. The iteration variables are P_s and U_s . The steam table Subroutine STH2X6 is called once during each iteration to obtain all the needed steam vapor properties, and Equations (3-137) and (3-138) are used to obtain the air properties. To save calculation time, only an approximate Jacobian is used inside the iteration loop. From Equation (3-140), it is clear that if the steam behaves as an ideal gas, i.e., $R_s = (V_s P_s / l_g)$ is constant, then Equation (3-140) is a simple linear equation determining P_s directly in terms of P and X_n . It simplifies the iteration if we neglect the derivatives of R_s in the Jacobian. This makes the Jacobian matrix equal to the left side matrix in Equation (3-141) with TERM1 and TERM2 terms absent. This iteration has been tested with P_s ranging from 2000 Pa to P and has always converged. The iteration is terminated when $|\Delta P_s|/P$ and $|\Delta V_s|/V_g$ are both < 0.0005 . Hand calculations have been performed to compare both the properties and derivatives with the code calculations.

Once the iteration has converged, the gaseous properties are determined from the formulas in this section. In the evaluation of all these derivatives, the full matrix in Equation (3-141) is used, including TERM1 and TERM2.

3.3 Constitutive Models

The constitutive relations include models for defining flow regimes and flow regime related models for interphase drag, wall friction, and interphase heat and mass transfer. Heat transfer regimes are defined and used for wall heat transfer and wall reflood heat transfer. For the vertical mass, a formula based on the void fraction is used.

3.3.1 Flow Regime Maps

The constitutive relations include flow regime effects for which simplified mapping techniques have been developed to control the use of constitutive relation correlations. The flow regime maps are based on the work of Taitel and Dukler^{3-19,20} and Ishii.^{3-21,22,23}

Taitel and Dukler have simplified flow regime classification and developed semi-empirical relations to describe flow regime transitions. However, some of their transition criteria are quite complex, and further simplification has been carried out in order to efficiently apply these criteria in SCDAP/RELAP5. In addition, post-critical heat flux (CHF) regimes as suggested by Ishii³⁻²¹ are included.

Three flow regime maps are used. They are vertical and horizontal maps for flow in pipes and a high mixing map for flow in pumps.

3.3.1.1 Vertical Flow Regime Map. The vertical flow regime map is for volumes whose elevation angle ϕ is such that $15.0 \text{ degrees} < |\phi| \leq 90 \text{ degrees}$. This map is modeled as seven regimes, three of which are for pre-CHF heat transfer, three of which are for post-CHF heat transfer, and one of which is for vertical stratification. For pre-CHF heat transfer, the regimes modeled are the bubbly, slug, and annular mist regimes. Formulations for these three regimes were utilized by Vince and Lahey³⁻²⁴ to analyze their data. For post-CHF heat transfer, the bubbly, slug, and annular mist regimes are transformed to the inverted annular, inverted slug, and mist regimes, respectively, as

suggested by Ishii.³⁻²¹ Unheated components are also modeled, utilizing the pre-CHF map. A schematic representing the pre- and post-CHF regimes of the vertical flow regime map is shown in Figure 3-3. The vertically stratified regime may exist at low flow conditions, and a schematic showing its relationship in the vertical flow regime map is given in Figure 3-4. The criteria for defining the boundaries for transition from one regime to another are given by the following correlations.

For the bubbly-to-slug transition, Taitel and Dukler^{3-19,20} suggested that bubbly flow may not exist in tubes of small diameter where the rise velocity of small bubbles exceeds that of Taylor bubbles. The small bubble rise velocity is given by the correlation³⁻²⁰

$$v_{sb} = 1.53 \left(\frac{D^* \sigma}{D \rho_f} \right)^{1/2} \quad (3-157)$$

and the Taylor bubble rise velocity is given by the correlation³⁻³

$$v_{tb} = 0.35 D^* \left(\frac{\sigma}{D \rho_f} \right)^{1/2} . \quad (3-158)$$

(Note: in Reference 3-20, $\rho_f - \rho_g$ is approximated as ρ_f , see also References 3-22 and 3-25.) Accordingly, the limiting tube diameter allowing the presence of bubbly flow is

$$D^* \geq 19 \quad (3-159)$$

where D^* is the dimensionless tube diameter,

$$D^* = D[g(\rho_f - \rho_g)/\sigma]^{1/2} . \quad (3-160)$$

Equation (3-160) is the dimensionless ratio of tube diameter to film thickness times the Deryagin number, where the Deryagin number is the ratio of film thickness to capillary length. Also, in the limit, as the fluid properties approach the thermodynamic critical pressure, $D^* = D$.

Figure 3-3. Sketch of vertical flow regime map.

Figure 3-4. Vertical flow regime map, including the vertically stratified regime.

For tubes with diameters satisfying the condition of Equation (413), the bubble-slug transition occurs at a void fraction $\alpha_g = 0.25$ for low mass fluxes of $G \leq 2000 \text{ kg/m}^2 \cdot \text{s}$. By combining this void criterion with Equation (3-159), the bubble-slug transition criterion can be defined such that

$$\alpha_L = 0.25 \text{ MIN } [1.0, (D^*/19)^8] \quad (3-161)$$

Hence, if the local void fraction, α_g , exceeds the criterion of Equation (161) then bubbly flow cannot exist since the rise velocity of small bubbles exceeds that of Taylor bubbles. The exponential power of 8 is used to provide a smooth variation of α_L as D^* decreases.

At high mass fluxes of $G \geq 3000 \text{ kg/m}^2 \cdot \text{s}$, bubbly flow with finely dispersed bubbles can exist up to a void fraction, α_g , of 0.5. Then, if the criterion is linearly interpolated between the upper and lower void limits, the bubbly-slug transition criterion can be written as

$$\alpha_{B-S} = \alpha_L \quad (3-162)$$

for mass fluxes of $G < 2000 \text{ kg/m}^2 \cdot \text{s}$,

$$\alpha_{B-S} = \alpha_L + 0.001 (G - 2000) (0.5 - \alpha_L) \quad (3-163)$$

for mass fluxes of $2000 < G < 3000 \text{ kg/m}^2 \cdot \text{s}$, and

$$\alpha_{B-S} = 0.5 \quad (3-164)$$

for mass fluxes of $G \geq 3000 \text{ kg/m}^2 \cdot \text{s}$. The flow regime can therefore be said to be in the bubbly regime if $\alpha_g < \alpha_{B-S}$ and in the slug regime if $\alpha_g \geq \alpha_{B-S}$.

The bubble-slug transition defined by Equations (3-162) to (3-164) is similar to that given by Taitel and Dukler,³⁻²⁰ except that their void fraction relation is converted into a form based on liquid and vapor superficial velocities, and finely dispersed bubbles are also distinguished from ordinary bubbles.

For the slug-to-annular-flow transition, Taitel and Dukler³⁻²⁰ developed a criterion based on the critical vapor velocity required to suspend a liquid droplet. The critical velocity, u_c , is written as

$$u_c = 3.1[\sigma g(\rho_f - \rho_g)]^{1/4} / \rho_g^{1/2} = (\alpha_g v_g)_c \quad (3-165)$$

The value 3.1 for the numerical coefficient is somewhat larger than the value of 1.4 reported by Wallis³⁻²⁶ but is a better fit to the data reported by Vince and Lahey.³⁻²⁴ In comparing RELAP5 code results to data, however, the coefficient value of 1.4 gives better results. The void fraction must also be >0.75 in order to get good comparisons between code results and data. Hence, solving Equation (3-165) for void fraction and imposing a lower void limit of 0.75 yields the slug-to-annular transition criterion for which

$$\alpha_{S-A} = \left\{ \text{MAX } 0.75, 1.4[\sigma g(\rho_f - \rho_g)]^{1/4} / (v_g \rho_g^{1/2}) \right\} \quad (3-166)$$

where the flow regime is said to be in the slug regime if $\alpha_g \leq \alpha_{S-A}$ and in the annular-mist regime if $\alpha_g > \alpha_{S-A}$.

For post-CHF heat transfer, the same formulations are used to define the inverted flow regime transition criteria in that Equations (3-162) through (3-164) also define the inverted-annular to inverted-slug regime transition and Equation (3-166) defines the inverted-slug-to-mist regime transition.

At low mass fluxes, the possibility exists for vertically stratified conditions. In SCDAP/RELAP5, vertical flow in a volume cell is considered

to be stratified if the difference in void fraction of the volumes above and below is >0.5 and if the magnitude of the volume average mixture mass flux is less than the Taylor bubble rise velocity mass flux. The Taylor bubble criterion is based on the Taylor bubble velocity given by Equation (3-158) such that

$$|G| < \rho v_{Tb} \quad (3-167)$$

where v_{Tb} is the Taylor bubble velocity, and

$$|G| = |\alpha_g \rho_g v_g + \alpha_f \rho_f v_f| \quad (3-168)$$

Hence, if Equation (3-167) is true, then transition to vertical stratification exists; and if Equation (3-167) is false, then transition to vertical stratification does not exist. Fixed numbers are not shown on Figure 3-4 for the mass flux limits for the vertical stratification region because these depend on v_{Tb} .

3.3.1.2 Horizontal Flow Regime Map. The horizontal flow regime map is for volumes whose elevation angle ϕ is such that $0 \text{ degrees} \leq |\phi| \leq 15.0 \text{ degrees}$. This map is similar to the vertical flow regime map except that the post-CHF regimes are not included and a horizontal stratification regime is modeled that replaces the vertical stratification regime. The horizontal flow regime map therefore consists of horizontally stratified, bubbly, slug, and annular mist regimes. The criteria for the bubbly-to-slug and the slug-to-annular mist regimes are also similar to those for the vertical map except that the bubbly to slug transition criterion is a constant

$$\alpha_{B-S} = \alpha_L = 0.25 \quad (3-169)$$

and the slug-to-annular-mist transition criterion is a constant

$$\alpha_{S-A} = 0.8 \quad (3-170)$$

The criterion defining the horizontally stratified regime is based on the one developed by Taitel and Dukler.³⁻¹⁹

According to Taitel and Dukler, the flow field is horizontally stratified if the vapor velocity satisfies the condition that

$$v_g < v_{gL}, \quad (3-171)$$

where

$$v_{gL} = \frac{1}{2} \frac{(\rho_f - \rho_g) S/B_{g\alpha} v_g A}{\rho D \sin \theta} (1 - \cos \theta) \quad (3-172)$$

This condition is modified in the code, and the flow is horizontally stratified so the phase velocity difference satisfies the condition

$$v_g - v_f < v_{gL}$$

and the mass flux satisfies the condition

$$G < 300 \text{ kg/m}^2\text{-s}.$$

These modifications were implemented to handle situations where the flow is stratified but the liquid is flowing.

The angle θ is related to the liquid level, ll , and the void fraction, α_g , by the relationships

$$ll = D (1 + \cos \theta)/2 \quad (3-173)$$

and

$$\alpha_g \pi = \theta - \sin \theta \cos \theta. \quad (3-174)$$

If the horizontal stratification conditions of Equations (3-172a) and (3-172b) are met, then the flow field undergoes a transition to horizontally stratified. If the conditions of Equations (3-172a) and (3-172b) are not met, then the flow field undergoes a transition to the bubbly, slug, or annular mist flow regime.

3.3.1.3 High Mixing Flow Regime Map. The high mixing flow regime map is based on vapor void fraction, α_g , and consists of a bubbly regime for $\alpha_g < 0.5$, a mist regime for $\alpha_g \geq 0.95$, and a transition regime for $0.5 < \alpha_g < 0.95$. The transition regime is modeled as a mixture of bubbles dispersed in liquid and droplets dispersed in vapor.

3.3.2 Interphase Drag

The interphase drag force per unit volume expressed in terms of relative phasic velocity is

$$FI_{gf} = - f_{gf} |v_g - v_f| (v_g - v_f) \quad (3-175)$$

with

$$f_{gf} = \frac{1}{8} \rho_c S_f a_{gf} C_D \quad (3-176)$$

where

ρ_c = density of the continuous phase

C_D = drag coefficient

a_{gf} = interfacial area per unit volume

S_f = shape factor.

The shape factor,³⁻²² is assumed to be unity (1.0). The evaluation of a_{gf} and C_D for different flow regimes is covered in the following discussion.

3.3.2.1 Dispersed Flow. The bubbly and mist flow regimes are both considered as dispersed flow. According to Wallis³⁻²⁶ and Shapiro,³⁻²⁷ the dispersed bubbles or droplets can be assumed to be spherical particles with a size distribution of the Nukiyama-Tanasawa form. The Nukiyama-Tanasawa distribution function in nondimensional form is

$$p^* = 4d^{*2} e^{-2d^*} \quad (3-177)$$

where $d^* = d/d'$; d' is the most probable particle diameter, and p^* is the probability of particles with nondimensional diameter of d^* . With this distribution, it can be shown that the average particle diameter $d_o = 1.5 d'$, and the surface area per unit volume is

$$a_{gf} = \frac{6\bar{\alpha}}{d'} - \frac{\int d^{*2} p^* dd^*}{\int d^{*3} p^* dd^*} = \frac{2.4\bar{\alpha}}{d'} \quad (3-178)$$

where $\bar{\alpha} = \alpha_g$ for bubbles and $\bar{\alpha} = \alpha_f$ for droplets. In terms of the average diameter, d_o , the interfacial area per unit volume, a_{gf} , is

$$a_{gf} = 3.6\bar{\alpha}/d_o \quad (3-179)$$

The average diameter d_o is obtained by assuming that $d_o = (1/2)d_{max}$. The maximum diameter, d_{max} , is related to the critical Weber number, We , by

$$We = d_{max} \rho_c (v_g - v_f)^2 / \sigma \quad (3-180)$$

where σ is the surface tension. The values for We are presently taken as $We = 10.0$ for bubbles and $We = 3.0$ for droplets.

The drag coefficient is given by a modification to Ishii and Chawla³⁻⁷⁸ for the viscous regime as

$$C_D = 24(1.67 + 0.123 \text{Re}_p^{0.75}) / \text{Re}_p \quad (3-181)$$

where the particle Reynolds number, Re_p , is defined as

$$\text{Re}_p = \left| v_g - v_f \right| d_o \rho_c / \mu_m \quad (3-182)$$

The mixture viscosity, μ_m , is $\mu_m = \mu_f / \alpha_f$ for bubbles and $\mu_m = \mu_g / (\alpha_g)^{2.5}$ for droplets.

3.3.2.2 Slug Flow. Slug flow is modeled as a series of Taylor bubbles separated by liquid slugs containing small bubbles. A sketch of a slug flow pattern is shown in Figure 3-5. The Taylor bubble has a diameter nearly equal to the pipe diameter and a length varying from one to one hundred pipe diameters.

Let α_{gs} be the average void fraction in the liquid film and slug region. The void fraction of a single Taylor bubble, α_b , in the total mixture is then

$$\alpha_b = (\alpha_g - \alpha_{gs}) / (1 - \alpha_{gs}) \quad (3-183)$$

By approximating the ratio of the Taylor bubble diameter to the tube diameter and the diameter-to-length ratio of a Taylor bubble, Ishii and Mishima³⁻²³ obtained the surface-to-volume ratio of a Taylor bubble as $4.5/D$. Consequently, the interfacial area per unit volume, a_{gf} , for slug flow is

$$a_{gf} = (4.5 C_t / D) \alpha_b + (3.6 \alpha_{gs} / d_o) (1 - \alpha_b) \quad (3-184)$$

Figure 3-5. Slug flow pattern.

where C_t is a roughness parameter that is introduced to account for irregularities in the surface of large Taylor bubbles. At the present time, C_t is assumed to be unity (1.0).

To provide a smooth transition into and out of slug flow, α_{gs} in Equation (3-183) is considered as a free parameter varying from α_{B-S} at the bubbly-to-slug flow regime transition to nearly zero at the slug-to-annular-mist flow regime transition. The variation is represented by the exponential expression

$$\alpha_{gs} = \alpha_{B-S} \exp[-8(\alpha_g - \alpha_{B-S}) / (\alpha_{S-A} - \alpha_{B-S})] \quad (3-185)$$

The drag coefficient for Taylor bubbles is given by Ishii and Chawla³⁻²² as

$$C_D = 9.8 (1 - \alpha_b)^3 \quad (3-186)$$

where α_b is given by combining Equations (3-183) and (3-183).

3.3.2.3 Annular Mist Flow. Annular mist flow is characterized by a liquid film along the wall and a vapor core containing entrained liquid droplets. Let α_{ff} be the average liquid volume fraction of the liquid film along the wall. Then, from simple geometric considerations, the interfacial area per unit volume can be shown to be

$$a_{gf} = (4C_{an}/D)(1 - \alpha_{ff})^{1/2} + (3.6\alpha_{fd} d_o)(1 - \alpha_{ff}) \quad (3-187)$$

where C_{an} is a roughness parameter introduced to account for waves in the liquid wall film and α_{fd} is the average liquid volume fraction in the vapor core, for which

$$\alpha_{fd} = (\alpha_f - \alpha_{ff}) / (1 - \alpha_{ff}) \quad (3-188)$$

A simple relation based on the flow regime transition criterion and liquid Reynolds number is used to correlate the average liquid film volume fraction. For vertical flow regimes, the entrainment relation is

$$\alpha_{ff} = \alpha_f C_f \exp \left[- 7.5 \times 10^{-5} (\alpha_g v_g / u_c)^6 \right] \quad (3-189)$$

where u_c is the entrainment critical velocity given by Equation (3-165) with the coefficient 3.1 replaced by 1.4. For horizontal flow regimes, the entrainment relation is

$$\alpha_{ff} = \alpha_f C_f \exp \left[- 4.0 \times 10^{-5} (v_g / v_{gL})^6 \right] \quad (3-190)$$

where v_{gL} is the horizontal stratification critical velocity given by Equation (3-172). The term C_f is expressed as

$$C_f = 10^{-4} \alpha_f \rho_f v_f \frac{D}{\mu_f} \quad (3-191)$$

The interfacial friction factor, f_i , for the liquid film takes the place of C_D in Equation (3-176) and is described by a correlation obtained by Bharathan et al.³⁻²⁸ for which

$$f_i = 4 \left[0.005 + A(\delta^*)^B \right] \quad (3-192)$$

where

$$\log_{10} A = -0.56 + 9.07/D^* \quad (3-193)$$

$$B = 1.63 + 4.74/D^* \quad (3-194)$$

$$\delta^* = \delta \left[\frac{(\rho_f - \rho_g)g}{\sigma} \right]^{1/2} \quad (3-195)$$

The term δ^* is the liquid wall film Deryagin number for which δ is the film thickness, and D^* is the dimensionless diameter given by Equation (3-161).

3.3.2.4 Vertical Stratified Flow. For vertically stratified flow, the previously discussed interphase drag relationships are applied except that for the junction above the vertically stratified volume, the interphase drag for the volume above the junction is used.

3.3.2.5 Horizontal Stratified Flow. By simple geometric consideration, one can show that the interfacial area per unit volume is

$$a_{gf} = 4C_{st} \sin\theta / (\pi D) \quad (3-196)$$

where C_{st} is a roughness parameter introduced to account for surface waves and is set to one at the present time.

The interface Reynolds number is defined with the vapor properties and regarding liquid as the continuous phase for which

$$Re_i = D_i \rho_g |v_g - v_f| / \mu_g \quad (3-197)$$

where the equivalent wetted diameter, D_i , for the interface is

$$D_i = \alpha \pi D / (\theta + \sin\theta) \quad (3-198)$$

The interfacial friction factor, f_i , replaces C_D in Equation (3-176) and is obtained by assuming typical friction factor relationships for which

$$f_i = 64 / Re_i \quad (3-199)$$

for laminar flow, where $Re_i \leq 1187$;

$$f_i = 0.3164/Re_i^{0.25} \quad (3-200)$$

for turbulent flow, where $Re_i \geq 4000$; and

$$f_i = 0.0539 \quad (3-201)$$

for the laminar-to-turbulent transition where $1187 < Re_i < 4000$.

3.3.2.6 Inverted Flow Regimes. The interphase drag relationships for post-CHF inverted flow regimes are treated in a similar fashion to the corresponding pre-CHF flow regimes except that the roles of vapor and liquid are interchanged.

3.3.2.7 Bubbly/Slug Flow for Rod Bundles. The interphase friction model in SCDAP/RELAP5 can be altered by the user through a volume control flag incorporating Bestion's³⁻²⁹ bubbly/slug interfacial friction correlation for bundles, as developed and modified by Analytis³⁻³⁰. This is recommended in rod bundle geometry when the normal bubbly/slug flow regime overpredicts core void fractions. It can best be described by first examining the finite-difference form of the momentum equations.

The normal sum and difference momentum equations for the semi-implicit scheme can be written in the following form:

$$A_j^n v_{g,j}^{n+1} + B_j^n v_{f,j}^{n+1} = -(P_L - P_K)^{n+1} \Delta t + D_j^n \quad (3-202)$$

$$\begin{aligned} E_j^n v_{g,j}^{n+1} - G_j^n v_{f,j}^{n+1} = & - \left(\frac{\rho_f - \rho_g}{\rho_f \rho_g} \right)_j^n (P_L - P_K)^{n+1} \Delta t \\ & - (\rho F I)_j^n (v_{g,k}^{n+1} - v_{f,j}^{n+1}) \Delta x \Delta t + H_j^n \end{aligned} \quad (3-203)$$

where the next to last term in Equation (3-203) is the interphase drag term (FI). The code currently uses an FI of the form

$$FI_j^n = \left(\frac{FIJ}{\alpha_g \rho_g \alpha_f \rho_f} \right)_j^n |v_{g,j}^n - v_{f,j}^n| \quad (3-204)$$

where the junction FIJ is a volume-weighted average of the volume interphase drag FIVOL (which is the flow regime dependent) from the two adjoining volumes. For rod bundles, the user can request the Bestion/Analytis model, which uses a FIVOL of the form

$$FIVOL_L^n = \frac{65 \rho_{g,L}^n \alpha_{g,L}^n (1 - \alpha_{g,L}^n)^3}{D_L} \quad (3-205)$$

and an FI of the form

$$FI_j^n = \left(\frac{FIJ}{\alpha_g \rho_g \alpha_f \rho_f} \right)_j^n |C_1 v_{g,j}^n - C_0 v_{f,j}^n| \quad (3-206)$$

with Equation (3-203) now becoming

$$\begin{aligned} E_j^n v_{g,j}^{n+1} - G_j^n v_{f,j}^{n+1} = & - \left(\frac{\rho_f - \rho_g}{\rho_f \rho_g} \right)_j^n (P_L - P_K)^{n+1} \Delta t \\ & - (\rho FI)_j^n (C_1 v_{g,j}^{n+1} - C_0 v_{f,j}^{n+1}) \Delta x \Delta t + H_j^n \end{aligned} \quad (3-207)$$

For the coefficients C_0 and C_1 , the values are

$$C_0 = 1.2 \quad (3-208)$$

$$C_1 = \max \left[\frac{1 - C_0 \alpha_g}{1 - \alpha_g}, 0.7 \right] \quad (3-209)$$

Regarding the units in Equation (3-205), using SI units, since E_j^n and G_j^n in Equation (3-203) have units of meters, the term $(\rho FI)_j^n (v_{g,j}^{n+1} - v_{f,j}^{n+1}) \Delta x \Delta t$ in Equation (3-203) has the units of m^2/s . Thus, FI has the units of $m^3/(kg \cdot s)$, and from Equation (3-204), FIJ and $FIVOL$ have units of kg/m^4 . Equation (3-205) also has these units for $FIVOL$.

With regard to the solution method, if the Bestion/Analytis model is requested, the coding checks to see if the flow regime is bubbly or slug. If it is, flags are set; and Equation (3-205) is used to calculate the volume interphase drag. Then, when the terms in the momentum equations are calculated, Equations (3-202) and (3-206) through (3-209) are used. If the nearly implicit scheme is used, this scheme's version of Equation (3-207) has the necessary changes to use this model.

It should be pointed out that Analytis modified Bestion's interphase drag correlation, as shown in Equation (3-205). Bestion used a value of 28.3 rather than 65. Analytis found that a value of 28.3 resulted in too low an interphase drag and hence overprediction of collapsed liquid levels in boil-off experiments. Analytis then found that a value of 65 gave better results.

3.3.3 Coefficient of Virtual Mass

The calculation of the drag due to the virtual mass effect is based on objective and symmetric formulation of the relative acceleration.³⁻⁹ The drag force in the momentum equation is written as

$$FA_{gf} = -C\alpha_g(1 - \alpha_g) \rho \frac{\partial}{\partial t} (v_g - v_f) + v_f \left(\frac{\partial v_g}{\partial x} \right) - v_g \left(\frac{\partial v_f}{\partial x} \right) \quad (3-210)$$

where

$$\rho = \alpha_g \rho_g + (1 - \alpha_g) \rho_f$$

FA_{gf} = force per unit volume due to dynamic drag.

The factor, $C\alpha_g(1 - \alpha_g)\rho$, is chosen to ensure a smooth transition between $\alpha_g = 0$ and $\alpha_g = 1.0$. This factor also gives the proper limit, $C\alpha_g\rho_f$, in the thinly dispersed bubbly flow and $C(1 - \alpha_g)\rho_g$ in the dispersed droplet flow. The virtual mass coefficient, C , is given³⁹⁶ as

$$C = 1/2 \frac{(1 + 2\alpha_g)}{(1 - \alpha_g)} \text{ for } 0 \leq \alpha_g \leq 1/2 \quad (3-211)$$

and

$$C = 1/2 \frac{(3 - 2\alpha_g)}{\alpha_g} \text{ for } 1/2 \leq \alpha_g \leq 1 \quad (3-212)$$

It may be appropriate to assume that $C = 0$ should be used for separated or stratified flow. At present, the value of C defined by Equations (3-211) or (3-212) is used without regard to the flow regime. As discussed in Section 3.1.1.1, the spatial derivative portion of the virtual mass term has been neglected.

3.3.4 Wall Friction

The wall friction force terms include only wall shear effects. Losses due to abrupt area change are calculated using mechanistic form loss models. Other losses due to elbows or complicated flow passage geometry are modeled using energy loss coefficients that must be input by the user.

Emphasis was placed on obtaining reasonable values for wall friction in all flow regimes in the development of the wall friction model. The flow regime models are discussed in Section 3.3.1.

The wall friction model is based on a two-phase multiplier approach in which the two-phase multiplier is calculated from the Heat Transfer and Fluid Flow Service (HTFS) modified Baroczy correlation.³⁻³¹ The individual phasic wall friction components are calculated by apportioning the two-phase friction between the phases using a technique derived by Chisholm³⁻³² from the Lockhart-Martinelli³⁻³³ model. The model is based on the assumption that the frictional pressure drop may be calculated using a quasi-steady form of the momentum equation.

3.3.4.1 The Two-Phase Friction Multiplier Approach. The overall friction pressure drop can be expressed in terms of the liquid-alone wall friction pressure drop

$$\left(\frac{\partial P}{\partial x}\right)_{2\phi} = \phi_f^2 \left(\frac{\partial P}{\partial x}\right)_f \quad (3-213)$$

or the vapor-alone wall friction pressure drop

$$\left(\frac{\partial P}{\partial x}\right)_{2\phi} = \phi_g^2 \left(\frac{\partial P}{\partial x}\right)_g \quad (3-214)$$

where ϕ_f and ϕ_g are the liquid-alone and vapor-alone two-phase friction multipliers, respectively. The phasic wall friction pressure gradients are expressed as

$$\left(\frac{\partial P}{\partial x}\right)_f = \frac{\lambda'_f M_f^2}{20 \rho_f A^2} \quad (3-215)$$

for the liquid-alone, and

$$\left(\frac{\partial P}{\partial x}\right)_g = \frac{\lambda'_g M_g^2}{20 \rho_g A^2} \quad (3-216)$$

for the vapor-alone, where the prime indicates the liquid and vapor-alone friction factors, respectively, calculated at the respective Reynolds numbers

$$Re'_f = \frac{\alpha_f \rho_f |v_f| D}{\mu_f} \quad (3-217)$$

and

$$Re'_g = \frac{\alpha_g \rho_g |v_g| D}{\mu_g} \quad (3-218)$$

The liquid and vapor mass flow rates, respectively, are defined as

$$M_f = \alpha_f \rho_f v_f A \quad (3-219)$$

and

$$M_g = \alpha_g \rho_g v_g A \quad (3-220)$$

Throughout the current literature, the overall two-phase friction pressure gradient is calculated using two-phase friction multiplier correlations. However, regardless of the correlation used, the multipliers may be interrelated using Equations (3-213) through (3-216) and the Lockhart-Martinelli³⁻³³ ratio defined as

$$x^2 \equiv \frac{(\frac{dP}{dx})_f}{(\frac{dP}{dx})_g} = \frac{\phi_g^2}{\phi_f^2} \quad (3-221)$$

These equations are used to apportion the overall wall friction into liquid and vapor wall friction coefficients.

3.3.4.2 Flow Regime Effects. Two-phase friction can be modeled in terms of two-phase friction multipliers and known friction factors using the method developed by Lockhart-Martinelli.³⁻³³ Chisholm³⁻³² also developed a theoretical basis for the Lockhart-Martinelli model that provides a rationale for relating the equations to empirical results.

From the theoretical basis developed by Chisholm, irrespective of flow regime, the quasi-steady phasic momentum equations can be expressed in scalar form as

$$\alpha_f A \left(\frac{\partial p}{\partial x} \right)_{2\phi} - \tau_f p_f + S_{FI} = 0 \quad (3-222)$$

for the liquid, and

$$\alpha_g A \left(\frac{\partial p}{\partial x} \right)_{2\phi} - \tau_g p_g - S_{FI} = 0 \quad (3-223)$$

for the vapor, where τ_f and τ_g are the liquid and vapor wall shear stresses, respectively, p_f and p_g are the liquid and vapor wetted wall perimeters, respectively, and S_{FI} is a stress gradient due to interphase friction. These equations can be expressed in terms of Darcy friction factors and simplified so that

$$\left(\frac{dp}{dx} \right)_{2\phi} \left(1 + S_R \frac{\alpha_g}{\alpha_f} \right) = \frac{\lambda_f \rho_f v_f^2}{2D} \left(\frac{\alpha_{fw}}{\alpha_f} \right) \quad (3-224)$$

for the liquid, and

$$\left(\frac{dp}{dx} \right)_{2\phi} (1 - S_R) = \frac{\lambda_g \rho_g v_g^2}{2D} \left(\frac{\alpha_{gw}}{\alpha_g} \right) \quad (3-225)$$

for the vapor, where the interphase friction term, S_R , is defined as

$$S_R = \frac{S_{FI}}{\alpha_g A \left(\frac{\partial P}{\partial x} \right)_{2\phi}} \quad (3-226)$$

The terms α_{fw} and α_{gw} are the liquid and vapor volume fractions, respectively, at the wall; and α_f and α_g are the overall liquid and vapor volume fractions, respectively. Taking the ratio of Equation (3-224) to (3-225) gives

$$Z^2 = \frac{\lambda_f \rho_f v_f^2 \left(\frac{\alpha_{fw}}{\alpha_f} \right)}{\lambda_g \rho_g v_g^2 \left(\frac{\alpha_{gw}}{\alpha_g} \right)} = \frac{1 + S_R \left(\frac{\alpha_g}{\alpha_f} \right)}{(1 - S_R)} \quad (3-227)$$

Consider the pure liquid case where $\alpha_g = 0$ and $\alpha_{fw} = \alpha_f$ and for which Equation (3-224) reduces to

$$\left(\frac{\partial P}{\partial x} \right)_{2\phi} = \left(\frac{\partial P}{\partial x} \right)_f = \frac{\lambda_f \rho_f v_f^2}{2D} \quad (3-228)$$

For this case, the friction factor, λ_f , can be precisely calculated based on a Reynolds number expressed in terms of D . Similarly, for the two-phase case, liquid and vapor friction factors can be calculated based on a Reynolds number of

$$R_f = \frac{\rho_f \left(\frac{\alpha_f}{\alpha_{fw}} \right) D |v_f|}{\mu_f}, \quad R_g = \frac{\rho_g \left(\frac{\alpha_g}{\alpha_{gw}} \right) D |v_g|}{\mu_g} \quad (3-229)$$

for the liquid and vapor, respectively. These terms have the property that as one phase or the other disappears, the friction factors calculated reduce to their single-phase formulations.

Equations (3-224) and (3-225) can be rewritten as

$$\left(\frac{dP}{dx}\right)_{2\phi} \frac{Z^2}{\alpha_g + \alpha_f Z^2} = \frac{\lambda_f \rho_f v_f^2}{2D} \left(\frac{\alpha_{fw}}{\alpha_f}\right) \quad (3-230)$$

$$\left(\frac{dP}{dx}\right)_{2\phi} \frac{1}{\alpha_g + \alpha_f Z^2} = \frac{\lambda_g \rho_g v_g^2}{2D} \left(\frac{\alpha_{gw}}{\alpha_g}\right) \quad (3-231)$$

for the liquid and vapor, respectively. However, these equations are now flow-regime-dependent, since knowledge of the wetted wall and overall void fractions is required in order to calculate the friction factors. The term Z^2 can also be considered as a correlating factor relating the overall two-phase friction pressure gradient to the known phasic friction factors.

The quasi-steady phasic momentum equations similar to Equations (3-230) and (3-231) can also be written in terms of the SCDAP/RELAP5 friction coefficient, where

$$\alpha_f \left(\frac{dP}{dx}\right)_{2\phi} \frac{Z^2}{\alpha_g + \alpha_f Z^2} = FWF(\alpha_f \rho_f v_f) \quad (3-232)$$

for the liquid, and

$$\alpha_g \left(\frac{dP}{dx}\right)_{2\phi} \frac{1}{\alpha_g + \alpha_f Z^2} = FWG(\alpha_g \rho_g v_g) \quad (3-233)$$

for the vapor. Taking the sum of these two equations gives the overall quasi-steady two-phase pressure gradient as

$$\left(\frac{dP}{dx}\right)_{2\phi} = FWF(\alpha_f \rho_f v_f) + FWG(\alpha_g \rho_g v_g) \quad (3-234)$$

It should be noted that the calculation of the phasic friction factors using the Reynolds numbers given by Equation (3-229) and the assumption

that two-phase flows behave similarly to single-phase flows in the laminar, transition, and turbulent regimes provides the rationale relating Equations (3-230) and (3-231) to empirical data. It is this same rationale that allows expressing the correlating term, Z^2 , in terms of friction factors that are independent of interphase friction as given by Equation (3-227). It is this equation that forms the basis for apportioning the overall two-phase wall friction between the phases.

3.3.4.3 Apportioning Wall Friction. Overall two-phase wall friction can be apportioned into phasic components by combining Equations (3-232) and (3-233) with Equations (3-213) through (3-216) and (3-227), (3-230), and (3-231), which results in

$$\phi_f^2 \frac{\lambda'_f \rho_f (\alpha_f v_f)^2}{2D} - \frac{\alpha_{fw} \lambda_f \rho_f v_f^2}{\alpha_{gw} \lambda_g \rho_g v_g^2 + \alpha_{fw} \lambda_f \rho_f v_f^2} = FWF(\alpha_f \rho_f v_f) \quad (3-235)$$

for the liquid, and

$$\phi_g^2 \frac{\lambda'_g \rho_g (\alpha_g v_g)^2}{2D} - \frac{\alpha_{gw} \lambda_g \rho_g v_g^2}{\alpha_{gw} \lambda_g \rho_g v_g^2 + \alpha_{fw} \lambda_f \rho_f v_f^2} = FWG(\alpha_g \rho_g v_g) \quad (3-236)$$

for the vapor, where the two-phase multiplier terms are calculated using a two-phase friction multiplier correlation. Flow regime effects are also included in the relationships between wetted wall and overall void fractions and their effect in calculating the friction factor terms.

3.3.4.4 The H.T.F.S. Two-Phase Friction Multiplier Correlation. Only the H.T.F.S. correlation³⁻³¹ is used to calculate two-phase friction multipliers. This correlation was chosen because it is correlated to empirical data over very broad ranges of phasic volume fractions, phasic flow rates and phasic flow regimes. The correlation has also been shown to give good agreement with empirical data.

The H.T.F.S. correlation for the two-phase friction multiplier³⁻³¹ is expressed as

$$\phi_f^2 = 1 + \frac{C}{x} + \frac{1}{x^2} \quad (3-237)$$

for the liquid-alone multiplier, or

$$\phi_g^2 = x^2 + Cx + 1 \quad (3-238)$$

for the vapor-alone multiplier, where C is the correlation term and x is the Lockhart-Martinelli ratio given by Equation (3-221). The correlation term is expressed in terms of scalar mass flux, G , and the Baroczy dimensionless property index, Λ , such that

$$2 \leq C = -2 + f_1(G) T_1 \quad (3-239)$$

where

$$f_1(G) = 28 - 0.3\sqrt{G} \quad (3-240)$$

$$T_1 = \exp \left[- \frac{(\log_{10} \Lambda + 2.5)^2}{2.4 - G(10^{-4})} \right] \quad (3-241)$$

$$\Lambda = \frac{\rho_g}{\rho_f} \left(\frac{\mu_f}{\mu_g} \right)^{0.2} \quad (3-242)$$

$$G = \left| \alpha_f \rho_f v_f + \alpha_g \rho_g v_g \right| \quad (3-243)$$

The terms ρ , μ , α and v denote the density, viscosity, volume fraction and velocity, respectively.

If the H.L.F.S. correlation is combined with the wall friction formulations by combining Equations (3-213) through (3-216), (3-219) through (3-221), (3-237), and (3-238), then

$$\begin{aligned} \left(\frac{dP}{dx}\right)_{2\phi} &= \phi_f^2 \left(\frac{dP}{dx}\right)_f = \phi_g^2 \left(\frac{dP}{dx}\right)_g \\ &= \frac{1}{2D} \left[\lambda'_f \rho_f (\alpha_f v_f)^2 + C \sqrt{\lambda'_f \rho_f (\alpha_f v_f)^2 \lambda'_f \rho_f (\alpha_g v_g)^2} + \lambda'_g \rho_g (\alpha_g v_g)^2 \right] \end{aligned} \quad (3-244)$$

Equation (3-244) can then be combined with Equation (3-235) and (3-236) and simplified such that

$$\begin{aligned} FWF(\alpha_f \rho_f) &= \alpha_{fw} \frac{\rho_f \lambda_f |v_f|}{2D} \left[\lambda'_f \rho_f (\alpha_f v_f)^2 + C \sqrt{\lambda'_f \rho_f (\alpha_f v_f)^2 \lambda'_g \rho_g (\alpha_g v_g)^2} \right. \\ &\quad \left. + \lambda'_g \rho_g (\alpha_g v_g)^2 \right] / \left[\alpha_{gw} \lambda_g \rho_g v_g^2 + \alpha_{fw} \lambda_f \rho_f v_f^2 \right] \end{aligned} \quad (3-245)$$

for the liquid, and

$$\begin{aligned} FWG(\alpha_g \rho_g) &= \alpha_{gw} \frac{\rho_g \lambda_g |v_g|}{2D} \left[\lambda'_f \rho_f (\alpha_f v_f)^2 + C \sqrt{\lambda'_f \rho_f (\alpha_f v_f)^2 \lambda'_g \rho_g (\alpha_g v_g)^2} \right. \\ &\quad \left. + \lambda'_g \rho_g (\alpha_g v_g)^2 \right] / \left[\alpha_{gw} \lambda_g \rho_g v_g^2 + \alpha_{fw} \lambda_f \rho_f v_f^2 \right] \end{aligned} \quad (3-246)$$

for the vapor.

The friction factor and velocity terms are calculated in such a manner that, as the velocity terms disappear, the equations give the correct limits. For example, the friction factor terms are evaluated such that

$$\lim_{\left| \left(\frac{\alpha_f}{\alpha_{fw}} \right) v_f \right| \rightarrow 0} \left(\lambda_f \left| \left(\frac{\alpha_f}{\alpha_{fw}} \right) v_f \right| \right) = \frac{64 \mu_f}{D \rho_f} = \lim_{\left| \alpha_f v_f \right| \rightarrow 0} (\lambda'_f |\alpha_f v_f|) \quad (3-247)$$

$$\lim_{|(\frac{\alpha_g}{\alpha_{gw}})v_g| \rightarrow 0} (\lambda_g |(\frac{\alpha_g}{\alpha_{gw}})v_g|) = \frac{64\mu_g}{D\rho_g} = \lim_{|\alpha_g v_g| \rightarrow 0} (\lambda_g' |\alpha_g v_g|) \quad (3-248)$$

and the velocity terms are evaluated such that

$$\lim_{v_f \rightarrow 0} |v_f| = \epsilon = \lim_{v_g \rightarrow 0} |v_g| \quad (3-249)$$

Hence, for stagnant flow or single-phase conditions, a positive and finite friction coefficient is always calculated. Thus, the numerical possibility of an infinite or negative friction coefficient is eliminated.

In Equations (3-245) and (3-246), flow regime effects are included in the terms (α_{fw}/α_f) and (α_{gw}/α_g) for the liquid and vapor, respectively. These terms are such that

$$\alpha_{fw} = 1 - \alpha_{gw} \quad (3-250)$$

$$\alpha_f = 1 - \alpha_g \quad (3-251)$$

Equations (3-250) and (3-251) are restricted such that as overall phasic volume fraction disappears its corresponding wall film volume fraction disappears, so that

$$\lim_{\alpha_f \rightarrow 0} (\frac{\alpha_{fw}}{\alpha_f}) = 1, \quad \lim_{\alpha_g \rightarrow 0} (\frac{\alpha_{gw}}{\alpha_g}) = 1 \quad (3-252)$$

and similarly,

$$\lim_{\alpha_g \rightarrow 0} (\frac{\alpha_{gw}}{\alpha_g}) = 1, \quad \lim_{\alpha_f \rightarrow 0} (\frac{\alpha_{fw}}{\alpha_f}) = 1 \quad (3-253)$$

3.3.4.5 Flow Regime Factors for Phasic Wall Friction. Phasic wall friction is expressed in terms of wall shear stress, which, in turn, requires knowledge of the surface area wetted by each phase. From the flow regime model discussed in Section 3.3.1, expressions for the wall film phasic volume fractions can be derived. Using these expressions, the phasic wall friction factors that appear in Equations (3-224) and (3-225) may then be computed.

In the flow regime map, seven flow regimes are modeled, which are: for pre-CHF heat transfer, the bubbly, slug, and annular mist; for post-CHF heat transfer, the inverted-annular, inverted-slug and mist; and for stratified flow, the vertically and horizontally stratified. For the transition regime between pre- and post-CHF heat transfer, an interpolation scheme is also implemented in the code.

To implement flow regime effects in the two-phase wall friction model, first consider the wall liquid and vapor volume fractions. These terms are

$$\frac{p_f}{p} = \alpha_{fw} \quad (3-254)$$

which represents the liquid volume fraction in the wall film, and

$$\frac{p_g}{p} = \alpha_{gw} \quad (3-255)$$

which represents the vapor volume fraction in the wall film, where the terms p_f , p_g , and p are the perimeters wetted by the liquid, vapor, and mixture, respectively. Then, from the flow regime model, these are formulated for all of the flow regimes as follows:

For the bubbly regime,

$$\alpha_{fw} = \alpha_f \text{ and } \alpha_{gw} = \alpha_g \quad (3-256)$$

where α_f , α_g are the overall liquid vapor volume fraction, respectively.

For the slug regime,

$$\alpha_{fw} = 1 - \alpha_{gs} \text{ and } \alpha_{gw} = \alpha_{gs} \quad (3-257)$$

where α_{gs} is given by Equation (3-195).

For the annular-mist regime,

$$\alpha_{fw} = (\alpha_{ff})^{\frac{1}{4}} \text{ and } \alpha_{gw} = 1 - (\alpha_{ff})^{\frac{1}{4}} \quad (3-258)$$

where α_{ff} is given by Equation (3-190).

For the inverted-annular regime,

$$\alpha_{gw} = (\alpha_{gg})^{\frac{1}{4}} \text{ and } \alpha_{fw} = 1 - (\alpha_{gg})^{\frac{1}{4}} \quad (3-259)$$

where α_{gg} is the inverted form of Equation (3-190).

For the inverted-slug regime,

$$\alpha_{fw} = \alpha_{fs} \text{ and } \alpha_{gw} = 1 - \alpha_{fs} \quad (3-260)$$

where α_{fs} is the inverted form of Equation (3-185).

For the mist regime,

$$\alpha_{fw} = \alpha_f \text{ and } \alpha_{gw} = \alpha_g \quad (3-261)$$

similar to the bubbly regime.

For the vertically stratified regime,

$$\alpha_{fw} = \alpha_f \text{ and } \alpha_{gw} = \alpha_g \quad (3-262)$$

For the horizontally stratified regime,

$$\alpha_{fw} = 1 - \frac{\theta}{\pi} \text{ and } \alpha_{gw} = \frac{\theta}{\pi} \quad (3-263)$$

where θ results from the solution of Equations (3-173) and (3-174).

3.3.4.6 The Friction Factor Model. In SCDAP/RELAP5, the friction factor is computed using a high-speed calculational scheme representing an engineering approximation to the Colebrook correlation.³⁻³⁴

The friction factor model is simply an interpolation scheme linking the laminar, laminar-turbulent transition, and turbulent-full turbulent transition regimes. The laminar friction factor is calculated as

$$\lambda_L = \frac{64}{R}, \quad 0 \leq R \leq 2000 \quad (3-264)$$

where R is the Reynolds number. The laminar-turbulent friction factor is interpolated as

$$\lambda_{L,T} = [1.189 - (\frac{4000}{R})^{0.25}] (\lambda_{t,4000} - \lambda_{L,2000}) + \lambda_{L,2000}, \quad 2000 < R < 4000 \quad (3-265)$$

where $\lambda_{L,2000}$ is the laminar factor at a Reynolds number of 2000 and where $\lambda_{t,4000}$ is the turbulent friction factor at a Reynolds number of 4000. The interpolation factor is defined such that

$$0 \leq (2 - 4000/R) \leq 1 \quad (3-266)$$

The turbulent-full turbulent friction factor is interpolated as

$$\lambda_{t,tt} = \frac{[1 - (\frac{4000}{R})^{0.25}]}{[1 - (\frac{4000}{R_c})^{0.25}]} (\lambda_{tt} - \lambda_{t,4000}) + \lambda_{t,4000}, \quad 4000 \leq R \leq R_c \quad (3-267)$$

where the interpolation factor is defined such that

$$0 \leq \frac{[1 - (\frac{4000}{R})^{0.25}]}{[1 - (\frac{4000}{R_c})^{0.25}]} \leq 1 \quad (3-268)$$

and R_c is the critical Reynolds number at which the Colebrook equation gives a constant friction factor of

$$\lambda_{tt} = [1.74 - 2\log_{10}(2\epsilon/D)]^{-2} \quad (3-269)$$

and where ϵ is the surface roughness.

The critical Reynolds number is given as

$$R_c = \frac{378.3}{\frac{2\epsilon}{D} \sqrt{\lambda_{tt}}} \quad (3-270)$$

If precise values for $\lambda_{t,4000}$ are used, Equations (3-264) and (3-265) are identical to the formulations used in the Colebrook friction factor model for the laminar and transition regimes. Equation (3-269) is also identical to the solution of the Colebrook model for Reynolds numbers greater than the critical Reynolds number. Therefore, the interpolation scheme in the friction factor model lies in the formulation of Equation (3-267), which is linear in $(1/R)^{0.25}$. The maximum deviation between the friction factor calculated using Equation (3-267) and that calculated using the Colebrook correlation is

within the third significant figure for a moderate ϵ/D of 0.0003. As ϵ/D increases, the deviation decreases; until at an ϵ/D such that $R_c < 4000$, the value given by Equation (3-267) is precisely that of Equation (3-269). In any case, the results calculated using Equation (3-267) are negligibly different from those calculated by the Colebrook equation. This accuracy is achieved using a good estimate for $\lambda_{t,4000}$ given by

$$\lambda_{t,4000} \sim \lambda_0 + K(\lambda_{tt} - \lambda_1) \quad (3-271)$$

where λ_0 is a constant evaluated from the Blasius smooth-pipe formula at a Reynolds number of 4000, such that

$$\lambda_0 = 0.0398 \quad (3-272)$$

The coefficients have been evaluated as

$$K = 0.558, \lambda_1 = 0.0158$$

using the method of least squares.

It is desirable in calculational schemes, to evaluate the friction factor in terms of $\lambda|\psi v|$ so that the limiting terms will be correctly calculated as defined by Equation (3-248). For this case, the Reynolds number must be defined as

$$R = \frac{\rho D}{\mu} |\psi v| \quad ; \quad (3-273)$$

and Equation (3-267) can be rewritten as

$$\begin{aligned} \lambda|\psi v| = & \lambda_L^* + L(2 - R^*) \quad L[(1 - R^*)/(1 - R_c^*)] (\lambda_{tt} - \lambda_{t,4000})|\psi v| \\ & + \lambda_{t,4000}|\psi v| - \lambda_L^* \end{aligned} \quad (3-274)$$

where $L(y)$ denotes a general limit function such that

$$0 \leq L(y) \leq 1 \quad (3-275)$$

$$R^* = (4000/R)^{0.25}, \quad R_C^* = (4000/R_C)^{0.25} \quad (3-276)$$

$$R \geq 2000, \quad R_C \geq 4000 \quad (3-277)$$

and where the laminar term is

$$\lambda_L^* = \frac{64\mu}{\rho D} \quad (3-278)$$

The accuracy of the improved friction factor model can be observed in Figure 3-6, which is a plot of results calculated by Equation (3-274) compared to similar results calculated by the Colebrook equation. Four curves are plotted for each model, representing roughness-to-diameter ratios of $2\epsilon/D = 0.0, 0.0006, 0.02, \text{ and } 0.1$, respectively. Equation (3-274) results are labeled as INTERP in the plot legend. Colebrook equation results are labeled as COLBRK in the plot legend. The axes of the plot are scaled logarithmically.

3.3.5 Heat Transfer Models

A boiling curve is used in SCDAP/RELAP5 to govern the selection of heat transfer correlations. In particular, the heat transfer regimes modeled are classified as pre-CHF and post-CHF regimes. Condensation heat transfer is also modeled, and the effects of noncondensable gases are modeled. Figure 3-7 gives a chart of the logic scheme for selecting the heat transfer models.

The pre-CHF regime consists of models for single-phase liquid convection, subcooled nucleate boiling, and saturated nucleate boiling. The model assumes that the wall is totally wetted by liquid and that the

Figure 3-6. Comparison of friction factors for the Colebrook and the improved SCDAP/RELAP5 friction factor models.

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Figure 3-7. Logic chart for wall heat transfer regime selection.

wall is not wetted by vapor. Therefore, the heat transfer rate per unit volume from the wall to the vapor, Q_{wg} , is equal to zero. The heat transfer rate per unit volume from the wall to the liquid, Q_{wf} , is given by the expression

$$Q_{wf} = h_{wf} A_w (T_w - T_f) / V \quad (3-279)$$

where h_{wf} is the heat transfer coefficient, A_w is the total wall heat transfer area, and T_w and T_f are the wall and liquid temperatures, respectively. V is the volume of the fluid cell adjacent to the heat slab. The heat transfer coefficients used for this regime are the Dittus-Boelter³⁻³⁵ and the Chen³⁻³⁶ correlations for the single-phase liquid convective heat transfer and the nucleate boiling regimes, respectively. It should be noted that the Chen correlation is also extended into the subcooled boiling regime by setting the Reynolds number factor to one.

The post-CHF regime consists of models for transition film boiling, film boiling, and single-phase vapor convection. A mechanistic model developed by Tong and Young³⁻³⁷ is adapted so that

$$Q_{wf} = h_{wf} A_w F_f (T_w - T_f) / V \quad (3-280)$$

$$Q_{wg} = h_{wg} A_w (1 - F_f) (T_w - T_g) / V \quad (3-281)$$

where A_w is the total wall heat transfer area and F_f is the fraction of wall surface contacted by the liquid. The heat transfer correlation and the liquid contact area correlation developed by Chen³⁻³⁸ are used in both the transition film boiling and the film boiling regime. For single-phase vapor convective heat transfer, the wall is assumed to be dry and the heat transfer area between the wall and the liquid is negligible. Therefore, the heat transfer rate per unit volume from the wall to the liquid, Q_{wf} , is equal to zero; and the heat transfer rate per unit volume from the wall to the vapor, Q_{wg} , is given by the expression

$$Q_{wg} = h_{wg} A_w (T_w - T_g)/V \quad (3-282)$$

The Dittus-Boelter correlation is used for h_{wg} .

In the condensation regime, heat transfer to the wall from liquid and vapor is dependent on the flow regime. Heat transfer from liquid to the wall is modeled by convection in the low void regime, and heat transfer from vapor to the wall is modeled by condensation in the high void regime. The heat transfer rate per unit volume from liquid to the wall is given by

$$Q_{wf} = [(1 - \alpha_g) h_{\text{Dittus-Boelter}} (T_w - T_f)] A_w / V \quad (3-283)$$

where $h_{\text{Dittus-Boelter}}$ is the Dittus-Boelter correlation heat transfer coefficient. The heat transfer rate per unit volume from the vapor to the wall is modeled by condensation or convection and expressed as

$$Q_{wg} = [\alpha_g \min [h_{\text{con}} (T_w - T_{\text{sat}}), h_{\text{Dittus-Boelter}} (T_w - T_g)]] A_w / V \quad (3-284)$$

where h_{con} is the condensation heat transfer coefficient.

The correlations used to calculate wall heat transfer are summarized in Table 3-1.

3.3.6 Interphase Mass Transfer

The interface mass transfer is modeled according to the thermodynamic process, interphase heat transfer regime, and flow regime. After the thermodynamic process is decided, the flow regime map discussed in Section 3.3.1 is used to determine the phasic interfacial area and to select the interphase heat transfer correlation.

The mass transfer model is formulated so that the net interfacial mass transfer rate is composed of two components, the mass transfer rate at the wall and the mass transfer rate in the bulk fluid, and is expressed as

TABLE 3-1. SCDAP/RELAP5 HEAT TRANSFER

Single-Phase Forced Convection for Wall to Liquid, Liquid to Wall, Vapor to Wall, or Wall to Vapor: Dittus-Boelter³⁻³⁵

$$h = 0.023 \frac{k}{D_e} Pr^{0.4} Re^{0.8} ,$$

where the physical properties are evaluated at fluid temperature (T_f or T_g) and where

h = heat transfer coefficient ($W/m^2 \cdot K$)

k = thermal conductivity ($W/m \cdot K$)

D_e = equivalent diameter (m)

Pr = Prandtl number = $C_p \mu / k$

C_p = specific heat at constant pressure ($J/kg \cdot K$)

μ = viscosity ($kg/m \cdot s$)

G = mass flux ($kg/m^2 \cdot s$)

Re = Reynolds number = GD_e / μ .

For single-phase liquid,

$$Q_{wf} = h \cdot A_{wf} (T_w - T_f) / V$$

TABLE 3-1. (continued)

$$Q_{wg} = h \cdot A_{wg} (T_w - T_g)/V = 0 \quad ,$$

where

$$A_{wf} = A_w$$

$$A_{wg} = 0$$

$$Q_{wf} = \text{wall to liquid volumetric heat flux (W/m}^3\text{)}$$

$$Q_{wg} = \text{wall to vapor volumetric heat flux (W/m}^3\text{)}$$

$$A_w = \text{total wall heat transfer area (m}^2\text{)}$$

$$A_{wf} = \text{wall to liquid heat transfer area (m}^2\text{)}$$

$$A_{wg} = \text{wall to vapor heat transfer area (m}^2\text{)}$$

$$V = \text{hydraulic volume (m}^3\text{)}$$

$$T_w = \text{wall temperature (K).}$$

For single-phase vapor,

$$Q_{wf} = h \cdot A_{wf} (T_w - T_f)/V = 0$$

TABLE 3-1. (continued)

$$Q_{wg} = h \cdot A_{wg} (T_w - T_g)/V ,$$

where

$$A_{wf} = 0$$

$$A_{wg} = A_w .$$

Saturated Nucleate Boiling: Chen³⁻³⁶

$$h = h_{mic} + h_{mac} ,$$

where

$$h_{mic} = 0.00122 \frac{k_f^{0.79} C_{pf}^{0.45} \rho_f^{0.49}}{\sigma^{0.5} \mu_f^{0.29} h_{fg}^{0.24} \rho_g^{0.24}} \Delta T_{sat}^{0.24} \Delta p^{0.75} S$$

$$h_{mac} = 0.023 \frac{k_f}{D_e} (Pr)_f^{0.4} (Re)_f^{0.8} F$$

F = Reynolds number factor

$$F = \begin{cases} 1.0 & x_{tt}^{-1} \leq 0.10 \\ 2.35 (x_{tt}^{-1} + 0.213)^{0.736} & x_{tt}^{-1} > 0.10 \end{cases}$$

$$x_{tt}^{-1} = \left[\frac{\alpha_g \rho_g v_g}{(1-\alpha_g) \rho_f v_f} \right]^{0.9} \left(\frac{\rho_f}{\rho_g} \right)^{0.5} \left(\frac{\mu_g}{\mu_f} \right)^{0.1}$$

TABLE 3-1. (continued)

S = suppression factor

$$S = \left\{ \begin{array}{ll} 1.0 & \alpha_g \leq 0.3 \\ [1 + 0.12 (\text{Re}_{TP})^{1.14}]^{-1} & \text{Re}_{TP} < 32.5 \\ [1 + 0.42 (\text{Re}_{TP})^{0.78}]^{-1} & 32.5 \leq \text{Re}_{TP} < 70.0 \\ 0.0797 & \text{Re}_{TP} \geq 70 \\ \text{interpolates } S(\text{Re}_{TP}) \text{ on } \alpha_g & 0.3 < \alpha_g < 0.8 \end{array} \right\} \begin{array}{l} \alpha_g \leq 0.3 \\ \alpha_g \geq 0.8 \\ 0.3 < \alpha_g < 0.8 \end{array}$$

$$\text{Re}_{TP} = \left(\frac{v_f \rho_f \alpha_f D_e}{\mu_f} \right) F^{1.25} \times 10^{-4}$$

ρ = density (kg/m³)

σ = surface tension (N/m)

h_{fg} = latent heat of vaporization (J/kg)

ΔT_{sat} = $T_w - T_{\text{sat}}$

T_{sat} = saturation temperature (K)

ΔP = difference in vapor pressure corresponding to ΔT_{sat} (Pa)

v = velocity (m/s)

α_g = void fraction

TABLE 3-1. (continued)

f = saturated liquid condition (subscript)

g = saturated vapor condition (subscript).

$$Q_{wf} = h \cdot A_{wf} \cdot (T_w - T_f) / V$$

$$Q_{wg} = h \cdot A_{wg} \cdot (T_w - T_g) / V = 0 ,$$

where

$$A_{wf} = A_w$$

$$A_{wg} = 0 .$$

Subcooled Nucleate Boiling: Modified Chen³⁻³⁹

$$Q_{wf} = \left[h_{mic} \Delta T_{sat} + h_{mac} (T_w - T_f) \right] A_{wf} / V$$

$$Q_{wg} = h \cdot A_{wg} \cdot (T_w - T_g) / V = 0 ,$$

where

$$A_{wf} = A_w$$

$$A_{wg} = 0 .$$

The modified Chen correlation is obtained by setting $F = 1$ in h_{mac} and evaluating the properties at T_f .

TABLE 3-1. (continued)

Critical Heat Flux (CHF) Correlation:

1. High Flow CHF correlation: Biasi³⁻³⁹ (for mass flux (G) $\geq 200 \text{ kg/m}^2\cdot\text{s}$)

$$q_{\text{crit}} = \frac{1.883 \times 10^7}{D_e^n G^{1/6}} \left[\frac{f(P)}{G^{1/6}} - x_e \right] ,$$

for the low quality region,

$$q_{\text{crit}} = \frac{3.78 \times 10^7 h(P)}{D_e^n G^{0.6}} [1 - x_e] ,$$

for the high quality region,

where the maximum value of the above q_{crit} 's is used and

where

$$n = 0.4, \text{ for } D_e \geq 1 \text{ cm}$$

$$n = 0.6, \text{ for } D_e < 1 \text{ cm}$$

$$f(P) = 0.7249 + 0.099 P \exp(-0.032P)$$

$$h(P) = -1.159 + 0.149 P \exp(-0.019P) + 8.99P/(10 + P^2)$$

$$D_e = \text{hydraulic diameter (cm)}$$

$$P = \text{pressure (bar)}$$

$$x_e = \text{equilibrium equality}$$

TABLE 3-1. (continued)

q_{crit} = critical heat flux (W/m^2)

G = mass flux ($g/cm^2 \cdot s$) .

2. Low Flow CHF Correlation: Modified Zuber³⁻⁴⁰ (for $G \leq 100 \text{ kg/m}^2 \cdot s$)

$$q_{crit} = 0.131 h_{fg} \rho_g^{0.5} [\sigma g (\rho_f - \rho_g)]^{0.25} (1.00 - \alpha_g)$$

If mass flux, G , is between 100 and 200 ($kg/m^2 \cdot s$), a linear interpolation with respect to G is used to evaluate q_{crit} .

Transition Film Boiling: Chen³⁻³⁸

$$Q_{wf} = q_{crit} \cdot A_{wf}/V + q_{rad,f} (A_{wf})_{rad}/V ,$$

where

$$A_{wf} = A_w \cdot e^{-\lambda \Delta T_{sat}}$$

$$\lambda = \lambda_1 \text{ or } \lambda_2, \text{ whichever is greater}$$

where the exponential term is the liquid contact area weighting factor and where

$$\lambda_1 = C_1 - C_2 \cdot \frac{G}{10^5}$$

$$\lambda_2 = C_3 \cdot \frac{G}{10^5}$$

TABLE 3-1. (continued)

$$C_2 = \frac{0.05}{1 - \alpha_g} + 0.075\alpha_g$$

$$C_1 = 2.4 C_2$$

$$C_3 = 0.2 C_2$$

also,

$$q_{\text{rad},f} = \epsilon_f B(T_w^4 - T_s^4) \quad (\epsilon \text{ is the gray factor})$$

$$(A_{wf})_{\text{rad}} = A_w (1 - \alpha_g)$$

It should be noted that the Chen transition film boiling correlation is expressed here in British units.

$$Q_{wg} = q_{vc} A_{wg}/V + q_{\text{rad},g} (A_{wg})_{\text{rad}}/V,$$

where

$$q_{vc} = 0.023 \left(\frac{k_g}{D_e} \right) \left[\left(\frac{\rho_g v_g \alpha_g}{\mu_g} \right) D_e \right]^{0.8} (Pr)_g^{0.4} (T_w - T_g)$$

$$A_{wg} = A_w (1 - e^{-\lambda \sqrt{\Delta T_{\text{sat}}}})$$

$$q_{\text{rad},g} = \epsilon_g B(T_w^4 - T_g^4)$$

TABLE 3-1. (continued)

$$(A_{wg})_{rad} = A_w \cdot \alpha_g$$

$$B = \text{Stefan-Boltzmann constant.}$$

Film Boiling: Modified Bromley-Pomeranz³⁻⁴¹ and Dougall-Rohsenow³⁻⁴²

$$Q_{wf} = q_{film} \cdot A_{wf} / V ,$$

where

$$A_{wf} = (1 - \alpha_g) A_w$$

$$q_{film} = h_{Bromley} (\Delta T_{sat})$$

$$h_{Bromley-Pomeranz} = 0.620 \left(\frac{D_e}{\lambda_c} \right)^{0.25} \left[\frac{k_g^3 \rho_g (\rho_f - \rho_g) h'_{fg} g}{D_e \mu_g \Delta T_{sat}} \right]^{0.25}$$

$$h'_{fg} = h_{fg} + 0.5 (\rho_g (T_w - T_{sat}))$$

$$\lambda_c = 2\pi \left[\frac{\sigma}{g(\rho_f - \rho_g)} \right]^{0.5}$$

$$g = \text{acceleration due to gravity (m/s}^2\text{)}.$$

$$Q_{wg} = q_{DFG} \cdot A_{wg} / V + q_{rad,g} (A_{wg})_{rad} / V ,$$

where

$$A_{wg} = \alpha_g A_w$$

TABLE 3-1. (continued)

$$A_{wg,rad} = \alpha_g A_w$$

$$q_{DFG} = h_{\text{Dougall-Rohsenow}} (T_w - T_g)$$

$$h_{\text{Dougall-Rohsenow}} = 0.023 \frac{k_g}{D_e} \left\{ \frac{\rho_g [\alpha_g v_g + (1-\alpha_g) v_f] D_e}{\mu_g} \right\}^{0.8} \left[\frac{\mu_g (C_p)_g}{k_g} \right]^{0.4}$$

$$q_{rad,g} = \epsilon_g (T_w^4 - T_g^4).$$

Condensation heat transfer: (See Reference 3-39)

$$Q_{wf} = [(1 - \alpha_g) h_{\text{Dittus-Boelter}} (T_w - T_f)] A_w / V,$$

$$Q_{wg} = \left\{ \alpha_g \min [h_{\text{con}} (T_w - T_{\text{sat}}), h_{\text{Dittus-Boelter}} (T_w - T_g)] \right\} A_w / V.$$

where

$$h_{\text{con}} = \max \begin{cases} \frac{3}{4} (1.47) (Re)_f^{-0.333} \left[\frac{\rho_f (\rho_f - \rho_g) g}{\mu_f^2} \right]^{0.333} k_f & \text{(free flow condensation)} \\ 0.065 \frac{\rho_f^{0.5}}{\mu_f} (Pr)_f^{0.5} \tau_i^{0.5} k_f & \text{(free flow condensation)} \end{cases}$$

$$\tau_i = \frac{0.0792}{(Re)_g^{0.25}} \left(\frac{\rho_g v_g}{2} \right)^2$$

$$\Gamma_g = \Gamma_w + \Gamma_{ig} \quad .$$

(3-285)

For system components in which wall heat transfer is modeled, mass transfer at the wall is calculated according to the wall heat transfer model and mass transfer to the bulk fluid is calculated according to the interphase heat transfer regime and flow regime. For system components in which wall heat transfer is not modeled, mass transfer at the wall is ignored and mass transfer in the bulk fluid is modeled according to the interphase heat transfer regime and flow regime.

For components modeling wall heat transfer processes, the interfacial mass transfer at the wall is calculated from the total wall-to-liquid heat transfer minus the wall-to-liquid convective heat transfer. For these processes, the heat transfer model developed by Chen, as discussed in Section 3.3.5, is used to model the total wall-to-liquid heat transfer. The Chen model assumes that the total wall-to-liquid heat transfer is composed of boiling and convective heat transfer and that the interfacial mass transfer at the wall is mainly due to boiling heat transfer. Consequently, the contribution due to convective heat transfer must be subtracted from the total wall-to-liquid heat transfer in order to calculate the interfacial mass transfer at the wall. Correlations used to calculate interfacial mass transfer at the wall for different heat transfer regimes are summarized in Table 3-2.

For components not modeling wall heat transfer and for the general bulk mass transfer processes, the interfacial mass transfer in the bulk fluid is modeled according to the flow regime. In the bubbly flow regime, for the liquid side, interfacial mass transfer is the larger of either the model for bubble growth developed by Plesset and Zwick³⁻⁴³ or the model for convective heat transfer for a spherical bubble.³⁻⁴⁴ For the vapor side, an interphase heat transfer coefficient is assumed that is high enough to drive the vapor temperature toward saturation. Analogously, in the annular mist regime, for the vapor side, a convective heat transfer model for a spherical droplet is used for the interphase heat transfer coefficient. For the liquid side, an interphase heat transfer coefficient

TABLE 3-2. SCDAP/RELAP5 INTERFACIAL MASS TRANSFER AT WALL

Subcooled and Saturated Boiling Heat Transfer Regimes:

$$\Gamma_{wf} = \frac{Q_{wf} - Q_c}{h_{fg} [1 + C_{\rho f} (T_s - T_f) j_f / (\rho_g h_{fg})]^2}$$

$$\Gamma_{wg} = 0 ,$$

where

Q_{wf} is defined in Table 3-1 for corresponding regimes

and

$$Q_c = h_{mac} \cdot (T_w - T_f) \cdot A_w / V$$

$$h_{mac} = \text{convective part of the Chen correlation (see Table 3-1)}$$

$$h_{fg} = \text{specific latent heat (J/kg).}$$

Transition Film and Film Boiling Regimes:

$$\Gamma_{wf} = \frac{Q_{wf}}{h_{fg} (1 + 0.5 C_{pg} \cdot \Delta T_{sat} / h_{fg})}$$

$$\Gamma_{wg} = 0$$

Condensation Regime:

$$\Gamma_{wg} = \frac{Q_{wg}}{h_{fg} [1 + 0.375 C_{pg} (T_g - T_s) / h_{fg}]}$$

TABLE 3-2. (continued)

$$\Gamma_{wf} = 0$$

where

$$Q_c = (1 - \alpha_g) h_{\text{Dittus-Boelter}} (T_w - T_f) \cdot A_w / V .$$

is assumed that is high enough to drive the liquid temperature toward saturation. Correlations used to calculate interfacial mass transfer in the bulk fluid are summarized in Table 3-3.

For condensation processes, the interfacial mass transfer in the bulk fluid, for the liquid side, is calculated by the Unal bubble collapse model³⁻⁴⁵ in the bubbly flow regime and by the Brown droplet model³⁻⁴⁶ and Theofanous interfacial condensation model³⁻⁴⁷ in the annular mist flow regime. For the vapor side, a large interphase heat transfer coefficient is assumed in order to drive the vapor temperature toward saturation.

3.3.7 Reflood Heat Transfer

A special reflood model is designed to specifically analyze the reflood process, which occurs normally at low pressures and low mass flow rates. To increase computational efficiency in the nucleate boiling and transition boiling regimes, the heat transfer correlations known to apply for the reflood process are employed. These correlations and a model for radiation heat transfer are described in the following.

The wall temperature, T_{IB} , at the incipience of boiling is determined by a criterion developed by Bergles and Rohsenow³⁻⁴⁸ expressed in British units as

$$T_{IB} = T_{sat} + \left(\frac{q}{15.6 p^{1.156}} \right)^{\left(\frac{p^{0.0234}}{2.30} \right)} \quad (3-286)$$

where the heat flux, q , is computed from the Dittus-Boelter correlation for single-phase convection to liquid. For wall temperatures higher than that at the incipience of boiling, the heat flux is computed from the equation,

$$q = h_c (T_w - T_f) + h_{NB} (T_w - T_{sat}) \quad (3-287)$$

TABLE 3-3. SCDAP/RELAP5 INTERFACIAL MASS TRANSFER IN BULK FLUID

Depressurization Process ($T_f > T_{sat}$)

1. Bubbly flow regimes:

$$Q_{if} = H_{if} (T_s - T_f)$$

$$H_{if} = a_{gf_b} \frac{k_f}{d_b} Nu$$

$$Nu = \max \left\{ \begin{array}{l} \frac{12}{\pi} \Delta T_{sat} \frac{\rho_f (C_p)_f}{\rho_g h_{fg}} \quad (\text{Plesset-Zwick})^{3-43} \\ 2 + 0.74 Re_b^{0.5} \\ \quad \quad \quad (\text{Force convection for single bubble})^{3-37} \end{array} \right.$$

$$Re_b = \frac{\rho_f d_b |v_g - v_f|}{\mu_f} \quad (\text{Bubble Reynolds number})$$

$$a_{gf_b} = \text{interfacial area per unit volume for bubbles}$$

$$d_b = \text{bubble diameter (m)}$$

$$Q_{ig} = H_{ig} (T_s - T_g) ,$$

where

$$H_{ig} = a_{gf_b} \frac{k_g}{d_b} Nu_{ib}$$

$$Nu_{ib} = 10^4 .$$

TABLE 3-3. (continued)

2. Annular-mist flow regime:

$$Q_{if} = H_{if} (T_s - T_f) \quad ,$$

where

$$H_{if} = a_{gf_d} \frac{k_f}{d_d} Nu_{ib}$$

$$a_{gf_b} = \text{interfacial area per unit volume for bubbles}$$

$$Nu_{id} = 10^5$$

$$Q_{ig} = H_{ig} (T_s - T_g)$$

where

$$H_{ig} = \frac{a_{gf_d}}{d_d} \frac{k_g}{d_d} (2. + 0.74 Re_d^{0.5} Pr_g^{0.33})$$

$$+ 0.023 (Re)_g^{0.8} \cdot k_g \cdot \frac{(\alpha_g)^{0.5}}{D_h^2}$$

$$Re_d = \frac{\rho_g d_d |v_g - v_f|}{\mu_g} \quad (\text{Droplet Reynolds Number})$$

$$d_d = \text{drop diameter (m)}$$

$$d_h = \text{hydraulic diameter (m).}$$

TABLE 3-3. (continued)

Heat Transfer Process ($T_f \leq T_{sat}$)

1. Bubbly flow regime:

$$Q_{if} = H_{if} (T_s - T_f) ,$$

where

$$H_{if} = \frac{3\phi C h_{fg} \alpha_g}{\frac{1}{\rho_g} - \frac{1}{\rho_f}} \quad (\text{Unal's correlation})^{3-45}$$

$$\phi = \begin{cases} 1 & v_f \leq 0.61 \text{ (m/s)} \\ [1.639 v_f]^{0.47} & v_f > 0.61 \text{ (m/s)} \end{cases}$$

$$C = \begin{cases} 61 - 6.489 \times 10^{-5} (P - 1.7 \times 10^5) & P \leq 10^6 \text{ (Pa)} \\ 2.3 \times 10^9 / P^{1.418} & P > 10^6 \text{ (Pa)} \end{cases}$$

P = pressure (Pa) .

$$Q_{ig} = H_{ig} (T_s - T_g) ,$$

where

$$H_{ig} = a_{gf_b} \frac{\text{kg}}{\text{d}_b} \text{Nu}_{ib}$$

$$\text{Nu}_{ib} = 10^4 .$$

2. Annular-mist flow regime:

Same as the depressurization process.

TABLE 3-3. (continued)

Condensation Process

1. Bubbly flow regime:

Same as the heat transfer process.

2. Annular-mist flow regime:

$$Q_{if} = H_{if} (T_s - T_f) ,$$

where

$$H_{if} = 6 \left[2.0 + \frac{8.0(T_s - T_f)}{T_m - T_f} \right] k_f (1 - \alpha_g) / d_d^2 \\ + 10^{-3} \cdot \rho_f \cdot v_f \cdot C_{pf} \cdot A_{film}$$

A_{film} = area of film per unit volume

$$T_m = \frac{T_s - T_f}{1 + C_{pg}(T_g - T_s)/h_{fg}} .$$

The first term of right side uses the condensation of a single droplet in superheated steam model developed by Brown.^{3 46} The second term of right side uses the film condensation model developed by Theofanous.³⁻⁴⁷

$$Q_{ig} = H_{ig} (T_s - T_g) ,$$

where

$$H_{ig} = a_{gf} \frac{kg}{d_b} \cdot Nu_{id}$$

$$Nu_{id} = 10^5 .$$

where h_c is a Dittus-Boelter convective heat transfer coefficient and h_{NB} is a nucleate boiling heat transfer coefficient. The nucleate boiling heat transfer coefficient is obtained using the McAdams³⁻⁴⁹ nucleate boiling correlation for low pressures, for which

$$q_{NB} = h_{NB} (T_w - T_{sat}) = 2.253 (T_w - T_{sat})^{3.86} \quad (3-288)$$

Nucleate boiling prevails up to a temperature, T_{CHF} , at which the boiling heat flux is equal to the critical heat flux, q_{CHF} , where

$$h_{NB} (T_{CHF} - T_{sat}) = q_{CHF} \quad (3-289)$$

The critical heat flux, q_{CHF} , is calculated according to the modified Zuber correlation,^{3-50,51,52,53} expressed as

$$q_{CHF} = 0.131 (1 - \alpha_g) h_{fg} \left(\frac{\rho_g \rho_f}{\rho_f + \rho_g} \right)^{1/2} \left[\sigma g (\rho_f - \rho_g) \right]^{1/4} \\ \times \max \left\{ [1, (G/G_{ref})^{0.33}] \right\} \quad (3-290)$$

where G is mass flux and G_{ref} is a reference mass flux and is equal to $67.8 \text{ kg/m}^2 \cdot \text{s}$.

For wall temperatures higher than the temperature, T_{CHF} , the heat flux is computed using the equation

$$q = h_c (T_w - T_g) + h_{TB} (T_w - T_{sat}) \quad (3-291)$$

where the convective heat transfer coefficient, h_c , is of a Dittus-Boelter form given by the Dougall-Rohsenow correlation shown in Table 3-1. The transition boiling heat transfer coefficient, h_{TB} , is calculated using a correlation developed by Weisman,³⁻⁵¹ for which

$$h_{TB} = h_m \exp(-0.055\Delta T) + 4500 (G/G_{ref})^{0.2} \exp(-0.012\Delta T) \quad (3-292)$$

Here, h_m and ΔT are

$$h_m = q_{CHF} / \Delta T_m \quad (3-293)$$

and

$$\Delta T = T_w - T_{sat} - \Delta T_m \quad (3-294)$$

respectively, and where

$$\Delta T_m = S (q_{CHF} / 2.253)^{1/3.86} \quad (3-295)$$

The term, S , is Chen's boiling suppression factor, shown in Table 3-1.

The transition boiling and film boiling formulas intersect at a temperature, T_Q , which is called the rewetting or quench temperature. The quench temperature is currently computed using the formula

$$T_Q = (T_{CHF} + T_{sat})/2 + 125.0 \quad (3-296)$$

where T_{sat} is the saturation temperature at atmospheric pressure.

Equation (3-296) yields a value of about 520 K, which is close to the value of 260°C suggested by Arrieta and Yadigaroglu.³⁻⁵⁴

For film boiling, the heat transfer coefficient, h_{FB} , is obtained from

$$h_{FB} = \text{MAX} (h_{TB}, h_{FBB}) \quad (3-297)$$

Here, h_{TB} is defined by Equation (3-292) and h_{FBB} is given by the modified Bromley correlation³⁻⁵⁵ for which

$$h_{FBB} = 0.62 \left[\frac{k_g^3 \rho_g (\rho_f - \rho_g) h'_{fg} g}{\mu_g (T_w - T_{sat})} \frac{1}{2\pi} \sqrt{\frac{g (\rho_f - \rho_g)}{\sigma}} \right]^{0.25} \quad (3-298)$$

where

$$h'_{fg} = h_{fg} [1 + 0.68 C_{pv} (T_w - T_{sat})/h_{fg}] \quad (3-299)$$

and h_{fg} is the heat of vaporization. In Equations (3-298) and (3-299), all of the vapor properties are evaluated at the film temperature, $(T_w + T_{sat})/2$. Note also that the true quench temperature is implied by the minimum film boiling heat transfer coefficient given by Equation (3-250). The value of T_Q defined by Equation (3-296) is for convenience, and its value is not important in the calculated results as long as the actual quench temperature implied from Equation (3-297) is higher than T_Q from Equation (3-296).

At high wall temperatures, radiation heat transfer is treated using a model developed by Sun.³⁻⁵⁶ The model considers the vapor-droplet mixture as an optically thin medium and uses an electric network analogy to analyze the radiation energy exchange among the wall, the liquid droplets, and the vapor. The radiation fluxes are expressed as

$$q_{wf} = F_{wf} \sigma (T_w^4 - T_{sat}^4) , \quad (3-300)$$

$$q_{wg} = F_{wg} \sigma (T_w^4 - T_g^4) , \text{ and} \quad (3-301)$$

$$q_{gf} = F_{gf} \sigma (T_g^4 - T_{sat}^4) . \quad (3-302)$$

In Equations (3-300) through (3-302), the term σ is the Stefan-Boltzman constant, T_g is the vapor temperature, and F_{wf} , F_{wg} and F_{gf} are gray body factors for which

$$F_{wf} = 1/[R_2 (1 + R_3/R_1 + R_3/R_2)] \quad (3-303)$$

$$F_{wg} = 1/[R_1 (1 + R_3/R_1 + R_3/R_2)] \quad (3-304)$$

$$F_{gf} = 1/[R_2 (1 + R_1/R_2 + R_1/R_3)] \quad (3-305)$$

In Equations (3-303) through (3-305), the resistance terms in the electrical analogy are given as

$$R_1 = (1 - \epsilon_g)/[\epsilon_g (1 - \epsilon_g \epsilon_f)] \quad (3-306)$$

$$R_2 = (1 - \epsilon_f)/[\epsilon_f (1 - \epsilon_g \epsilon_f)] \quad (3-307)$$

$$R_3 = 1/(1 - \epsilon_g \epsilon_f) + (1 - \epsilon_w)/\epsilon_w \quad (3-308)$$

for which the emissivities are given as

$$\epsilon_g = 1 - \exp(-a_g L_m) \quad (3-309)$$

$$\epsilon_f = 1 - \exp(-a_f L_m) \quad (3-310)$$

$$\epsilon_w = 0.9 \quad (3-311)$$

where L_m is a mean length and a_g and a_f are vapor and liquid absorption coefficients, respectively. The mean length L_m is roughly equal to $0.9 D_{hy}$, where D_{hy} is the hydraulic diameter of the fluid channel. The absorption coefficient, a_f , for droplets is given by

$$a_f = 1.11 \alpha_f / D_d \quad (3-312)$$

where α_f is the liquid volume fraction and D_d is the droplet diameter. The absorption coefficient, a_g , for vapor³⁻⁵⁷ is given by

$$a_g = 1.8 \times 10^{-4} P (555.56/T_g)^2 [1 - 0.054(555.56/T_g)^2] \quad (3-313)$$

where P is pressure.

3.4 Special Process Models

Certain models in SCDAP/RELAP5 have been developed to simulate special processes. These models are described in the following subsections.

3.4.1 Choked Flow

A choked-flow model developed by Ransom and Trapp^{3-58,10} is included primarily for calculation of the mass discharge from the system at a pipe break or a nozzle. Generally, the flow at the break or nozzle is choked until the system pressure nears the containment pressure. The choked-flow model is used to predict if the flow is choked at break or nozzle and, if it is, to establish the discharge boundary condition. In addition, the choked-flow model can be used to predict existence of and calculate choked flow at internal points in the system.

Choking is defined as the condition wherein the mass flow rate becomes independent of the downstream conditions (that point at which further reduction in the downstream pressure does not change the mass flow rate). The fundamental reason that choking occurs is that acoustic signals can no longer propagate upstream. This occurs when the fluid velocity equals or exceeds the propagation velocity. The choked-flow model is based on a definition that is established by a characteristic analysis using time-dependent differential equations.

Consider a system of n first-order, quasi-linear, partial differential equations of the form

$$A(U) (\partial U / \partial t) + B(U) (\partial U / \partial x) + C(U) = 0 \quad (3-314)$$

The characteristic directions (or characteristic velocities) of the system are defined^{3-59,60} as the roots, $\lambda_i (i \leq n)$, of the characteristic polynomial

$$(A\lambda - B) = 0 \quad . \quad (3-315)$$

The real part of any root, λ_i , gives the velocity of signal propagation along the corresponding characteristic path in the space/time plane. The imaginary part of any complex root, λ_i , gives the rate of growth or decay of the signal propagating along the respective path. For a hyperbolic system in which all the roots of Equation (3-315) are real and nonzero, the number of boundary conditions required at any boundary point equals the number of characteristic lines entering the solution region as time increases. If we consider the system [Equation (3-313)] for a particular region $0 \leq x \leq L$ and examine the boundary conditions at $x = L$, as long as any λ_i are less than zero, we must supply some boundary information to obtain the solution. If λ_i are greater than or equal to zero, no boundary conditions are needed at $x = L$; and the interior solution is unaffected by conditions beyond this boundary.

A choked condition exists when no information can propagate into the solution region from the exterior. Such a condition exists at the boundary point, $x = L$, when

$$\lambda_j \geq 0 \text{ for all } j \leq n \quad . \quad (3-316)$$

These are the mathematical conditions satisfied by the equations of motion for a flowing fluid when reduction in downstream pressure ceases to result in increased flow rate. It is well-known³⁻⁶⁹ that the choked condition for single-phase flow occurs when the fluid velocity just equals the local sound speed. For this case, one of the λ_j 's is just equal to zero. For the two-phase case, it is possible for all λ_j 's to be greater than zero under special conditions which can exist during discharge of a subcooled liquid.

Extensive investigation was carried out to determine a two-phase choked-flow criterion under two assumed conditions:^a (a) thermal equilibrium between phases, and (b) adiabatic phases without phase change (frozen).³⁻⁶² The frozen assumption was in poor agreement with data, compared to the thermal equilibrium assumption. Therefore, the thermal equilibrium assumption with slip is used as the basis for the SCDAP/RELAP5 choked-flow criterion. In the following subsections, theoretical aspects of choked flow are discussed.

3.4.1.1 Choking Criterion for Nonhomogeneous, Equilibrium Two-Phase Flow. The two-fluid model for the conditions of thermal equilibrium (equilibrium interphase mass transfer) is described by the overall mass continuity equation, two-phasic momentum equations, and the mixture entropy equation. This system of equations is

$$\partial(\alpha_g \rho_g + \alpha_f \rho_f) / \partial t + \partial(\alpha_g \rho_g v_g + \alpha_f \rho_f v_f) / \partial x = 0 \quad (3-317)$$

$$\begin{aligned} & \alpha_g \rho_g [\partial v_g / \partial t + v_g (\partial v_g / \partial x)] + \alpha_g (\partial P / \partial x) \\ & + C \alpha_g \alpha_f \rho \left[(\partial v_g / \partial t + v_f (\partial v_g / \partial x) - \partial v_f / \partial t) - v_g (\partial v_f / \partial x) \right] = 0 \end{aligned} \quad (3-318)$$

$$\begin{aligned} & \alpha_f \rho_f [\partial v_f / \partial t + v_f (\partial v_f / \partial x)] + \alpha_f (\partial P / \partial x) \\ & + C \alpha_f \alpha_g \rho \left\{ [\partial v_f / \partial t + v_f (\partial v_g / \partial x) - \partial v_g / \partial t - v_f (\partial v_g / \partial x)] \right\} = 0 \end{aligned} \quad (3-319)$$

$$\partial(\alpha_g \rho_g S_g + \alpha_f \rho_f S_f) / \partial t + \partial(\alpha_g \rho_g S_g v_g + \alpha_f \rho_f S_f v_f) / \partial x = 0 \quad (3-320)$$

The momentum equations include the interphase force terms due to relative acceleration.³⁻⁸ These force terms have a significant effect on

a. The hydrodynamic model is not based on either of these assumptions. However, the purpose of this analysis is simply to establish a criterion for a choked flow; thus, there is no conflict with the basic hydrodynamic model.

wave propagation velocity and consequently on the choked flow velocity. The particular form chosen is frame invariant and symmetrical; and the coefficient of virtual mass, $C\alpha_g\alpha_f\rho$, is chosen to ensure a smooth transition between pure vapor and pure liquid. For a dispersed flow, the constant, C , has a theoretical value of 0.5; whereas for a separated flow, the value may approach zero. The energy equation is written in terms of mixture entropy, which is constant for adiabatic flow. (The energy dissipation associated with interphase mass transfer and relative phase acceleration is neglected.)

The nondifferential source terms, $C(U)$, in Equation (3-314) do not enter into the characteristic analysis or affect the propagation velocities. For this reason, the source terms associated with wall friction, interphase drag, and heat transfer are omitted for brevity in Equations (3-317) through (3-320).

In the thermal equilibrium case, ρ_g , ρ_f , S_g , and S_f are known functions of the pressure only (the vapor and liquid values along the saturation curve). The derivatives of these variables are designated by an asterisk as follows

$$\rho_f^* = d\rho_f^S/dP, \quad \rho_g^* = d\rho_g^S/dP \quad (3-321)$$

$$S_f^* = dS_f^S/dP, \quad S_g^* = dS_g^S/dP \quad . \quad (3-322)$$

The system of governing equations [Equations (3-317) through (3-320)] can be written in terms of the four dependent variables, α_g , P , v_g , and v_f , by application of the chain rule and the property derivatives [Equations (3-321) and (3-322)]. Thus, the system of equations can be written in the form of Equation (3-314) where the A and B are fourth-order square coefficient matrices.

The characteristic polynomial that results is fourth-order in λ , and factorization can only be carried out approximately to obtain the roots for λ and establish the choking criterion. The first two roots are

$$\lambda_{1,2} = \frac{\left\{ \alpha_f \rho_g + \rho C/2 \pm \left[(\rho C/2)^2 - \alpha_g \alpha_f \rho_g \rho_f \right]^{1/2} \right\} v_g + \left\{ \alpha_g \rho_f + \rho C/2 \pm \left[(\rho C/2)^2 - \alpha_g \alpha_f \rho_g \rho_f \right]^{1/2} \right\} v_f}{(\alpha_f \rho_g + \rho C/2) + (\alpha_g \rho_f + \rho C/2)} \quad (3-323)$$

These two roots are obtained by neglecting the fourth-order factors relative to the second-order factors in $(\lambda - v_g)$ and $(\lambda - v_f)$. There are no first- or third-order factors. Inspection of Equation (3-323) shows that $\lambda_{1,2}$ have values between v_g and v_f ; thus, the fourth-order factors, $(\lambda - v_g)$ and $(\lambda - v_f)$, are small (i.e., neglecting these terms is justified). The values for $\lambda_{1,2}$ may be real or complex depending on the sign of the quantity $[(\rho C/2)^2 - \alpha_g \alpha_f \rho_g \rho_f]$.

The remaining two roots are obtained by dividing out the quadratic factor containing $\lambda_{1,2}$, neglecting the remainder, and factoring the remaining quadratic terms. [This procedure can be shown to be analogous to neglecting the second- and higher-order terms in the relative velocity, $(v_g - v_f)$.] The remaining roots are

$$\lambda_{3,4} = v + D(v_g - v_f) \pm a \quad (3-324)$$

where

$$v = (\alpha_g \rho_g v_g + \alpha_f \rho_f v_f) / \rho \quad (3-325)$$

$$a = a_{HE} \left\{ \left[C \rho^2 + \rho(\alpha_g \rho_f + \alpha_f \rho_g) \right] / (C \rho^2 + \rho_g \rho_f) \right\}^{1/2} \quad (3-326)$$

and

$$D = 0.5 \left[\frac{(\alpha_g \rho_f - \alpha_f \rho_g)}{(\rho C + \alpha_f \rho_g + \alpha_g \rho_f)} + \frac{\rho_g \rho_f (\alpha_f \rho_f - \alpha_g \rho_g)}{\rho \rho_g \rho_f + C \rho^2} - a_{HE}^2 \frac{\rho (\alpha_g \rho_g^2 S_g^* + \alpha_f \rho_f^2 S_f^*)}{\rho_g \rho_f (S_g - S_f)} \right] \quad (3-327)$$

The quantity, a_{HE} , is the homogeneous equilibrium speed of sound. The roots, $\lambda_{3,4}$, have only real values.

The general nature and significance of these roots is revealed by applying the characteristic considerations. The speed of propagation of small disturbances is related to the values of the characteristic roots. In general, the velocity of propagation corresponds to the real part of a root, and the growth or attenuation is associated with the complex part of the root. Choking will occur when the signal, which propagates with the largest velocity relative to the fluid, is just stationary, i.e.,

$$\lambda^R = 0 \text{ for } j \leq 4 \quad (3-328)$$

and

$$\lambda^R \geq 0 \text{ for all } i \neq j \quad (3-329)$$

The existence of complex roots for $\lambda_{1,2}$ makes the initial boundary value problem ill-posed. This problem has been discussed by many investigators,^{3-5,12} and the addition of any small, second-order viscous effects renders the problem well-posed.^{3-5,13} The whole phenomenon of systems with mixed orders of derivatives and a first-order system with the addition of a small, second-order term has been discussed and analyzed by Whitham.³⁻⁶⁰ He has shown that the second-order viscous terms give infinite characteristic velocities. However, very little information is propagated along these characteristic lines; and the bulk of the information is propagated along characteristic lines defined by the first-order system. We conclude that the ill-posed nature of Equations (3-317) through (3-320) can be removed by the addition of small, second-order viscous terms that have little effect upon the propagation of information. Therefore, the choking criterion for the two-phase flow system analyzed here is established from Equation (3-328).

The explicit character of the choking criterion for the two-phase flow model defined by Equations (3-317) through (3-320) is examined. Since the

two roots, $\lambda_{1,2}$, are between the phase velocities, v_f and v_g , the choking criterion is established from the roots, $\lambda_{3,4}$, and Equation (3-328). The choking criterion is

$$v + D(v_g - v_f) = \pm a \quad (3-330)$$

The choking criterion can be rewritten in terms of the mass mean and relative Mach numbers

$$M_v = v/a, \quad M_r = (v_g - v_f)/a \quad (3-331)$$

as

$$M_v + DM_r = \pm 1 \quad (3-332)$$

This relation is similar to the choking criterion for single-phase flow where only the mass average Mach number appears and choking corresponds to a Mach number of unity.

The choking criterion [Equation (3-332)] is a function of the two parameters, D and a . In Figure 3-8, a is plotted as a function of the void fraction, α_g , for a typical steam/water system at 7.5 MPa, with C equal to zero (the stratified equilibrium sound speed), C equal to 0.5 (the typical value for a dispersed flow model), and in the limiting case when C becomes infinite (homogeneous equilibrium sound speed). From Figure 3-8, it is evident that the virtual mass coefficient has a significant effect upon the choked-flow dynamics in two-phase flow.³⁻⁶

To establish the actual choked-flow rate for two-phase flow with slip, the relative velocity term in Equation (3-332) must also be considered. The relative Mach number coefficient, D , is shown plotted in Figure 3-9 for values of C equal to 0, 0.5 and infinity. It is evident from these results that the choked-flow velocity can differ appreciably from the mass mean velocity when slip occurs. It is significant that the variation of the

Figure 3-8. Equilibrium speed of sound as a function of void fraction and virtual mass coefficient.

Figure 3-9. Coefficient of relative Mach number for thermal equilibrium flow as a function of void fraction and virtual mass coefficient.

choked-flow criterion from the homogeneous result is entirely due to velocity nonequilibrium, since these results have been obtained under the assumption of thermal equilibrium. The particular values of these parameters used in the model are further discussed later in this section.

3.4.1.2 Subcooled Choking Criterion. The previous analysis assumes two-phase conditions exist throughout the break flow process. However, initially and in the early phase of blowdown, the flow approaching the break or break nozzle will be subcooled liquid. Under most conditions of interest in LWR systems, the fluid undergoes a phase change at the break. The transition from single- to two-phase flow is accompanied by a discontinuous change in the fluid bulk modulus. This is especially true for the liquid-to-liquid/vapor transition. For example, at 600 KPa, the ratio of the single- to two-phase sound speed at the liquid boundary is 339.4. Thus, considerable care must be exercised when analyzing a flow having transitions to or from a pure phase. (A discontinuity is also present at the vapor boundary, but the ratio is only 1.069.)

To understand the physical process that occurs for subcooled upstream conditions, consider the flow through a converging/diverging nozzle connected to an upstream plenum with subcooled water at a high pressure. For a downstream pressure only slightly lower than the upstream pressure, subcooled liquid flow will exist throughout the nozzle. Under these conditions, the flow can be analyzed using Bernoulli's equation, which predicts a minimum pressure, P_t , at the throat.^a As the downstream pressure is lowered further, a point is reached where the throat pressure equals the local saturation pressure, P_{sat} . If the downstream pressure is lowered further, vaporization will take place at the throat.^b When

a. For all practical cases of choking, the subcooled water can be considered incompressible with infinite sound speed.

b. An idealized one-dimensional homogeneous equilibrium model is assumed in the example.

this happens, the fluid sound speed lowers drastically; but continuity considerations dictate that the velocity, v_t , of the two-phase mixture (at the point of minuscule void fraction) just equals the velocity of the subcooled water slightly upstream of the throat. When this occurs, v_t in the subcooled region is less than the water sound speed; but in the two-phase region, v_t can be greater than the two-phase sound speed. Hence, the subcooled water has a Mach number (M) less than one, whereas the two-phase mixture at the throat has a Mach number greater than one. Under these conditions (Mach numbers greater than one in the two-phase region), downstream pressure effects are not propagated upstream and the flow is choked. In particular, the supersonic two-phase fluid at the throat must increase in velocity and the pressure must drop as it expands in the diverging section.^a (Transition back to subsonic flow can occur in the nozzle as a result of a shock wave.) The choked condition is shown in Figure 3-10a. Contrary to the usual single-phase choked flow in a converging/diverging nozzle, there is no point in the flow field where $M = 1$. This is because in the homogeneous equilibrium model the fluid undergoes a discontinuous change in sound speed from single-phase subcooled conditions to two-phase conditions, although the fluid properties are continuous through the transition point.

When this condition prevails, the flow rate can be established from application of Bernoulli's equation ($1/2 \rho v_t^2 = P_{up} - P_{sat}$). For further decrease in the downstream pressure, no further increase in upstream fluid velocity will occur as long as the upstream conditions are maintained constant.

Now consider the process where a subcooled choked flow, as described above, initially exists (with a very low downstream pressure) and the upstream pressure is lowered. As the upstream pressure decreases, the pressure at the throat will remain at P_{sat} , and Bernoulli's equation will give a smaller subcooled water velocity (v_t) at the throat. As P_{up} is

a. In a supersonic flow, a diverging nozzle implies an increase in velocity.

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Figure 3-10. Subcooled choking process.

lowered further, a point is reached where $v_t = a_{HE}$ and $M = 1$ on the two-phase side of the throat. (The Mach number in the subcooled portion upstream of the throat is much less than one.) This situation is shown schematically in Figure 3-10b.

As the upstream pressure is lowered further, the point where the pressure reaches P_{sat} must move upstream of the throat [see Figure 3-10c]. The subcooled water velocity at the P_{sat} location is smaller than the two-phase sound speed, and the flow is subsonic. In the two-phase region between the point at which P_{sat} is reached and the throat, the Mach number is less than 1 but increases to $M = 1$ at the throat; that is, the two-phase sonic velocity is reached at the throat (as in the case of choked flow having a continuous variation of sound speed with pressure). As P_{up} is lowered still further, the P_{sat} point moves upstream until the flow becomes completely two-phase.

The homogeneous assumption applied in the above subcooled choking description is very close to the real situation when vapor is first formed. However, nonequilibrium can result in a superheated liquid state at a throat pressure, P_t , much lower than the saturation pressure, P_{sat} . The onset of vaporization occurs at P_t instead of P_{sat} .

The pressure undershoot, $P_{sat} - P_t$, can be described by the Alamgir-Lienhard-Jones correlation^{3-63,64,65}

$$P_{sat} - P_t = \max (\Delta P, 0) \quad (3-333)$$

with

$$\Delta P = 0.258 \sigma^{3/2} T_R^{13.76} \left(1 + 13.25 \sum^{0.8} \right)^{1/2} / \left[(k_B T_c)^{1/2} (1 - v_f/v_g) \right] \\ - 0.07 (A_t/A)^2 (\rho v_c^2) \quad (3-334)$$

The first term in ΔP represents the static depressurization effect and is derived by Alamgir and Lienhard³⁻⁶⁴ based on classical nucleation theory. For a steady flow in a nozzle, the depressurization rate, Σ' , can be shown to be

$$\Sigma = \left(\rho v_c^3 / A_t \right) (dA/dx)_t \quad (3-335)$$

Note that in Equation (3-334) Σ' is in units of Matm/s, but in Equation (3-335) Σ' is in units of Pa/s. Here, $(dA/dx)_t$ is the variation of area with respect to axial length and is to be evaluated at the throat. The second term in ΔP [Equation (3-335)] represents the turbulence effect and is developed by Jones.³⁻⁶⁵

The choking velocity, based upon the process shown in Figure 3-10a, can be calculated by applying Bernoulli's equation

$$v_c = \left[v_{up}^2 + 2 (P_{up} - P_t) / \rho \right]^{1/2} \quad (3-336)$$

where P_t is to be computed from Equation (3-333).

For the process shown in Figures 3-10b and 3-10c,

$$v_c = a_{HE} \quad (3-337)$$

and the two-phase choking criterion applies.

To determine which of the above situations exists, both v_c 's are calculated and the larger is used as the choking velocity to be imposed at the throat. This velocity is imposed numerically at the throat in exactly the same manner as the choking criterion used for the two-phase condition described previously.

The subcooled choking model is very similar in concept to the model proposed by Burnell³⁻⁶⁶ in that both models assume a Bernoulli expansion to the point of vapor inception at the choke plane. The criterion for transition from subcooled choking to two-phase choking is now better understood and is in agreement with the physics of two-phase flow. The model here is also in agreement with cavitating venturi experience (experimentally confirmed behavior). The SCDAP/RELAP5 subcooled choking model is somewhat different than the model proposed by Moody³⁻⁶⁷ in that the Moody model assumes that an isentropic process occurs to the choke plane.

3.4.1.3 Horizontal Stratified Choked Flow. Under stratified conditions, the void fraction of the flow out of a small break may be quite different from the upstream void fraction. The usual definition of the outlet void fraction as a donored void fraction is no longer applicable. A simple approach based on the height of the liquid level and a criterion for the stability of small disturbances are used to determine the junction void fraction for stratified break flow.

By balancing the upward pressure force due to the Bernoulli effect and the downward gravitational force acting on a small surface perturbation, Taitel and Dukler³⁻¹⁹ developed the following criterion for transition from the stratified horizontal flow regime in a round pipe:

$$v_g > \left[\frac{(\rho_f - \rho_g) B_y A_g}{\rho_g dA_f / dH_f} \right]^{1/2} \left(1 - \frac{H_f}{D} \right) . \quad (3-338)$$

In the code, Equation (3-338) is modified to use $v_g - v_f$ rather than v_g . This was implemented to handle the situation where the flow is stratified but the liquid is flowing. In addition, stratification can exist only when the mass flux G is less than $3000 \text{ kg/m}^2\text{-s}$.

In Equation (3-338), A_g and A_f are the flow areas of vapor and liquid, respectively. The right side of Equation (3-338) is the limiting

vapor velocity, designated by v_{gL} . The following geometrical relationships define H_g and H_f :

$$H_g = D (1 - \cos\theta)/2 \quad (3-339)$$

and

$$H_f = D (1 + \cos\theta)/2 \quad (3-340)$$

where θ is the central angle formed by a vertical cord and a radius to the liquid vapor interface. It can be shown that dA_f/dH_f equals $D \sin \theta$; hence, v_{gL} becomes

$$v_{gL} = 1/2 \left[\frac{(\rho_f - \rho_g) B_y \alpha_g A}{\rho_g D \sin \theta} \right]^{1/2} (1 - \cos \theta) \quad (3-341)$$

Let D_t be the diameter of the break area. When the liquid level is above the break [that is, $H_f > (D + D_t)/2$], the outlet void fraction, $\alpha_{g,j}$, which accounts for the pull-through of vapor, is defined as

$$\alpha_{g,j} = \alpha_{g,K} (v_g/v_{gL})^{1/2} \quad (3-342)$$

where $\alpha_{g,K}$ and v_g are the void fraction and vapor velocity upstream of the outlet. If the liquid level falls below the break [that is, $H_f < (D - D_t)/2$], liquid entrainment is modeled by defining the outlet liquid fraction, $\alpha_{f,j}$, as

$$\alpha_{f,j} = \alpha_{f,K} (v_g/v_{gL})^{1/2} \quad (3-343)$$

where $\alpha_{f,K}$ is the liquid volume fraction upstream of the outlet. The equality, $\alpha_{g,j} + \alpha_{f,j} = 1$ is used to obtain $\alpha_{g,j}$ ($\alpha_{f,j}$), if $\alpha_{f,j}$ ($\alpha_{g,j}$) is known. When the liquid level lies within the outlet

area [that is, $(D + D_t)/2 > H_f > (D - D_t)/2$], the void fraction is obtained by interpolation of the two void fractions computed at the boundaries.

3.4.1.4 Implementation of Choked Flow Model. Ideally, the two-phase choking criterion [Equation (3-330)] can be used as a boundary condition for obtaining flow solutions. However, the applicability of Equation (3-330) has not been fully explored. Instead, an approximate criterion

$$(\alpha_g \rho_f v_g + \alpha_f \rho_g v_f) / (\alpha_g \rho_f + \alpha_f \rho_g) = \pm a_{HE} \quad (3-344)$$

has been applied extensively and has produced good code/data comparisons. Equation (3-344) can be derived from Equation (3-330) by neglecting the third term in D and setting $C = 0$ (stratified) on the left side of Equation (3-330) and $C = \infty$ (homogeneous) on the right side. Because of extensive experience with this approximate model, Equation (3-344) is currently used in SCDAP/RELAP5 choked-flow calculations.

At each time step and at each flow junction where two-phase cocurrent flow exists, the choking criterion [Equation (3-344)] is checked using explicitly calculated values. When choking occurs, Equation (3-344) is solved semi-implicitly with the upstream vapor and liquid momentum equations for v_g , v_f , and P_t , throat pressure, at the point of flow choking (upstream with reference to v_g and v_f). As P_t is not needed in system calculations, we can eliminate $\partial P / \partial x$ from the vapor and liquid momentum equations to obtain

$$\begin{aligned} & \rho_g (\partial v_g / \partial t + 1/2 \partial v_g^2 / \partial x) - \rho_f (\partial v_f / \partial t + 1/2 \partial v_f^2 / \partial x) \\ &= (\rho_g - \rho_f) B_x + \Gamma_g (v_I - \alpha_f v_g - \alpha_g v_f) / \alpha_f \alpha_g \\ & - \rho_g v_g^{FWG} + \rho_f v_f^{FWF} - \rho_f \rho_g (v_g - v_f) FI \end{aligned}$$

$$- C \rho \partial(v_g - v_f)/\partial t \quad (3-345)$$

The finite-difference form of this equation is obtained by integrating with respect to the spatial variable from the upstream volume center to the junction. In this finite-difference equation, all junction velocities are evaluated implicitly; $a_{HE,j}^{n+1}$ is approximated by

$$a_{HE,j}^{n+1} \approx a_{HE,j}^n + (\partial a_{HE}/\partial P)_j^n (P_k^{n+1} - P_k^n) \quad (3-346)$$

where P_k is the upstream volume pressure. The finite-difference equations corresponding to Equations (3-344) and (3-345) can be solved for $v_{g,j}^{n+1}$ and $v_{f,j}^{n+1}$ in terms of P_k^{n+1} and old time values.

In the case of subcooled choking, the choking criterion [Equation (3-344)] and the velocity equation [Equation (3-345)] reduce to

$$v_f = v_g = \pm v_c \quad (3-347)$$

Here, v_c is determined according to the procedures described previously. The frictional pressure losses and gravity head, which do not appear in ideal Equation (3-336), are properly taken into account in the actual calculation.

In general, there is a large drop in critical velocity when the fluid changes from a subcooled state to a two-phase state. This sudden change often leads to unrealistic velocity oscillations and causes the time step size to be reduced considerably. To provide a smooth transition from subcooled to two-phase, a transition region is defined as in the low void region. Within the transition region, an underrelaxation scheme,

$$\begin{aligned} v_{g,j}^{n+1} &\rightarrow v_{g,j}^n + 0.1 \left(v_{g,j}^{n+1} - v_{g,j}^n \right) \\ v_{f,j}^{n+1} &\rightarrow v_{f,j}^n + 0.1 \left(v_{f,j}^{n+1} - v_{f,j}^n \right) \end{aligned} \quad (3-348)$$

is implemented. Experience with this scheme indicates that it works satisfactorily.

3.4.2 Horizontal Stratification Entrainment Model

Under stratified conditions in horizontal components, the void fraction of flow through a junction may be different from the upstream volume void fraction. Consequently, the regular donoring scheme for junction void fraction is no longer appropriate because vapor may be pulled through the junction and liquid may also be entrained and pulled through the junction. The correlations describing the onset of vapor pull-through and liquid entrainment for various geometrical conditions were summarized by Zuber.³⁻⁶⁹

The condition for the onset of liquid entrainment is determined by the criterion that

$$v_g \geq v_{ge} \quad (3-349)$$

where v_{ge} is given by the expressions

$$v_{ge} = 5.7 \left(\frac{D - \ell\ell}{d} \right)^{3/2} \left[\frac{B_y (\rho_f - \rho_g) (D - \ell\ell)}{\rho_g} \right]^{1/2} \quad (3-350)$$

for an upwardly oriented (top) junction³⁻⁷⁰ and

$$v_{ge} = 3.25 \left(\frac{D/2 - \ell\ell}{d} \right)^2 \left[\frac{B_y (\rho_f - \rho_g) (D/2 - \ell\ell)}{\rho_g} \right]^{1/2} \quad (3-351)$$

for a centrally oriented (side) junction.^{3-71,72} In these expressions, $\ell\ell$ is the liquid level.

The condition for the onset of vapor pull-through is determined by the criterion

$$v_f \geq v_{fp} \quad (3-352)$$

where v_{fp} is given by the expression

$$v_{fp} = 3.25 \left(\frac{22 - D\zeta/2}{d} \right)^{5/2} \left[\frac{B_y (\rho_f - \rho_g)d}{f \rho} \right]^{1/2} \quad (3-353)$$

and where

$\zeta = 1$ for a centrally located or side junction, and

$\zeta = 0$ for a downward-oriented junction. ^{3-72,73}

Equations (3-349) through (3-353), together with the horizontal stratification criterion [Equation (3-171)] from Section 3.3.1], form the basis for calculating the junction void fraction under stratification conditions.

For liquid entrainment, the junction liquid fraction, $\alpha_{f,j}$, is related to the donor volume liquid fraction, $\alpha_{f,K}$, by the expression

$$\alpha_{f,j} = \alpha_{f,K} \left[1 - \exp \left(-C_1 v_g / v_{ge} - 12 v_g^2 / v_{gL}^2 \right) \right] \quad (3-354)$$

where v_{gL} is from Equation (3-172). For vapor pull-through, the junction void fraction, $\alpha_{g,j}$, is given by the expression

$$\alpha_{g,j} = \alpha_{g,K} \left[1 - \exp \left(-C_2 v_f / v_{fp} - 12 v_g^2 / v_{gL}^2 \right) \right] \quad (3-355)$$

The constants C_1 and C_2 for Equations (3-354) and (3-355) are obtained by comparisons of code calculations with experimental data. ^{3-74,75,76}

Currently, $C_1 = 1$ for a top junction, $C_1 = 20.1$ for a side junction, $C_2 = 1$ for a bottom junction, and $C_2 = 2.01$ for a side junction.

3.4.3 Abrupt Area Change

The general reactor system contains piping networks with many sudden area changes and orifices. To apply the SCDAP/RELAP5 hydrodynamic model to such systems, analytical models for these components have been developed.³⁻⁷⁷ The basic hydrodynamic model is formulated for slowly varying (continuous) flow area variations; therefore, special models are not required for this case.

The abrupt area change model, discussed here and developed in detail in Reference 3-77, is based on the Bourda-Carnot³⁻⁷⁸ formulation for a sudden enlargement and standard pipe flow relations, including the vena-contracta effect for a sudden contraction or an orifice or both. Quasi-steady continuity and momentum balances are employed at points of abrupt area change. The numerical implementation of these balances is such that hydrodynamic losses are independent of upstream and downstream nodalization. In effect, the quasi-steady balances are employed as jump conditions that couple fluid components having abrupt changes in cross-sectional area. This coupling process is achieved without change to the basic linear semi-implicit numerical time-advancement scheme.

3.4.3.1 Abrupt Area Change Modeling Assumptions. The basic assumption used for the transient calculation of two-phase flow in flow passages with points of abrupt area change is: the transient flow process can be approximated as a quasi-steady flow process that is instantaneously satisfied by the upstream and downstream conditions (that is, transient inertia, mass, and energy storage are neglected at abrupt area changes). However, the upstream and downstream flows are treated as fully transient flows.

There are several bases for the above assumption. A primary consideration is that available loss correlations are based on data taken during steady flow processes; however, transient investigations³⁻⁷⁹ have verified the adequacy of the quasi-steady assumption. The volume of fluid and associated mass, energy, and inertia at points of abrupt area change is

generally small compared with the volume of upstream and downstream fluid components. The transient mass, energy, and inertia effects are approximated by lumping them into upstream and downstream flow volumes. Finally, the quasi-steady approach is consistent with modeling of other important phenomena in transient codes (that is, heat transfer, pumps, and valves).

3.4.3.2 Review of Single-Phase Abrupt Area Change Models. The modeling techniques used for dynamic pressure losses associated with abrupt area change in single-phase flow are reviewed briefly before discussing the extension of these methods to two-phase flows. In a steady incompressible flow, losses at an area change are modeled by the inclusion of an appropriate dynamic head loss term, h_L , in the one-dimensional modified Bernoulli equation

$$(v^2/2 + P/\rho)_1 = (v^2/2 + P/\rho)_2 + h_L \quad (3-356)$$

The particular form of the dynamic head loss is obtained by employing the Bourda-Carnot³⁻⁷⁸ assumption for calculating losses associated with the expansion part of the flow process. Losses associated with the contracting part of the flow process are small relative to the expansion losses and are neglected.

The most general case of an abrupt area change is a contraction with an orifice at the point of contraction. Such a configuration is shown in Figure 3-11. Three area ratios are used throughout this development. The first is the contraction area ratio at the vena-contracta relative to the minimum physical area, $\epsilon_c = A_c/A_1$. The second is the ratio of the minimum physical area to the upstream flow area, $\epsilon_1 = A_1/A_1$. The third is the ratio of the downstream to upstream area, $\epsilon = A_2/A_1$.

The loss associated with the contracting fluid stream from Station 1 to c (the point of vena-contracta) is neglected. (Measurements indicate that the contracting flow experiences a loss no larger than $\Delta P_f \sim 0.05 (1/2 \rho v_c^2)$ where v_c is the velocity at the vena-contracta.] The dynamic

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Figure 3-11. Orifice at abrupt area change.

pressure loss associated with the expansion from the vena-contracta to the downstream section is given by

$$\Delta P_f = 1/2 \rho (1 - A_c/A_2)^2 v_c^2 \quad (3-357)$$

The contraction ratio, $\epsilon_c = A_c/A_T$, is an empirical function of $\epsilon_T = A_T/A_1$. The function is $\epsilon_c = 0.62 + 0.38 (\epsilon_T)^3$. Using the continuity equations,

$$v_c = \frac{A_T v_T}{A_c} = v_T / \epsilon_c \quad \text{and} \quad v_T = \frac{A_2 v_2}{A_1} = \frac{\epsilon}{\epsilon_T} v_2, \quad \text{Equation (3-357) can be written as}$$

$$\Delta P_f = 1/2 \rho \left(1 - \frac{\epsilon}{\epsilon_c \epsilon_T} \right)^2 v_2^2 \quad (3-358)$$

Equation (3-358) is applicable to all the cases of interest. For a pure expansion, $\epsilon_T = 1$, $\epsilon_c = 1$, and $\epsilon > 1$; for a contraction, $\epsilon_T = \epsilon < 1$ and $\epsilon_c < 1$. Each of these is a special case of Equation (3-358). The two-phase dynamic pressure loss model is based on an adaptation of the general single-phase head loss given by Equation (611).

3.4.3.3 Two-Phase Abrupt Area Change Model. The two-phase flow through an abrupt area change is modeled in a manner very similar to that for single-phase flow by defining phasic flow areas. The two phases are coupled through the interphase drag, a common pressure gradient, and the requirement that the phases coexist in the flow passage.

The one-dimensional phasic stream-tube momentum equations are given in Section 3.1.1. The flow at points of abrupt area change is assumed to be quasi-steady and incompressible. In addition, the terms in the momentum equations due to body force, wall friction, and mass transfer are assumed to be small in the region affected by the area change. The interphase drag terms are retained, since the gradient in relative velocity can be large at points of abrupt area changes.

Equations (3-5) and (3-6) can be integrated approximately for a steady incompressible, smoothly varying flow to obtain modified Bernoulli-type equations

$$\begin{aligned} \left(\frac{1}{2} \rho_f v_f^2 + p \right)_1 &= \left(\frac{1}{2} \rho_f v_f^2 + p \right)_2 + \left(\frac{FI'}{\alpha_f} \right)_1 (v_{f1} - v_{g1}) L_1 \\ &+ \left(\frac{FI'}{\alpha_f} \right)_2 (v_{f2} - v_{g2}) L_2 \end{aligned} \quad (3-359)$$

and

$$\begin{aligned} \left(\frac{1}{2} \rho_g v_g^2 + p \right)_1 &= \left(\frac{1}{2} \rho_g v_g^2 + p \right)_2 + \left(\frac{FI'}{\alpha_f} \right)_1 (v_{g1} - v_{f1}) L_1 \\ &+ \left(\frac{FI'}{\alpha_f} \right)_2 (v_{g2} - v_{f2}) L_2 \end{aligned} \quad (3-360)$$

where $FI' = \alpha_f \alpha_g \rho_f \rho_g FI$. The interphase drag is divided into two parts associated with the upstream and downstream parts of the flow affected by the area change.

3.4.3.4 General Model. Consider the application of Equations (3-359) and (3-360) to the flow of a two-phase fluid through a passage having a generalized abrupt area change (the flow passage shown in Figure 3-12a). Here, the area A_T is the throat or minimum area associated with an orifice located at the point of the abrupt area change. Since each phase is governed by a modified Bernoulli-type equation, it is reasonable to assume that losses associated with changes in the phasic flow area can be modeled by separate dynamic pressure loss terms for both the liquid and gas phases. Hence, we assume that the liquid sustains a loss as if it alone (except for interphase drag) were experiencing an area change from $\alpha_{f1} A_1$ to $\alpha_{fT} A_T$ to $\alpha_{f2} A_2$; and the gas phase experiences a loss as

Figure 3-12. Schematic flow of two-phase mixture at abrupt area change.

if it alone were flowing through an area change from $\alpha_{g1} A_1$ to $\alpha_{g1} A_1$ to $\alpha_{g2} A_2$. The area changes for each phase are the phasic area changes (see Figure 3-12). When the losses for these respective area changes [based on the Bourda-Carnot model and given by Equation (3-358)] are added to Equations (3-359) and (3-360), the following phasic momentum equations are obtained:

$$\begin{aligned} \left(\frac{1}{2} \rho_f v_f^2 + p \right)_1 &= \left(\frac{1}{2} \rho_f v_f^2 + p \right)_2 + \frac{1}{2} \rho_f \left(1 - \frac{\alpha_{f2} \epsilon}{\alpha_{f1} \epsilon_{fc} \epsilon_T} \right)^2 (v_{f2})^2 \\ &+ \left(\frac{FI'}{\alpha_f} \right)_1 (v_{f1} - v_{g1}) L_1 + \left(\frac{FI'}{\alpha_f} \right)_2 (v_{f2} - v_{g2}) L_2 \quad (3-361) \end{aligned}$$

and

$$\begin{aligned} \left(\frac{1}{2} \rho_g v_g^2 + p \right)_1 &= \left(\frac{1}{2} \rho_g v_g^2 + p \right)_2 + \frac{1}{2} \rho_g \left(1 - \frac{\alpha_{g2} \epsilon}{\alpha_{g1} \epsilon_{gc} \epsilon_T} \right)^2 (v_{g2})^2 \\ &+ \left(\frac{FI'}{\alpha_g} \right)_1 (v_{g1} - v_{f1}) L_1 + \left(\frac{FI'}{\alpha_g} \right)_2 (v_{g2} - v_{f2}) L_2 \quad (3-362) \end{aligned}$$

These phasic momentum equations are used across an abrupt area change. In Equations (3-361) and (3-362), ϵ_{fc} and ϵ_{gc} are the same tabular function of area ratio as in the single-phase case except the area ratios used are the phasic area ratios

a. In Figure 3-12, the flow is shown as a separated flow for clarity. The models developed are equally applicable to separated and dispersed flow regimes.

$$\epsilon_{fT} = (\alpha_{fT}/\alpha_{f1}) \epsilon_T \quad (3-363)$$

and

$$\epsilon_{gT} = (\alpha_{gT}/\alpha_{g1}) \epsilon_T \quad (3-364)$$

respectively. The area ratios, $\epsilon = A_2/A_1$ and $\epsilon_T = A_T/A_1$, are the same as for single-phase flow.

The interphase drag effects in Equations (3-361) and (3-362) are important. These terms govern the amount of slip induced by an abrupt area change; and, if they are omitted, the model will always predict a slip at the area change appropriate to a completely separated flow situation and give erroneous results for a dispersed flow.

3.4.3.5 Model Application. A few remarks concerning the way Equations (3-361) and (3-362) are applied to expansions and contractions, both with and without an orifice, are necessary. In a single-phase steady flow situation, given the upstream conditions, v_1 and P_1 , using the continuity equation ($v_1 A_1 = v_2 A_2$) and Equation (3-356) one can solve for v_2 and P_2 . Equations (3-361) and (3-362,) along with the two phasic continuity equations, can be used in a similar manner except now that the downstream void fraction is an additional unknown which must be determined.

3.4.3.5.1 Expansion--For the purpose of explanation, consider the case of an expansion ($\alpha_{fT} = \alpha_{f1}$, $\epsilon > 0$, $\epsilon_T = 1$, $\epsilon_{fc} = \epsilon_{gc} = 1$, $FI'_1 = 0$, $L_1 = 0$) for which Equations (3-361) and (3-362) reduce to

$$\begin{aligned} \left(\frac{1}{2} \rho_f v_f^2 + P \right)_1 &= \left(\frac{1}{2} \rho_f v_f^2 + P \right)_2 + \frac{1}{2} \rho_f \left(1 - \frac{\alpha_{f2} \epsilon}{\alpha_{f1}} \right)^2 (v_{f2})^2 \\ &+ \left(\frac{FI'}{\alpha_f} \right)_2 (v_{f2} - v_{g2}) L_2 \end{aligned} \quad (3-365)$$

and

$$\begin{aligned} \left(\frac{1}{2} \rho_g v_g^2 + P \right)_1 &= \left(\frac{1}{2} \rho_g v_g^2 + P \right)_2 + \frac{1}{2} \rho_g \left(1 - \frac{\alpha_{g2} \epsilon}{\alpha_{g1}} \right)^2 (v_{g2})^2 \\ &+ \left(\frac{FI'}{\alpha_g} \right)_2 (v_{g2} - v_{f2}) L_2 \quad . \end{aligned} \quad (3-366)$$

These two equations with the incompressible continuity equations

$$\alpha_{f1} v_{f1} A_1 = \alpha_{f2} v_{f2} A_2 \quad (3-367)$$

and

$$\alpha_{g1} v_{g1} A_1 = \alpha_{g2} v_{g2} A_2 \quad (3-368)$$

are a system of four equations having four unknowns, α_{f2} ($\alpha_{g2} = 1 - \alpha_{f2}$), v_{f2} , v_{g2} , and P_2 , in terms of the upstream conditions, α_{f1} ($\alpha_{g1} = 1 - \alpha_{f1}$), v_{f1} , v_{g1} , and P_1 . (The interphase drag, FI' , is a known function of the flow properties.) It is important to note that the downstream value of the liquid fraction (α_{f2}) is an additional unknown compared with the single-phase case and is determined (with the downstream velocities and pressure) by simultaneous solution of Equations (3-365), through (3-368), without additional assumptions. It is reassuring that by taking a proper linear combination of Equations (3-361) and (3-362) the usual overall momentum balance obtained using the Bourda-Carnot³⁻⁷⁸ assumption can be obtained.^{3-80,81}

If, as in the cited literature,^{3-80,81,82,83} only the overall momentum balance is used at an expansion, there will be an insufficient number of equations to determine all the downstream flow parameters, α_{f2} , v_{f2} , v_{g2} , and P_2 . The indeterminacy has been overcome in cited works by means of several different assumptions concerning the downstream void fraction.^a In the model developed here [Equations (3-365) and (3-366)], division of the overall loss into liquid and gas parts, respectively, results in sufficient conditions to determine all downstream flow variables, including α_{f2} . In addition, the present model includes force terms due to interphase drag in Equations (3-365) and (3-366), which are necessary to predict the proper amount of slip and void redistribution that occurs at points of area change.

3.4.3.5.2 Contraction--Consider the application of Equations (3-364) and (3-365) to a contraction. To determine both the downstream conditions and throat conditions from the upstream values of α_{f1} (α_{g1}), v_{f1} , v_{g1} , and P_1 , an additional consideration needs to be made. To obtain the throat values, apply the momentum equations valid for the contracting section of flow. (Here, the L_1 portion of the interphase force is associated with the contraction.)

$$\left(\frac{1}{2} \rho_f v_f^2 + P \right)_1 = \left(\frac{1}{2} \rho_f v_f^2 + P \right)_T + \left(\frac{F I'}{\alpha_f} \right)_1 (v_{f1} - v_{g1}) L_1 \quad (3-369)$$

$$\left(\frac{1}{2} \rho_g v_g^2 + P \right)_1 = \left(\frac{1}{2} \rho_g v_g^2 + P \right)_T + \left(\frac{F I'}{\alpha_f} \right)_1 (v_{g1} - v_{f1}) L_1 \quad (3-370)$$

$$\alpha_{f1} v_{f1} A_1 = \alpha_{fT} v_{fT} A_T \quad (3-371)$$

$$\alpha_{g1} v_{g1} A_1 = \alpha_{gT} v_{gT} A_T \quad (3-372)$$

a. J. G. Collier³⁻⁸⁰ mentions three different assumptions that have been used: (i) $\alpha_{f2} = \alpha_{f1}$, (ii) α_{f2} is given by a homogeneous model, and (iii) α_{f2} is given by the Hughmark void fraction correlation.

These four equations are solved simultaneously for the values of $\alpha_{fT}(\alpha_{gT})$, v_{fT} , v_{gT} , P_T at the throat section (the minimum physical area). No additional or special assumptions are made concerning the throat conditions, since they follow as a direct consequence of the unique head loss models for each phase. After the throat values have been obtained, the conditions, at the point of vena-contracta are established, assuming the void fraction is the same as at the throat. Thus, ϵ_{fc} and ϵ_{gc} are established using the tabular function in Appendix A of Reference 3-77 and the throat area ratios, ϵ_{fT} and ϵ_{gT} , defined by Equations (3-363) and (3-364). To determine the downstream values, Equations (3-361) and (3-362) can be applied directly from Stations 1 to 2 with the throat values known, or the expansion loss equations can be used from the throat section to Station 2. Both approaches produce identical downstream solutions. As in the case of an expansion, because the proper upstream and downstream interphase drag is included, this modeling approach establishes the phase slip and resulting void redistribution. An orifice at an abrupt area change is treated exactly as the contraction explained above (that is, with two separate calculations to establish first the throat and then the downstream flow variables).

3.4.3.5.3 Countercurrent Flow--The preceding development implicitly assumed a cocurrent flow. For countercurrent flow, Equations (3-361) and (3-362) are applied exactly as in cocurrent flow except that the upstream sections for the respective phases are located on different sides of the abrupt area change. The difference appears in how the throat and downstream voids are determined. To determine the throat properties, equations similar to Equations (3-369) through (3-372) are used with the upstream values appropriate for each phase. These four equations are then solved for $\alpha_{fT}(\alpha_{gT})$, v_{fT} , v_{gT} , and P_T . To determine the downstream values for each phase, only the head loss terms are needed for the downstream voids. (The downstream v_f , v_g , and P do not appear.) For countercurrent flow, these voids are set such that the downstream void of each phase plus the upstream void of the opposite phase adds to one. (Both phases together must fill the flow channel.) With the

throat and downstream voids now known, Equations (3-361) and (3-362) can be used directly to determine the total loss for each phase at the abrupt area change.

3.4.4 Crossflow Junction

The SCDAP/RELAP5 numerical scheme is generally formulated using one-dimensional elements. However, there are several applications where an approximate treatment of crossflow provides an improved physical simulation. Three different applications for a crossflow formulation are described in the following paragraphs.

The first application concerns a small crossflow between two essentially axial flow streams. This situation is typical of regions such as a reactor core or a steam generator, because the component geometry provides a large resistance to crossflow and a small resistance to axial flow. Hence, simplified crossflow momentum equations can be used to couple a hot flow channel to a bulk flow channel.

The second application of a crossflow junction is to provide a tee model. In this case, the momentum flux in the side branch is assumed to be perpendicular to the main stream; thus, the main stream momentum flux does not contribute to the crossflow momentum formulation.

The third application is modeling of leak flow paths. In this case, the flow is small and governed primarily by pressure differential, gravity, and flow resistance. Thus, the momentum flux terms can be neglected.

The vapor momentum finite difference equation used in the basic numerical scheme is

$$\begin{aligned}
 & (\alpha_g \rho_g)_j^n (v_g^{n+1} - v_g^n)_j \Delta x_j^n + \frac{1}{2} (\alpha_g \rho_g)_j^n [(v_g^2)_L^n - (v_g^2)_K^n] \Delta t + \text{VISCOUS TERMS} \\
 & = - \alpha_{g,j}^n (p_L^{n+1} - p_K^{n+1}) \Delta t
 \end{aligned}$$

$$\begin{aligned}
& - (\alpha_g \rho_g)_j^n \left[(FWG_K^n + FWG_L^n) \Delta x_j + HLOSSG_j^n \right] v_{g,j}^{n+1} \Delta t \\
& - (\alpha_g \rho_g)_j^n FIG_j^n (v_{g,j}^{n+1} - v_{f,j}^{n+1}) \Delta x_j \Delta t + (\alpha_g \rho_g)_j^n B_x \Delta x_j \Delta t \\
& + \text{ADDED MASS} + \text{MASS TRANSFER MOMENTUM} \\
& + \text{HORIZONTAL STRATIFIED PRESSURE GRADIENT EFFECT} \tag{3-373}
\end{aligned}$$

where

$$\Delta x_j = \frac{1}{2}(\Delta x_K + \Delta x_L) \quad . \tag{3-374}$$

A parallel equation holds for the liquid phase. It should be noted that the momentum Equation (3-373) is in reality the sum of half the K cell momentum plus half the L cell momentum. This is the reason for Equation (3-374).

There are two areas in which the crossflow modeling affects the numerical scheme. One concerns the approximations made in the junction momentum equations, and the other concerns the volume average velocities in a volume.

If the junction is to model crossflow perpendicular to the main or axial flow direction, then the volume average velocity in the K and L cells, which represents the axial flow velocity, should not include crossflow junction velocity components. For the simple leak flow situation shown in Figure 3-13, this requires that $v_{j,3}$ not be included in the volume average (axial) velocity calculation for the L cell.

The second area of numerical modification relates to the reduced form of the momentum equations to be used at a crossflow junction. In crossflow junctions, just as in the normal junctions, the cross product momentum flux terms are neglected, i.e., there is no x-direction transport of momentum due to the y velocity.

EC000083

Figure 3-13. Simplified tee crossflow.

For the case of a small crossflow junction between two axial flow streams (J2 in Figure 3-14) all the geometric input (AVOL, DX, DZ) for both of the volumes relates to the axial flow direction, as do the wall drag and code-calculated form losses. Since the crossflow has a different flow geometry and resistance (for example, crossflow resistance in a rod bundle), the friction and form losses must be user-specified and must be appropriate for the crossflow direction geometry. For crossflow junctions, the user-specified form losses should include all crossflow resistance (form losses and wall drag). The normal terms representing wall drag and abrupt area change losses are not included in the formulation of the momentum equation at a crossflow junction, as these refer to the axial properties of the K and L volumes.

Since the connecting K and L volumes are assumed to be predominantly axial flow volumes, the crossflow junction momentum flux (related to the axial volume velocity in K and L) is neglected along with the associated numerical viscous term. In addition, the horizontal stratified pressure gradient is neglected.

All lengths and elevation changes in the one-dimensional representation are based upon the axial geometry of the K and L volumes, and the crossflow junction is assumed to be perpendicular to the axial direction and of zero elevation change. Thus, no gravity force term is included.

The resulting vapor momentum finite difference equation for a crossflow junction is

$$\begin{aligned}
 (\alpha_g \rho_g)_j^n (v_g^{n+1} - v_g^n)_j \Delta x_j = & - \alpha_{g,j}^n (P_L - P_K)^{n+1} \Delta t - (\alpha_g \rho_g)_j^n HLOSSG_j^n v_{g,j}^{n+1} \Delta t \\
 & - (\alpha_g \rho_g)_j^n FIG_j^n (v_{g,j}^{n+1} - v_{f,j}^{n+1}) \Delta x_j \Delta t \\
 & + \text{ADDED MASS} + \text{MASS TRANSFER MOMENTUM} .
 \end{aligned}
 \tag{3-375}$$

A similar equation can be written for the liquid phase. In

EC000084

Figure 3-14. Modeling of crossflows or leak.

Equation (3-375), $HLOSS_j^n$ contains only the user-specified crossflow resistance. The Δx_j term that is used to estimate the inertial length associated with crossflow is defined using the diameters of volumes K and L,

$$\Delta x_j = \frac{1}{2} [D(K) + D(L)] \quad . \quad (3-376)$$

The crossflow option can be used with the crossflow junction perpendicular to the axial flow in volume L (or K) but parallel to the axial flow in volume K (or L) (see Figure 3-13). Here, the situation regarding the half cell momentum contribution in volume L is the same as described above. The half cell momentum contribution associated with volume K is the same as for a normal junction. Hence, this crossflow junction has all the terms in Equation (3-373) except that; (a) wall friction, momentum flux, and gravity only include the K cell contribution; (b) the $HLOSS_j^n$ term is only the user-specified loss; and (c) the Δx used in the inertial term and interphase drag includes the normal K cell contribution and a term of the form in Equation (3-376) for the L cell. This type of crossflow modeling can be used for a 90-degree tee simulation.

For leak flows and minor flow paths, the modeling approach shown in Figure 3-15 is recommended. Here, J_3 is the normal flow path, whereas junction J_1 , volume M, and junction J_2 represent the leak flow path. Junctions J_1 and J_2 should be modeled as tee junctions described above. The only reason for using volume M is to obtain a correct representation of the gravity head from K to L. If a crossflow junction were modeled directly between volumes K and L, then there would be no gravity head in the leak flow junction equation. Leak paths may also be modeled using a crossflow junction that is perpendicular to both the K and L volumes when the leak flow is between volumes having the same volume center elevation.

3.4.5 Vertical Stratification Model

The vertical stratification model has been installed so that the nonequilibrium modeling capability can include repressurization transients

EC000085

Figure 3-15. Leak flow modeling.

in which subcooled liquid and superheated vapor may coexist in the pressurizer and/or other locations in the primary coolant system. A preliminary version³⁻⁸⁴ of this model has been modified, and this modified version is described in this section.

For this model, a vertically stratified flow regime is included in the vertical flow regime map, as shown in Figure 3-4. A vertical volume is detected as being vertically stratified when the difference between the void fraction in the volume above and that in the volume below is >0.5 and if the magnitude of the volume mixture mass flux is less than the Taylor bubble rise velocity³⁻²⁰ mass flux. The Taylor bubble criterion is based on the Taylor bubble velocity given by Equation (3-158) such that

$$|G| < \rho V_{Tb} \quad (3-377)$$

where V_{Tb} is the Taylor bubble velocity and $|G| = |\alpha_g \rho_g V_g + \alpha_f \rho_f V_f|$.

If Equation (3-377) is false and the void fraction difference is <0.5 , then the vertical stratification model is not used and the normal vertical flow regime map is used. If Equation (3-377) is true and the void fraction difference is ≥ 0.5 , then a linear interpolation is used between the normal flow regime values and the vertical stratification flow regime values for the interphase mass transfer, wall heat transfer, and the interphase drag coefficients.

For a vertically stratified volume, the interphase mass transfer, wall heat transfer, and interphase drag coefficients are modified. The interphase mass transfer is given in terms of the interphase heat transfer [see Equation (3-25)]. The interphase heat transfer rate per unit volume (neglecting contribution from the wall) is given as

$$Q_{if} = h_{if} \frac{A_c}{V} (T^s - T_f) \quad (3-378)$$

$$Q_{ig} = h_{ig} \frac{A_c}{V} (T^s - T_g) \quad (3-379)$$

where h_{if} and h_{ig} are the liquid side and vapor side interface heat transfer coefficients, A_c is the cross-sectional flow area (equal to the interfacial area when stratified), and V is the volume. The values for h_{if} and h_{ig} used in the vertical stratification model are $h_{if} = 14.7 k_f$ and $h_{ig} = 81.4 k_g$. The wall heat transfer coefficients, h_{wf} , and h_{wg} , are partitioned with respect to their corresponding vapor and liquid fractions (α_f and α_g) when vertical stratification occurs. For the junction above the vertically stratified volume, the interphase drag coefficient for the volume above is used.

There is no specific edit information output for a vertically stratified volume.

3.4.6 Water Packing Mitigation Scheme

Large pressure spikes that cannot be explained by known physical phenomena are at times encountered when Eulerian-type codes are used to analyze integral systems tests or reactor accidents. These spikes usually do not affect overall transient behavior but, in some cases, may affect important localized behavior (e.g. delivery of coolant to the reactor core). A water packing scheme has been installed to mitigate these spikes.

The water packing scheme closely follows the method used in the TRAC code.^{3-85,86} It involves a detection scheme to determine when a pressure change occurs in a volume containing mostly liquid. It then imposes changes to the momentum equations, followed by a recalculation of the pressure solution using the sparse matrix solver.

The detection logic used in the water packing scheme evolved from experience gained in running a vertical fill problem.³⁻⁸⁷ The scheme requires a pressure increase of 0.23% or more, a void fraction (α_g) ≤ 0.12 , the liquid temperature (T_f) to be less than the saturation temperature (T^s), the volume to be flagged as vertically stratified, and the volume above to be highly voided. Thus a legitimate water hammer would not be detected in the water packing scheme.

The next part of the scheme involves altering the momentum equations so that only small pressure changes will occur in the volume that fills with water. The scheme involves modifying the coefficient that multiplies the pressure change in the filling volume. The modification multiplies this coefficient by 10^6 and is discussed in more detail in the next paragraph. Since the pressure solution is rejected when water packing occurs, the pressure calculation is repeated using the sparse matrix solver.

The finite difference form of the phasic momentum equations used can be written

$$v_{f,j}^{n+1} = v_{f,j}^{n,exp} - (VFDP)_j^n \left[(P_L^{n+1} - P_L^n) - (P_K^{n+1} - P_K^n) \right] \quad (3-380)$$

$$v_{g,j}^{n+1} = v_{g,j}^{n,exp} - (VGDP)_j^n \left[(P_L^{n+1} - P_L^n) - (P_K^{n+1} - P_K^n) \right] \quad (3-381)$$

where $v_{f,j}^{n,exp}$ and $v_{g,j}^{n,exp}$ contain all the old time terms and $(VFDP)_j^n$ and $(VGDP)_j^n$ contain all the terms that multiply the pressure change. Consider the filling example in Figure 3-16 where volume K is full of liquid and volume L is full of steam. The change to the momentum equations is to multiply the $(P_K^{n+1} - P_K^n)$ terms by 10^6 , which forces P_K^{n+1} to be approximately the same as P_K^n . Thus, the water-filled K volume will not show a pressure spike. The momentum equations then have the form

$$v_{f,j}^{n+1} = v_{f,j}^{n,exp} - (VFDP)_j^n (P_L^{n+1} - P_L^n) + (VFDP)_j^n (10^6) (P_K^{n+1} - P_K^n) \quad (3-382)$$

$$v_{g,j}^{n+1} = v_{g,j}^{n,exp} - (VGDP)_j^n (P_L^{n+1} - P_L^n) + (VGDP)_j^n (10^6) (P_K^{n+1} - P_K^n) \quad (3-383)$$

In addition to the modification of the momentum equation, the interphase drag for junction j uses the interphase drag for volume L.

EC000086

Figure 3-16. Two vertical vapor/liquid volumes.

3.4.7 Countercurrent Flow Limitation Model

There are several structures internal to RCSs where gravity drainage of liquid can be impeded by upward flowing vapor. These include the upper core tie plate, downcomer annulus, steam generator tube support plates, and the entrance to the tube sheet in the steam generator inlet plenum. A completely mechanistic approach to determine the onset of flow limiting for all structural configurations is impractical. Both the Wallis and Kutateladze forms of the general flooding limit equation have been found to provide acceptable results when constants applicable to specific geometries are used in conjunction with them. Wallis³⁻²⁶ discusses the phenomenon of flooding, which can occur when liquid is falling in a vertical structure and gas is moving upward. For a specified liquid downflow rate, there is a certain gas upward flow rate at which very large waves appear on the interface, the flow becomes chaotic, gas pressure drop increases, and liquid flows upward. Figure 3-17 is a reproduction of Wallis' Figure 11.11 and shows this phenomena. Wallis points out that the flooding point is not approached as the limit of a continuous process (which occurs in drops or bubbles), but it is the result of a marked instability.

A general countercurrent flow limitation (CCFL) model is implemented that allows the user to select the Wallis form, the Kutateladze form, or a form in between the Wallis and Kutateladze forms. This general form was proposed by Bankoff, et al.³⁻⁸⁸ and is used in the TRAC-PF1 code³⁻⁸⁹. It has the structure

$$H_g^{1/2} + m H_f^{1/2} = c \quad (3-384)$$

where H_g is the dimensionless gas flux, H_f is the dimensionless liquid flux, c is the gas intercept (value of $H_g^{1/2}$ when $H_f = 0$, i.e., complete flooding), and m is the "slope", that is the gas intercept divided by the liquid intercept (the value of $H_f^{1/2}$ when $H_g = 0$). A typical plot of $H_g^{1/2}$ versus $H_f^{1/2}$ is shown in Figure 3-18. Quotes are used around the word "slope" because in a strict mathematical sense, the

Figure 3-17. Pressure-drop characteristics near the boundary between countercurrent and cocurrent flow (from Wallis,³⁻²⁶ p. 337).

Figure 3-18. Plot of $H_g^{1/2}$ versus $H_f^{1/2}$ for a typical CCFL correlation.

slope is negative for Equation (3-384) and $m = -\text{slope}$. The constant m will be called the slope in this report and in the input cards and output edit, but one should think of this as $-\text{slope}$. The dimensionless fluxes have the form

$$H_g = j_g \left[\frac{\rho_g}{gw(\rho_f - \rho_g)} \right]^{1/2} \quad (3-385)$$

$$H_g = j_f \left[\frac{\rho_f}{gw(\rho_f - \rho_g)} \right]^{1/2} \quad (3-386)$$

where j_g is the gas superficial velocity ($\alpha_g v_g$), j_f is the liquid superficial velocity ($\alpha_f v_f$), ρ_g is the gas density, ρ_f is the liquid density, α_g is the gas volume fraction, α_f is the liquid volume fraction, g is the gravitational acceleration, and w is given by the expression

$$w = D_j^{1-\beta} L^\beta \quad (3-387)$$

In Equation (3-387), D_j is the junction hydraulic diameter and L is the Laplace capillary constant, given by

$$L = \left[\frac{\sigma}{g(\rho_f - \rho_g)} \right]^{1/2} \quad (3-388)$$

where σ is the surface tension. In Equation (3-387), β can be a number from 0 to 1. For $\beta = 0$, the Wallis form of the CCFL equation is obtained; and for $\beta = 1$, the Kutateladze form of the CCFL equation is obtained. For $0 < \beta < 1$, a combination of the Wallis and Kutateladze forms is obtained; and Bankoff³⁻⁸⁸ suggests that β be correlated to data for the particular geometry of interest. He has included a possible function for β , although it is somewhat restrictive. The form of Equations (3-384) through (3-388) is general enough to allow the Wallis or Kutateladze form to appear at either small or large diameters. Other approaches (e.g., Tien, et al.³⁻⁹⁰) appear to be more restrictive by defaulting to the Wallis form at small diameters and the Kutateladze form at large diameters.

With regard to the solution method, if the CCFL model is requested by the user, the coding checks if countercurrent flow exists and if the liquid downflow exceeds the limit imposed by Equation (3-384). If this is true, the sum momentum equation and the flooding limit equation are applied. This approach was suggested by Trapp,^a who observed that the CCFL model is similar to the choking model in that both place limits on the momentum equations. He observed that since the flooding phenomenon can be incorporated by altering the interphase friction (as is done in TRAC-PF1), it can also be incorporated by replacing the code's difference momentum equation with the flooding limit equation. The difference equation contains the interphase friction, whereas the sum equation does not. (In the choking model, the sum momentum equation is replaced with the choking model, and the sum momentum equation is replaced with the choking limit equation.) This method is advantageous in that the phasic velocities still must satisfy the sum momentum equation which contains gravity and pressure terms. The numerical form of Equation (3-384) needed by the code is obtained by letting $c_g = H_g/v_g$ and $c_f = H_f/v_f$, solving for $mH_f^{1/2}$, and squaring the equation, which results in

$$m^2 c_{f,j}^n v_{f,j}^{n+1} = c^2 - 2c (c_{g,j}^n)^{1/2} (v_{g,j}^{n+1})^{1/2} + c_{g,j}^n v_{g,j}^{n+1} \quad (3-389)$$

Linearization of $(v_{g,j}^{n+1})^{1/2}$ gives

$$(v_{g,j}^{n+1})^{1/2} = (v_{g,j}^n)^{1/2} + (1/2) (v_{g,j}^n)^{-1/2} (v_{g,j}^{n+1} - v_{g,j}^n) \quad (3-390)$$

and substitution into Equation (3-389) gives

$$\begin{aligned} m^2 c_{f,j}^n v_{f,j}^{n+1} + \left[c (c_{g,j}^n)^{1/2} (v_{g,j}^n)^{-1/2} - c_{g,j}^n \right] v_{g,j}^{n+1} \\ = c^2 - c (c_{g,j}^n)^{1/2} (v_{g,j}^n)^{1/2} \end{aligned} \quad (3-391)$$

3.5 Component Models

SCDAP/RELAP5 consists of a variety of generic models which are used to build system models. These include the pipe, annulus, branch, single volume, single junction, etc. These will be discussed in more detail in Volume III of this manual. The general philosophy has been to avoid system component models such as pressurizer, steam generator, core, etc. However, certain subsystem components are unavoidable due to unique processes or performance. SCDAP/RELAP5 contains models for subsystem components such as a branch, separator, jet mixer, pump, turbine, valve, and accumulator. A brief summary of each of these models is included here.

3.5.1 Branch

The branch component is a model designed for convenient interconnection of hydrodynamic components. The identical result can be obtained by using a single-volume component and several single-junction components. Thus, the branch is a separate component only in the input processing scheme.

The crossflow junction has been added in which the junction velocities are assumed to be normal to the one-dimensional flow path of the hydrodynamic volume. Thus, the branch component can include multiple connections at the inlet, outlet, or in the crossflow direction.

Specialized modeling considerations are applied to any volume having multiple junctions connected at either volume end. (The ends of a hydrodynamic volume are the inlet and outlet, as defined in Section 3.1.1.)

These special calculations include both the method for calculating the volume average velocities and the method for partitioning the volume cross-sectional area between the multiple inlet or multiple outlet junctions. The partitioned volume areas are used both in the abrupt area change model, to calculate junction kinetic loss factors, and in the momentum equations, to simulate the stream-tube area.

In applications, the multiple junction and crossflow models are used in three distinct ways to model branching flows. These are the one-dimensional branching, a tee branch, and a crossflow branch. Combination of the three basic branches may also occur. Each of the three basic models will be discussed in turn.

3.5.1.1 One-Dimensional Branching. This basic branch model is consistent with the one-dimensional approximation for a piping network and assumes that multidimensional effects at branches are small compared to system interaction effects. In the case of branched flows that occur in headers or plena, the model gives an accurate physical description of the flow division or merging process; and the one-dimensional branch model is intended primarily for use in modeling such branched flows. Examples of such situations in LWR systems are flow division at the core inlet if parallel flow paths through the core are modeled, steam generator inlet and outlet plena when several parallel tube groups are modeled (for the effect of tube height and length), or at a wye connection.

The one-dimensional branch is illustrated in Figure 3-19 for a volume having two inlet junctions and one outlet junction. The junctions J_1 and J_2 are the inlet junctions, and junction J_3 is the outlet junction. The multiple flows are assumed to merge in such a way that they come to the common velocity equal to the inlet volume average velocity for volume V_3 . The volume cross-sectional area is then divided in proportion to the volume flow of the respective inlet junctions. This method of apportioning volume cross-sectional area satisfies continuity but does not conserve momentum, particularly for high velocity differences between the merging streams. (For flow splitting, however, the method does preserve momentum.) For this reason, the special jet mixer component was developed for merging flows having high relative velocities, such as in a jet pump. The jet mixer can be used for one-dimensional mixing but is limited to two inlet streams and a single outlet stream. (See Section 3.5.3 for a description of the jet mixer model.) The volume partitioned areas are calculated as follows:

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Figure 3-19. One-dimensional branch.

$$(A_K)_j = \left[|(\dot{\alpha}_f)_j^n (v_f)_j^n| + |(\dot{\alpha}_g)_j^n (v_g)_j^n| \right] A_j A_K$$

$$\sum_{i=J_1}^{J_N} \left[|(\dot{\alpha}_f)_i^n (v_f)_i^n| + |(\dot{\alpha}_g)_i^n (v_g)_i^n| \right] A_i \quad (3-39?)$$

The apportioned volume areas for each junction are used with the abrupt area change model, Section 3.4.2, to calculate energy loss coefficients for the liquid and vapor streams at each junction.

3.5.1.2 Ninety-Degree Tee Model. The crossflow junction (see Section 3.4.4) is used to form a 90-degree tee, as shown in Figure 3-13. In this particular application, the side connection to the tee is modeled using a junction in which only one-half of the junction momentum equation has the crossflow form. (The half of junction J_3 associated with volume V_L is a crossflow junction and is designated by an X, see Figure 3-13.)

No special component is provided to accomplish the input associated with a model, such as illustrated in Figure 3-13. The volume, V_L , may be specified as a branch with the associated junctions or as a single volume with single junctions used to specify the connecting junctions. In either case, junctions J_1 and J_2 should be specified as smooth unless actual abrupt changes in area occur at either junction. Junction J_3 should be specified as smooth with a user-specified form loss factor to account for the turning and entrance losses. In addition, junction J_3 must be specified so that the half of the junction associated with volume V_L is modeled as a crossflow junction and the half associated with volume V_K is a normal junction. These options are specified through input of junction control flags.

It is also possible to model a 90-degree tee without using a crossflow junction; however, unphysical numerical results have been obtained at times

for reasons that are not fully understood. Thus, the 90-degree tee model using the crossflow junction is recommended and is a closer approximation to the actual fluid momentum interaction that occurs at a tee.

3.5.1.3 Gravity Effects at a Tee. In some branching situations where the throughflow is small or where the flow is constrained by the geometry, body force effects may be significant. Examples that occur in PWR systems are the cold leg connections to the inlet annulus and downcomer and the hot leg connection to the upper plenum and core. This type of branched flow is modeled as shown in Figure 3-20. Here the vertical direction is modeled as the throughflow direction (indicated by the volume orientation arrows). The cold or hot leg connections are modeled by crossflow junctions. The throughflow direction of volume V_3 is chosen to correspond to the major flow path. In the case of a PWR inlet annulus, throughflow in the horizontal direction is inhibited by the annular structure; in the case of the upper-plenum-to-core connection, the area for flow in the vertical direction is large compared to the flow area in the horizontal direction. Some judgment is required to select the orientation. However, the crossflow branch connection will permit throughflow in the horizontal direction but with some accompanying pressure rise and drop associated with the fact that the momentum flux terms are neglected in the crossflow part of the junction.

The model illustrated in Figure 3-20 has the additional advantage that the effect of vertical void gradients in the flow out of the horizontal connections may be more sharply defined as a result of the central volume, V_3 , which has a vertical height equal to the diameter of branch Volumes V_1 and V_4 .

No special component model is provided for modeling the vertical tee, and either a branch or a single volume may be used for volume V_3 . The branch component is more convenient, since all junctions connecting to volume V_3 can be specified with the branch component.

EC000088

Figure 3-20. Gravity effects on a tee.

3.5.1.4 Crossflow Branch. A fourth type of branched flow path can be created by the use of a crossflow junction to couple two volumes. This type of branch is used to model crossflow between parallel core channels and leak paths between volumes having centers at the same vertical elevation. The crossflow junction is assumed to have no elevation change, thus one limitation of this type of branch is that the volume centers that are coupled must be at the same elevation. If volumes of differing elevations are coupled, an input processing error will occur in the loop elevation checking routines. The application of the crossflow junction for crossflow or leak path modeling is illustrated in Figure 3-14. The length scale associated with the crossflow junction is one half the diameter of the K volume plus one half the diameter of the L volume. This length is only used for modeling the fluid inertia terms in the momentum equation and is always assumed to lie in a horizontal plane.

The pure crossflow branch is most easily modeled using a single-junction component for the crossflow junction. However, either volume, V_1 or V_2 in Figure 3-14 can be modeled using the branch component and specifying the coupling junctions with that component.

3.5.2 Separator

The separator model is a nonmechanistic or black-box model consisting of a special volume with junction flows, as pictured in Figure 3-21. A steam-water inflowing mixture is separated by defining the quality of the outflow streams using empirical functions. No attempt is made to model the actual separation process from first principles.

The separator vapor outlet performance is defined by means of a special function for the vapor void fraction at J_1 . The donored junction vapor void fraction used to flux mass through the steam outlet is related to the vapor void fraction in the separator volume using the curve in Figure 3-22. For separator volume void fractions above the value of $VOVER$ (an input parameter), a perfect separation is assumed and pure vapor is fluxed out junction J_1 . For separator volume void fractions less than

Figure 3-21. Typical separator volume and junctions.

EC000090

Figure 3-22. Donor junction voids for outflow.

VOVER, a two-phase mixture is fluxed out. The VOVER parameter governs the vapor void fraction of the outflow. If VOVER is small, the vapor outflow corresponds to an ideal separator. If VOVER equals 1.0, the vapor outlet junction behaves as a normal junction; and the vapor outlet junction void fraction is equal to the separator volume average void fraction.

The flow of the separator liquid drain junction is modeled in a manner similar to the steam outlet except that pure liquid outflow is assumed when the volume liquid void fraction is greater than the value of VUNDER (see Figure 3-22). Normal donored fluxes are used for the separator inlet junction. Although the void fractions used to flux mass and energy from the separator volumes are modified, the normal junction momentum equations are used to calculate the flow velocities.

3.5.3 Jet Mixer

There are several components in a typical reactor plant where the momentum effects due to the mixing of two parallel streams of fluid at different velocities may be important. An example of this is the jet pump in a BWR. In this component, the pumping action is caused by the momentum transfer between the two fluid streams. Momentum effects may also be important for mixing at ECC injection points or for the aspirators present in some steam generators. The JEIMIXER component was developed for these cases.

3.5.3.1 Basic Jet Mixing Model. To derive the momentum equations needed to model a jet mixing situation, consider the schematic shown in Figure 3-23, which illustrates a mixing volume connected to a drive and a suction volume.^a The suction junction (with velocity v_s and area A_s) connects the last upstream suction region volume, KS, to the mixing volume, L. The drive junction (with velocity v_d and area A_d) connects the last

a. The drive and suction junctions should be the high-speed and low-speed junctions respectively when the JEIMIXER component is used for other than jet pump applications.

EC000091

Figure 3-23. Schematic of mixing junctions.

8 stream drive line volume, KD, to the mixing volume, L. Figure 3-23 shows the drive junction as a smooth junction and the suction junction as abrupt. The user can model either junction either way if the appropriate loss factors are included (see input guidelines in Volume 2 of this manual). Void fractions and densities subscripted by a D or S are donored values; a subscript a indicates an average value.

The mixing of the drive and suction flows between cross section 1 and 2 requires a reevaluation of the momentum flux terms. The wall drag, interphase drag, temporal acceleration, momentum exchange due to mass transfer, and gravity head terms for the drive and suction junctions are treated exactly as they are at any other junction. Only the pressure and momentum flux terms will be examined in the following momentum equation development.

Consider a control volume in the mixing region between cross sections 1 and 2 and assume the following: (a) steady single-phase flow; (b) one-dimensional flow at cross sections 1 and 2; and (c) equal pressures at junctions D and S. If we apply the conservation of momentum principle for this control volume with these assumptions, the momentum equation becomes

$$(P_L - P_1) A_L + \rho_L v_L^2 A_L - \rho_S v_S^2 A_S - \rho_D v_D^2 A_D = 0 \quad . \quad (3-393)$$

Conservation of mass applied with these same assumptions gives

$$\rho_L v_L A_L - \rho_S v_S A_S - \rho_D v_D A_D = 0 \quad . \quad (3-394)$$

Equation (3-394) can be used to write Equation (3-393) in its nonconservative form, obtaining

$$(P_L - P_1) + \rho_S v_S A_S (v_L - v_S)/A_L + \rho_D v_D A_D (v_L - v_D)/A_L = 0 \quad . \quad (3-395)$$

Equation (3-395) gives the momentum equation (pressure and flux terms) for the upstream half of the mixing volume. To develop the momentum equation for the suction junction, a normal half-cell momentum equation is written from KS to cross section 1, i.e.,

$$(P_1 - P_{KS}) + 1/2 \rho_{KS}(v_S^2 - v_{KS}^2) = 0 \quad . \quad (3-396)$$

Adding this to the half cell momentum Equation (3-395) for cross section 1 to L, gives

$$P_L - P_{KS} + 1/2 \rho_{KS}(v_S^2 - v_{KS}^2) + \rho_S v_S A_S (v_L - v_S)/A_L + \rho_D v_D A_D (v_L - v_D)/A_L = 0 \quad . \quad (3-397)$$

This equation shows how the pressure and momentum flux terms should be calculated for the suction junction equation.

If the suction junction were a normal junction, its momentum equation (pressure and flux terms) would be

$$(P_L - P_{KS}) + 1/2 \rho_{Sa}(v_L^2 - v_{KS}^2) = 0 \quad . \quad (3-398)$$

The velocity terms in Equation (3-398) must be replaced by the velocity terms in Equation (3-397) to correctly model the momentum equation at the suction junction. Similar equations for the drive junction can be obtained.

3.5.3.2 Jet Mixing in Two-Phase Flows. If a derivation similar to the previous section is carried out for the pressure and momentum flux terms in the two-phase case, the following equations are obtained for the liquid phase in the mixing region:

Conservation of momentum (from cross section 1 to L)

$$\alpha_{fL} A_L (P_L - P_1) + \alpha_{fL} \rho_{fL} v_{fL}^2 A_L - \alpha_{fS} \rho_{fS} v_{fS}^2 A_S - \alpha_{fD} \rho_{fD} v_{fD}^2 A_D = 0 \quad (3-399)$$

Conservation of mass (from cross section 1 to L)

$$\alpha_{fL} \rho_{fL} v_{fL} A_L - \alpha_{fS} \rho_{fS} v_{fS} A_S - \alpha_{fD} \rho_{fD} v_{fD} A_D = 0 \quad (3-400)$$

Using Equation (3-400) in Equation (3-399) and rewriting Equation (3-164) in nonconservative form yields

$$\alpha_{fL} (P_L - P_1) + \alpha_{fS} \rho_{fS} v_{fS} A_S (v_{fL} - v_{fS})/A_L + \alpha_{fD} \rho_{fD} v_{fD} A_D (v_{fL} - v_{fD})/A_L = 0 \quad (3-401)$$

Equation (3-401) can now be combined with the appropriate half-cell momentum equation for the upstream volume to obtain the final momentum equation for the liquid flow at the suction junction. A parallel development gives the gas phase momentum equation at the suction junction.

The momentum equations used consist of the sum of the phasic momentum equations and the difference of the phasic momentum equations.

To derive the sum momentum equation (pressure and flux terms only) for the suction junction, Equation (3-401) for the liquid phase is added to a similar equation for the gas phase to obtain

$$(P_L - P_1) + \alpha_{fS} \rho_{fS} v_{fS} A_S (v_{fL} - v_{fS})/A_L + \alpha_{fD} \rho_{fD} v_{fD} A_D (v_{fL} - v_{fD})/A_L + \alpha_{gS} \rho_{gS} v_{gS} A_S (v_{gL} - v_{gS})/A_L + \alpha_{gD} \rho_{gD} v_{gD} A_D (v_{gL} - v_{gD})/A_L = 0 \quad (3-402)$$

The normal half-cell sum momentum equation (pressure and flux terms only) for the upstream suction volume can then be added to Equation (3-402) to give

$$\begin{aligned}
 (P_L - P_{KS}) + \alpha_{fS} \rho_{fS} v_{fS} A_S (v_{fL} - v_{fS}) / A_L + \alpha_{fD} \rho_{fD} v_{fD} A_D (v_{fL} - v_{fD}) / A_L \\
 + \alpha_{gS} \rho_{gS} v_{gS} A_S (v_{gL} - v_{gS}) / A_L + \alpha_{gD} \rho_{gD} v_{gD} A_D (v_{gL} - v_{gD}) / A_L \\
 + 1/2 \alpha_{fKS} \rho_{fKS} (v_{fS}^2 - v_{fKS}^2) + 1/2 \alpha_{gKS} \rho_{gKS} (v_{gS}^2 - v_{gKS}^2) = 0 \quad (3-403)
 \end{aligned}$$

as the final form for the pressure and momentum flux terms in the new sum momentum equation for the suction junction. The pressure term in this equation has exactly the same form as the pressure term in the normal sum momentum equation. A parallel equation holds for the drive junction. Hence, at the drive and suction mixing junctions, the normal momentum flux terms in the sum momentum equation must be replaced by those in Equation (3-403).

The difference momentum equation for the suction junction is derived by dividing the liquid momentum mixing Equation (3-401) by α_{fL} and adding it to the half-cell liquid momentum equation for the upstream suction volume (also divided by the appropriate void fraction, α_{fKS}) to obtain

$$\begin{aligned}
 (P_L - P_{KS}) + \alpha_{fS} \rho_{fS} v_{fS} A_S (v_{fL} - v_{fS}) / \alpha_{fL} A_L + \alpha_{fD} \rho_{fD} v_{fD} A_D (v_{fL} - v_{fD}) / \alpha_{fL} A_L \\
 + 1/2 \rho_{fKS} (v_{fS}^2 - v_{fKS}^2) = 0 \quad (3-404)
 \end{aligned}$$

Next, Equation (3-404) is divided by the average junction liquid density, ρ_{fa} , and subtracted from the corresponding gas equation to obtain

$$\begin{aligned}
& \left(\frac{\rho_f - \rho_g}{\rho_f \rho_g} \right)_a (P_L - P_{KS}) + \alpha_{gS} \rho_{gS} v_{gS} A_S (v_{gL} - v_{gS}) / \alpha_{gL} \rho_{ga} A_L \\
& + \alpha_{gD} \rho_{gD} v_{gD} A_D (v_{gL} - v_{gD}) / \alpha_{gL} \rho_{ga} A_L + \frac{1}{2} \rho_{gKS} (v_{gS}^2 - v_{gKS}^2) / \rho_{ga} \\
& - \alpha_{fS} \rho_{fS} v_{fS} A_S (v_{fL} - v_{fS}) / \alpha_{fL} \rho_{fa} A_L - \alpha_{fD} \rho_{fD} v_{fD} A_D (v_{fD} - v_{fD}) / \alpha_{fL} \rho_{fa} A_L \\
& - \frac{1}{2} \rho_{fKS} (v_{fS}^2 - v_{fKS}^2) / \rho_{fa} = 0 \tag{3-405}
\end{aligned}$$

as the final difference momentum equation to be used at Junction S. A parallel equation must be used at the drive junction. The pressure term in Equation (3-405) has exactly the same form as the pressure term in the normal difference momentum equation. Hence, at the drive and suction mixing junctions the normal momentum flux terms in the difference momentum equation must be replaced by those in Equation (3-405).

3.5.3.3 Associated Flow Losses. The flow in the mixing region of volume L can in reality be either a true jet mixing or a flow split (for reverse flow). The flow split case is governed by different physics than the jet mixing case considered in the previous discussions. The redistribution that occurs when the flow splits is primarily determined by the effective resistances downstream of the separation point in the suction and drive flow paths. The mixing terms derived above do not apply. For this reason, the additional mixing terms are applied only for the positive drive flow regimes. The normal momentum flux calculations are used for the negative drive flow regimes.

The junctions associated with the JETMIXER component can be modeled as smooth or abrupt. If the junctions are input as smooth, then the appropriate flow resistances should be calculated in a standard fashion and input as form loss coefficients at the appropriate junctions by the user.

If the junctions in the JETMIXER component are input as abrupt area changes, then the code will calculate form loss coefficients as usual except that (a) the forward loss coefficients at the drive and suction junctions are set to zero and (b) the reverse loss coefficients for the suction and drive junctions are those associated with the expansions from the junction areas to the suction or drive volume areas. The forward losses at these junctions are actually associated with the expansion from the vena-contracta to the downstream mixing volume flow area. For parallel mixing streams, this loss is no longer appropriate. The losses associated with any contraction from the mixing volume to the suction or drive junctions are neglected for the same reason.

If the above normal flow losses are used when the suction flow reverses, it will be found that jet pump performance (head ratio) in this regime is significantly below the experimental data. The reverse flow loss coefficient applied in the suction junction has a significant effect on the jet pump performance in this flow situation. This loss coefficient (in addition to the normal loss coefficient associated with the expansion from A_S to area A_{KS}) represents all the irreversible losses associated with the turning and expansion of the flow from the drive junction. Because this flow regime is an important regime in the accident analysis of a BWR, it was decided to include an approximation for this flow-dependent loss in the jet mixing model.

This reverse suction flow loss was based upon the expansion losses experienced by the flow as it moves from the drive to the suction junction. Two flow situations with reversed suction flow and positive drive flow are possible, depending upon the flow direction in the mixing section (Figure 3-24). In the first situation, the expansion loss associated with the area change A_D to A_S , i.e.,

$$K = (A_S/A_D - 1)^2 \quad (3-406)$$

Regime 1

Regime 2

EC000093

Figure 3-24. Flow regimes and dividing streamline.

is added to the user-specified reverse loss coefficient (or the standard abrupt area change loss factor if the junction is input as abrupt) for the suction junction. In the second situation, the effective area for the suction flow that comes from the drive junction is less than A_S because the discharge flow is reversed. In this situation, the effective areas for the expansion loss are A_D and $A_S|W_D/W_S|$. Hence, for the second situation, the loss coefficient

$$K = \left(\frac{A_S|W_D/W_S|}{A_D} - 1 \right)^2 \quad (3-407)$$

is added to the user-specified reverse loss coefficient (or the abrupt area loss factor if the junction is input as abrupt) at the suction junction only if $A_S|W_D/W_S|$ is $>A_D$. If $A_S|W_D/W_S|$ is $<A_D$, the drive-to-suction flow is effectively a contraction; and the additional loss coefficient is set to zero.

Since the jet mixing and effective resistances are modeled by special terms in the suction and drive junction momentum equations, the normal losses associated with the partitioning of volume L are not included in these junction equations. However, the normal losses associated with the area ratios experienced by the flow upstream of the suction and drive junctions are retained in the junction momentum equations.

3.5.3.4 Numerical Implementation. The basic numerical algorithm used to evaluate the new momentum flux terms in Equations (3-403) and (3-405) is similar to the numerical evaluation of the normal momentum flux terms. The normal momentum flux terms are calculated explicitly at the n -th time level. The new momentum flux terms in Equations (3-403) and (3-405) are also explicitly evaluated, and the spatial location of each variable is indicated by its subscript.

3.5.4 Pump Model

The SCDAP/RELAP5 pump model is almost identical to the RELAP5/MOD1 pump model,³⁻⁹¹ which was originally taken from the RELAP4 pump model.³⁻⁹² The only difference is that in SCDAP/RELAP5, a shaft component has been added to the control system component. The pump can be linked to the shaft and thus driven by either a motor or a turbine. However, the SCDAP/RELAP5 options for a motor-driven pump were retained so that input changes to an existing plant model using the pump are not required unless it is desired to make use of the shaft coupling.

The pump is a volume-oriented component, and the head developed by the pump is apportioned equally between the suction and discharge junctions that connect the pump volume to the system. The pump model is interfaced with the two-fluid hydrodynamic model by assuming the head developed by the pump is similar to a body force. Thus, the head term appears in the mixture momentum equation; but, like the gravity body force, it does not appear in the difference of momentum equation used in SCDAP/RELAP5. The term that is added to the mixture momentum equation is

$$\frac{1}{2} \rho g H \quad (3\ 408)$$

where H is the total head rise of the pump (m), ρ is the fluid density (kg/m^3), and g is the acceleration due to gravity (m/s^2). The factor $1/2$ is needed because the term is applied at both the suction and discharge junctions.

In the semi-implicit numerical scheme, the pump is coupled explicitly so the numerical equivalent of Equation (3 408) is

$$\frac{1}{2} \rho^n g H^n \Delta t \quad (3\ 409)$$

where the n designates the previous time level and Δt is the time integration interval. This term is added to the right side of the mixture momentum equation, Equation (3-79).

In the nearly implicit numerical scheme, the pump is coupled implicitly by way of its dependence on the volumetric flow rate, Q . It is assumed that the head depends on the volumetric flow rate, and a first order Taylor series expansion is used,

$$H^{n+1} = H^n + \left(\frac{dH}{dQ} \right)^n (Q^{n+1} - Q^n) \quad . \quad (3-410)$$

Thus, the numerical equivalent of Equation (3-408) in the nearly implicit scheme is

$$\frac{1}{2} \rho^n g H^n \Delta t + \frac{1}{2} \rho^n g \left(\frac{dH}{dQ} \right)^n (Q^{n+1} - Q^n) \Delta t \quad . \quad (3-411)$$

This term is added to the right side of the mixture momentum Equation (3-79), which uses the linear implicit convection term from Equation (3-100).

The pump dissipation is calculated for the pump volume as

$$\tau \omega - gH (\alpha_f \rho_f v_f + \alpha_g \rho_g v_g) A \quad (3-412)$$

where τ is the pump torque and ω is the pump speed.

This term is evaluated explicitly in both the semi-implicit and nearly implicit schemes, and it is partitioned between the liquid and vapor thermal energy equations in such a way that the rise in temperature due to dissipation is equal in each phase. (The details of the dissipation mechanism in a two-phase system are unknown, so the assumption is made that the mechanism acts in such a way that thermal equilibrium between the phases is maintained without phase change.) Thus, the terms that are added to the right sides of the liquid and vapor thermal energy equations, Equations (3-68) and (3-69), are

$$\left[\tau^n \omega^n - gH^n \left(\alpha_f^n \rho_f^n \bar{v}_f^n + \alpha_g^n \rho_g^n \bar{v}_g^n \right) A \right] \Delta t \left(\alpha_f^n \rho_f^n C_{pf}^n \right) \\ \left(\alpha_f^n \rho_f^n C_{pf}^n + \alpha_g^n \rho_g^n C_{pg}^n \right) \quad (3-413)$$

and

$$\left[\tau^n \omega^n - gH^n \left(\alpha_f^n \rho_f^n \bar{v}_f^n + \alpha_g^n \rho_g^n \bar{v}_g^n \right) A \right] \Delta t \left(\alpha_g^n \rho_g^n C_{pg}^n \right) \\ \left(\alpha_f^n \rho_f^n C_{pf}^n + \alpha_g^n \rho_g^n C_{pg}^n \right), \quad (3-414)$$

respectively.

The pump head, H , and torque, τ , are defined by means of an empirical homologous pump performance model; and the pump speed, ω , is defined by a pump drive model. The derivative of the pump head with respect to the volumetric flow rate, dH/dQ , is obtained from the empirical homologous pump performance model, using the assumption that the pump speed is constant.

3.5.4.1 Centrifugal Pump Performance Model. The basic pump performance data must be generated experimentally. Analytical programs have been developed that are reasonably successful in predicting near-design pump performance for single-phase fluids. For off-design operation or for operation with a two-phase fluid, the problems of analytical pump performance prediction are nearly insurmountable. The basic parameters that characterize the pump performance are the rotational speed, ω or N , the volumetric throughflow, Q , the head rise, H , and the shaft torque, τ . The relationship between these four parameters can be uniquely displayed by a four-quadrant representation of such data. A typical four-quadrant curve is shown in Figure 3-25. Both positive and negative values for each of the four parameters are represented. The

Figure 3-25. Typical pump characteristic four-quadrant curves.

disadvantages in using such a data map for numerical purposes are the need for two-dimensional interpolation, the large number of points needed to define the entire range, and the fact that the map is infinite in extent. These objections can be largely overcome by use of a homologous transformation based on the centrifugal pump similarity relationships. Such a transformation collapses the four quadrant data onto a single, bounded, dimensionless curve having eight basic octants. Typical homologous curves for the head and torque are illustrated in Figures 3-26 and 3-27, respectively, where ω_r , Q_R , H_R , and τ_R are the rated values for the pump speed, volumetric flow rate, head, and torque, respectively. The homologous transformation is not unique, and not all points of Figure 3-25 lie on the curves of Figures 3-26 and 3-27. However, the data are closely grouped; and the single curve is a good approximation for the global pump performance.

The pump model allows the user the option of accounting for cavitation or two-phase degradation effects on pump performance. The user must supply a separate set of homologous, two-phase curves for head and torque that are in the form of difference curves. Difference curves are used because analysis of available two-phase pump data indicated that when the fluid being pumped had a void fraction between 0.2 and 0.9, little head was developed by the pump being tested. Outside this range of void fraction, the pump-developed head varied from zero to undegraded single-phase performance. To consider the degraded performance, a set of dimensionless homologous curves was fit to the head data. Thus the fully degraded, two-phase head was expressed as a function of the standard pump model arguments.

To consider the ranges of void fraction where the pump was able to develop head (0 to 0.2 and 0.9 to 1.0), a multiplier as a function of void fraction was used. The multiplier varied from 0 to about 1.0 as the void fraction varied from 0 to 0.2; and the multiplier varied from about 1.0 to 0 as the void fraction varied from 0.9 to 1.0.

Figure 3-26. Typical pump homologous head curves.

9-7358

Figure 3-27. Typical pump homologous torque curves.

Available pump data from the 1-1/2 Loop Model Semiscale and Westinghouse Canada Limited (WCL) experiments were used in developing the two-phase pump data. Assumptions inherent in the pump model for two-phase flow include:

- o The head multiplier, $M_H(\alpha_g)$, determined empirically for the normal operating region of the pump, is also valid as an interpolating factor in all other operating regions.
- o The relationship of the two-phase to the single-phase behavior of the Semiscale pump is applicable to large reactor pumps. This assumes that the pump model of two-phase flow is independent of pump specific speed.

The single-phase pump head (dimensionless) curve for the Semiscale pump is shown in Figure 3-28, and the fully degraded two-phase pump head curves are shown in Figure 3-29. These represent complete pump characteristics (except for the reverse pump fully degraded region) for the Semiscale pump operating under two-phase conditions, with the average of the void fractions of the pump inlet and outlet mixtures between 0.2 and 0.9. The lines drawn through the data were determined by least-squares polynomial fits to the data using known constraints.

A comparison of the two-phase data in Figure 3-29 with the single-phase data in Figure 3-28 shows that the two-phase dimensionless head ratio (h/v^2 or h/α^2) is significantly less than the single-phase dimensionless head ratio for the normal pump operation region (HAN and HVN). For negative ratios of v/α , such as those that occur in the HAD region, the pump flow becomes negative. When the pump flow is negative, the two-phase dimensionless head ratio is greater than the single-phase dimensionless head ratio. Two-phase flow friction losses are generally greater than single-phase losses, and friction is controlling in this energy dissipation region (HAD). The other regions of two-phase dimensionless head ratio data show similar deviations from single-phase data.

Normal pump	$(+Q, +\alpha)$	$\left\{ \begin{array}{l} \text{HAN} \\ \text{HVN} \end{array} \right.$
Energy dissipation	$(-Q, +\alpha)$	$\left\{ \begin{array}{l} \text{HAD} \\ \text{HVD} \end{array} \right.$
Normal turbine	$(-Q, -\alpha)$	$\left\{ \begin{array}{l} \text{HAT} \\ \text{HVT} \end{array} \right.$
Reverse pump	$(+Q, -\alpha)$	$\left\{ \begin{array}{l} \text{HAR} \\ \text{HVR} \end{array} \right.$

5 2301

Figure 3-28. Single-phase homologous head curves for 1 1/2 loop MOD1 Semiscale pumps.

Figure 3-29. Fully degraded, two-phase homologous head curves for 1 1/2 loop MOD1 Semiscale pumps.

Table 3-4 shows the difference between the single and two-phase dimensionless head ratio data as a function of v/α and α/v for the various pumping regions shown in Figures 3-28 and 3-29. The differences shown in Table 3-4 are for the eight curve types used for determining pump head.

The head multiplier, $M_H(\alpha_g)$, and void fraction data shown in Table 3-5 were obtained in the following manner. The Semiscale and WCL pump data³⁻⁹² were converted to dimensionless head ratios of h/α^2 or h/v^2 . Values of the dimensionless head ratios were obtained for pump speeds and volumetric flow rates within 50% of the rated speed and flow rate for the pumps. The difference between the single- and two-phase dimensionless ratios was developed as a function of the average void fractions for the pump inlet and outlet mixtures. The difference between the single- and two-phase dimensionless ratios was then normalized to a value between 0 and 1.0. The normalized result was tabulated as a function of the void fraction.

If the two-phase option is selected, the pump head and torque are calculated from

$$H = H_{1\phi} - M_H(\alpha_g) (H_{1\phi} - H_{2\phi}) \quad (3-415)$$

$$\tau = \tau_{1\phi} - M_\tau(\alpha_g) (\tau_{1\phi} - \tau_{2\phi}) \quad (3-416)$$

where

1ϕ = single-phase value

2ϕ = two-phase, fully degraded value, $0.2 < \alpha_g < 0.9$

M = multiplier on difference curve

α_g = average volume void fraction.

TABLE 3-4. SEMISCALE DIMENSIONLESS HEAD RATIO DIFFERENCE
DATA (single-phase minus two-phase)

$$x = \frac{v}{\alpha} \text{ or } \frac{\alpha}{v}$$

$$y = \frac{h}{\alpha^2} \bigg|_{1\phi} - \frac{h}{\alpha^2} \bigg|_{2\phi} \text{ or } \frac{h}{v^2} \bigg|_{1\phi} - \frac{h}{v^2} \bigg|_{2\phi}$$

Curve Type	x	y	Curve Type	x	y
1 (HAN)	0.00	0.00	4 (HVD)	-1.00	-1.16
	0.10	0.83		-0.90	-0.78
	0.20	1.09		-0.80	-0.50
	0.50	1.02		-0.70	-0.31
	0.70	1.01		-0.60	-0.17
	0.90	0.94		-0.50	-0.08
	1.00	1.00		-0.35	0.00
2 (HVN)	0.00	0.00	5 (HAT)	-0.20	0.05
	0.10	-0.04		-0.10	0.08
	0.20	0.00		0.00	0.11
	0.30	0.10		0.00	0.00
	0.40	0.21		0.20	-0.34
	0.80	0.67		0.40	-0.65
	0.90	0.80		0.60	-0.95
3 (HAD)	1.00	1.00		0.80	-1.19
	-1.00	-1.16		1.00	-1.47
	-0.90	-1.24	6 (HVT)	0.00	0.11
	-0.80	-1.77		0.10	0.13
	-0.70	-2.36		0.25	0.15
	-0.60	-2.79		0.40	0.13
	-0.50	-2.91		0.50	0.07
	-0.40	-2.67		0.60	-0.04
	-0.25	-1.69		0.70	-0.23
	-0.10	-0.50		0.80	-0.51
	0.00	0.00		0.90	-0.91
				1.00	-1.47
			7 (HAR)	-1.00	0.00
				0.00	0.00
			8 (HVR)	-1.00	0.00
				0.00	0.00

TABLE 3-5. HEAD MULTIPLIER AND VOID FRACTION DATA

α_g	$M_H(\alpha_g)$
0.000	0.00
0.070	0.00
0.080	0.74
0.165	1.00
0.900	1.00
1.000	0.00

3.5.4.2 Centrifugal Pump Drive Model. The pump torque is used to calculate the pump speed after the pump has been shut off by the input trip signal. The speed is calculated by the deceleration equation

$$I \frac{d\omega}{dt} = \tau \quad (3-417)$$

The solution of this equation is

$$\omega_{t+\Delta t} = \omega_t + \frac{\tau \Delta t}{I} \quad (3-418)$$

where

τ = net torque

I = moment of inertia

t = time

Δt = time step

ω = angular velocity.

The rate of energy addition to the pump system is given by $\omega\tau$ and has been used in Equation (3-412) to calculate the pump dissipation.

The total pump torque is calculated by considering the hydraulic torque from the homologous curves and the pump frictional torque. The net torque with the drive motor shut off is

$$\tau = \tau_{hy} + \tau_{fr} \quad (3-419)$$

where

τ_{hy} = hydraulic torque

τ_{fr} = frictional torque.

The frictional torque is in the form of a cubic equation. The value of the frictional torque is also dependent on the sign of the pump speed. An option is available to specify whether reverse rotation of the pump is allowed.

The electric drive motor will affect the speed behavior of the pump while the motor remains connected to its power source. The net torque with the drive motor on is incorporated into the pump model by adding the value of motor torque, τ_m , to the torque summation

$$\tau = \tau_{hy} + \tau_{fr} - \tau_m \quad (3-420)$$

where the sign of the motor torque is the same as that of the hydraulic and frictional torque for steady operating conditions, that is, zero net torque.

Induction motors are used to drive primary coolant pumps. At constant voltage, the motor torque is an explicit function of speed. This torque/speed relationship is normally available from the motor manufacturer.

Motor torque is supplied to the pump model as a tabular function of torque versus speed as given by the manufacturer's data. A typical torque/speed curve for an induction motor is shown in Figure 3-30.

The capability to simulate a locked rotor condition of the pump is included in SCDAP/RELAP5. This option provides for simulation of the pump rotor lockup as a function of input elapsed time, maximum forward speed, or maximum reverse speed. At the time the rotor locks (and at all times thereafter), the pump speed is set equal to zero.

EC000094

Figure 3-30. Torque versus speed, Type 93A pump motor (rated voltage).

3.5.5 Turbine Component

A steam turbine is a device that converts thermal energy contained in high-pressure, high-temperature steam to mechanical work. The complicated configuration of a steam turbine precludes a complete first-principles model, at least for the purpose of system transient calculations. A lumped-parameter turbine model is used in SCDAP/RELAP5 wherein a sequence of turbine stages (henceforth referred to as a stage group) is treated as a single junction and volume. The stage group is then represented using modified energy, continuity, and momentum equations. An efficiency factor based upon simple momentum and energy considerations is used to represent the nonideal internal processes.

A turbine can be modeled using a single stage group, i.e., a single volume and junction, or several stage groups depending upon the resolution required. If turbine steam is extracted to preheat the feedwater, then several stage groups may be needed to obtain the correct steam properties at the feedwater heating bleed points. All such steam bleed points are modeled as crossflow junctions in the SCDAP/RELAP5 model.

3.5.5.1 Model Design. The normal unmodified volume continuity equations are used for the stage group, with a representative nozzle throat area for the inlet junction and the last stator nozzle throat discharge area as the outlet junction area. It is important to use the same representative nozzle area at both junctions.

Unlike the continuity equations, the momentum equations are modified by the work extracted in the rotating blade system of each stage group. To develop the general form for the momentum equations, we first consider a steady-state total energy balance for a homogeneous fluid passing through a stage group (Figure 3-31). We will subsequently extend this general form to that used for the two-fluid system.

Although the fluid particles follow a tortuous path through the turbine, we can still write a total energy balance between cross sections 1 and 2 (Figure 3-31). For a steady-state situation, this gives

EC000128

Figure 3-31. A schematic of a stage group with idealized flow path between Points 1 and 2.

$$\rho v A \left(\frac{1}{2} v^2 + h \right)_1 = \rho v A \left(\frac{1}{2} v^2 + h \right)_2 + \rho v A W \quad (3-421)$$

where ρ is the density, v is the velocity, h is the enthalpy, and A is the cross-sectional area. The term W represents the shaft work per mass flow rate extracted from the fluid. Heat loss is neglected in this ideal analysis. From continuity considerations, $\rho v A$ is constant. Dividing Equation (3-421) by $\rho v A$, we obtain

$$\frac{1}{2} v_2^2 - \frac{1}{2} v_1^2 = -(h_2 - h_1) - W \quad (3-422)$$

In this way, the energy balance is converted into an equivalent force balance (power = force x velocity).

In this idealized process where external heat loss and internal dissipation are neglected, the process is isentropic and

$$dh = \frac{1}{\rho} dP \quad (3-423)$$

Integrating Equation (3-423) approximately between points 1 and 2 gives

$$h_2 - h_1 = \frac{1}{\rho} (P_2 - P_1) \quad (3-424)$$

where ρ is an average density.

The actual work, W , produced by the fluid on the rotating blades as its momentum is changed, is usually written as an efficiency factor times the isentropic enthalpy change across the stage and becomes

$$W = -\eta \int_{S=\text{const}} dh = -\eta \int_{S=\text{const}} \frac{1}{\rho} dP \quad (3-425)$$

If a constant efficiency for the stage group is assumed, Equation (3-425) can be approximated as

$$W = -\eta \frac{1}{\rho} (P_2 - P_1) \quad (3-426)$$

When Equations (3-424) and (3-426) are substituted into Equation (3-425), we obtain

$$\frac{1}{2} v_2^2 - \frac{1}{2} v_1^2 = - \frac{(1-\eta)}{\rho} (P_2 - P_1) \quad (3-427)$$

as the momentum equation for this steady-state case. Equation (3-427) shows that only a small fraction, $(1 - \eta)$, of the pressure gradient contributes to changes in the kinetic energy of the fluid. The larger fraction, η , of the pressure gradient results in turbine work [Equation (3-426)].

Using Equation (3-427) as a prototype, the full two-fluid momentum equations which are used in the turbine model are (in differential form)

$$\begin{aligned} (\alpha_g \rho_g) \left(\frac{\partial v_g}{\partial t} + v_g \frac{\partial v_g}{\partial x} \right) = & - \alpha_g (1 - \eta) \frac{\partial P}{\partial x} \\ & - \alpha_g \rho_g H_{LOSSG} v_g - \alpha_g \rho_g F_{IG} (v_g - v_f) \end{aligned} \quad (3-428)$$

$$\begin{aligned} (\alpha_f \rho_f) \left(\frac{\partial v_f}{\partial t} + v_f \frac{\partial v_f}{\partial x} \right) = & - \alpha_f (1 - \eta) \frac{\partial P}{\partial x} \\ & - \alpha_f \rho_f H_{LOSSF} v_f - \alpha_f \rho_f F_{IF} (v_f - v_g) \end{aligned} \quad (3-429)$$

The application guidelines will be summarized in Volume III of this report, but it seems appropriate at this point to mention three guidelines that are related to the momentum equation development:

1. In practice, a steam turbine does not usually contain significant liquid water, and the tortuous path precludes accurate modeling

of the interphase drag. Therefore, it is recommended that the homogeneous option be used at all axial turbine junctions. The effect of condensation could be included in the efficiency factor, if desired. At present, it is not included, as the effect is usually small.

2. The fluid path through the turbine volume is very tortuous. This, coupled with the large number of blades, makes the standard wall friction calculation meaningless. For this reason, the wall friction terms have not been shown in Equations (3-428) and (3-429). It is recommended that the turbine volume wall friction flag be set to use the zero wall friction option. If the user wants to include any momentum effects due to frictional or form losses, it should be done with an appropriate user-specified form loss.
3. The area changes in a turbine are gradual, so the smooth junction option should be used.

The inefficiency of the turbine gives rise to some dissipation that is a source of internal energy. The dissipation is a small effect and is neglected in the present turbine model formulation. The only effect on the internal energy equations is the dissipative source term due to any user-specified form loss.

The only equations that are modified as a result of the turbine model are the momentum equations, in which the pressure gradient terms are multiplied by the coefficient $(1 - \eta)$.

3.5.5.2 Efficiency Formulas. The basic efficiency formulas can be derived from velocity diagrams with assumed nozzle and blade efficiency factors. The derivations are fairly straightforward and are found in standard texts. The efficiency formulas recorded here were obtained from Reference 3-93. The efficiency factors for three turbine designs are described in the following paragraph.

3.5.5.2.1 Single-Stage Turbine--The first model considered is the most general. We consider a single row fixed-blade system followed by a single row rotating-blade system. Let r be the reaction fraction, i.e., the fraction of the stage energy released (enthalpy change) in the moving-blade system. If r is zero, we have a pure impulse stage with no pressure drop in the moving-blade system, i.e., the moving blades only change the fluid flow direction. A turbine stage with nonzero r at design conditions is commonly called a reaction stage. A value of $r = 0.5$ is a common design.

If all blading angles are ideal and all nozzle losses are zero, the ideal efficiency, as given in Reference 3-93, is

$$\eta = \left[(v_b - v_t) + \sqrt{(v_b - v_t)^2 + rv^2} \right] \left(\frac{2v_t}{v^2} \right) \quad (3.430)$$

where v is the fluid velocity at the nozzle exit, v_t is the tangential or rim velocity of the moving blades, and

$$b = \sqrt{1 - r} \quad (3.431)$$

In general, due to nozzle losses, entrance effects, and nonideal blading angles, the efficiency is less than that given by Equation (3.430). The maximum efficiency ($\eta = 1.0$) given by Equation (3.430) can be found by differentiation to occur when

$$\frac{v_t}{v} = \frac{0.5}{\sqrt{1 - r}} \quad (3.432)$$

For an impulse stage, the maximum efficiency occurs at $v_t/v = 0.50$. For a reaction turbine designed with $r = 0.5$, the maximum efficiency occurs at $v_t/v = 0.707$.

In general, the actual efficiency is less than the ideal value derived above. A first approximation to the actual efficiency (see Reference 3-93) is to include a constant factor, η_0 , in Equation (3-430) that represents the actual efficiency at the maximum point, i.e.,

$$\eta = \eta_0 \frac{2v_t}{v^2} \left[(vb - v_t) + \sqrt{(vb - v_t)^2 + rv^2} \right] \quad (3-433)$$

Equation (3-433) is the general efficiency formula that is applied to a single-row impulse or reaction turbine. This formula is applied to a stage group that may consist of a single-blade passage or multiple-blade passages. If the stage group contains multiple-blade passages, the efficiency represents some average value.

3.5.5.2.2 Two-Stage Impulse Turbine--The second turbine design considered is a two-row impulse stage, i.e., a nozzle, a moving constant area blade passage, a fixed constant area stationary passage, and a final constant area moving blade passage. This blading system is modeled as a single stage group. This type of stage design is sometimes used as the first stage in a turbine for governing purposes. Reference 3-93 records the efficiency formula for this design as

$$\eta = \eta_0 \frac{8v_t}{v^2} (v - 2v_t) \quad (3-434)$$

3.5.5.2.3 Constant Efficiency--The final efficiency option that is included is a constant efficiency independent of the reaction, nozzle fluid velocity, and rim speed, i.e.,

$$\eta = \eta_0 \quad (3-435)$$

It should be noted that a turbine stage, designed to operate with a given reaction fraction r at design conditions, will have a different reaction fraction for off-design conditions. The change in reaction

fraction with v_t/v can be calculated [Reference 3-93, p. 207, Equation (14)]. For reaction stages the change is small. In all cases, this change in r is neglected in the above efficiency formulas.

3.5.5.2.4 Power/Torque Output of Turbine--In general, the relationship between power and torque for a rotating shaft is

$$P = \tau \omega \quad (3-436)$$

The power extracted from the fluid per mass flow rate for a given stage group is

$$\eta \int_{S=\text{const}} dh \quad (3-437)$$

so we have for the torque

$$\tau = (\rho v A) \frac{\eta}{\rho} (P_2 - P_1) / \omega \quad (3-438)$$

or

$$\tau = (\rho v A) \frac{\eta}{\rho} (P_2 - P_1) \frac{R}{v_t} \quad (3-439)$$

where R is the mean stage radius at the nozzle and the approximation in Equation (3-426) has been used.

Equation (3-439) gives the torque that is extracted from a given stage group in terms of the stage efficiency, mean stage radius R , mean blade tangential velocity v_t , and pressure drop. This is the torque that is applied by the turbine component when it is coupled to the shaft component.

3.5.5.2.5 Numerical Implementation--As noted in the model design section, a stage group is modeled as a single junction (j) and volume (L) (see Figure 3-32).

EC000129

Figure 3-32. Schematic of lumped model for turbine stage group.

The continuity and internal energy equations in Section 3.1 are unchanged from their standard form. The normal finite difference form of the momentum equations for junction j is modified in two ways:

1. The pressure gradient term in the sum and difference numerical equations is multiplied by $(1 - \eta)$.
2. The numerical differencing of the convective terms has been modified. At a normal junction, the convective terms are approximated as

$$v \frac{\partial v}{\partial x} = \left(\frac{1}{2} v_L^2 - \frac{1}{2} v_K^2 \right) / \Delta x + \frac{1}{2} \text{VIS} \quad (3-440)$$

The small viscous term VIS is numerically calculated so as to give a donored formulation of the momentum flux term in a straight pipe. For a variable area channel, it is formulated so that it vanishes for a variable area channel with a constant density fluid. In a turbine, the area is slowly varying; but the fluid experiences large pressure changes (due to the work extraction), hence large density changes. A numerical simulation with the above convective terms used at the turbine junctions resulted in a viscous term that is larger than the kinetic energy terms. The normal viscous terms for a variable area channel are inaccurate in the turbine situation with large density changes and dominate the physical kinetic energy change. An alternative form of the convective terms which is sufficiently accurate and stable for the variable area turbine model is

$$v \frac{\partial v}{\partial x} = v_j (v_j - v_{j-1}) / \Delta x \quad (3-441)$$

when the flow is from left to right in Figure 3-32.

This difference form is used for all turbine junctions. If the v_j multiplying the numerical gradient is assumed to be approximately equal to $\frac{1}{2} (v_j + v_{j-1})$, then Equation (3-441) yields

$$v \frac{\partial v}{\partial x} = \frac{1}{2} (v_j^2 - v_{j-1}^2) / \Delta x \quad (3-442)$$

and a reasonable approximation to the kinetic energy change between $j-1$ and j results.

The algebraic efficiency formulas in Equations (3-433) through (3-435) are coded with v , η_o , r , ω , and R (where $v_t = R\omega$) as arguments. The type of the turbine stage group is fixed at input time.

The stage torque that is applied to the shaft is calculated from Equation (3-339). The torques from each stage group are added using the SHAFL component that integrates the angular momentum equation. The power is calculated from Equation (3-436). This variable is not needed in the integration scheme but is printed in the major edits.

3.5.6 Valves

Valves are quasi-steady models that are used either to specify an option in a system model or to simulate control mechanisms in a hydrodynamic system. The valve models can be classified into two categories; (a) valves that open or close instantly and (b) valves that open or close gradually. Either type can be operated by control systems or by flow dynamics.

Valves in the first category are trip valves and check valves. The model for these valves does not include valve inertia or momentum effects. If the valve is used as a junction with an abrupt area change, then the abrupt area change model is used to calculate kinetic loss factors when the valve is open.

Valves in the second category are the inertial swing check valve, the motor valve, the servo valve, and the relief valve. The inertial valve and relief valve behavior is modeled using Newton's second law of motion. The abrupt area change model controls losses through the valve as the

cross-sectional flow area varies with valve assembly movement. The motor and servo valve use differential equations to control valve movement. These two valves include the options to use the abrupt area change model to calculate losses across the valve or to use flow coefficients (C_v) specified by the user. The C_v 's are converted to energy loss coefficients within the numerical scheme.

Valves are modeled as junction components. The types of valves are defined as follows.

3.5.6.1 Trip Valve. The operation of a trip valve is solely dependent on the trip selected. With an appropriate trip, an abrupt full opening or full closing of the valve will occur. A latch option is also included for latching the valve in the open or closed position.

3.5.6.2 Check Valve. The operation of a check valve can be specified to open or close by static differential pressure, to open by static differential pressure and close by flow reversal, or to open by static differential pressure and close by dynamic differential pressure.

All of the check valves will be opened based on static differential pressure across the junction according to

$$\left(P_K + \Delta P_{K_g} \right) - \left(P_L + \Delta P_{L_g} \right) - PCV > 0, \text{ valve opens} \quad (3-443)$$

where

P_K, P_L = junction from and to volume thermodynamic pressures

$\Delta P_{K_g}, \Delta P_{L_g}$ = static pressure head due to gravity

PCV = back pressure required to close the valve (user input).

For a static pressure controlled check valve, the valve will open if Equation (3-443) becomes positive and will close if Equation (3-443) becomes negative. If Equation (3-443) is zero, the valve will remain as previously defined.

For a flow controlled check valve, the valve will open if Equation (3-443) is positive and will close only if a flow reversal occurs such that

$$GC < 0 \quad (3-444)$$

where GC is the dynamic pressure given as

$$GC = \frac{1}{2}(\overline{\rho v})_j = \frac{1}{2} |\alpha_f \rho_f v_f + \alpha_g \rho_g v_g| (\alpha_f v_f + \alpha_g v_g)_j \quad (3-445)$$

For a dynamic pressure controlled check valve, the valve opens if Equation (3-443) is greater than zero. Once the valve is open, the forces due to pressure differential and momentum hold the valve open until

$$\left(P_K - \Delta P_{K_g} \right) - \left(P_L + \Delta P_{L_g} \right) + GC - PCV < 0, \text{ valve closes} \quad (3-446) \\ = 0, \text{ remains as previously defined} \quad .$$

The terms α_f and α_g are the junction liquid and vapor volume fractions, respectively; ρ_f and ρ_g are the junction liquid and vapor densities, respectively; and v_f and v_g are the junction liquid and vapor velocities, respectively.

Flow and dynamic pressure controlled valves exhibit a hysteresis effect with respect to the forces opening and closing the valve. The static pressure controlled valve, however, has no hysteresis effect.

All check valves may be initialized as either open or closed. Leakage is also allowed if the valve is closed, and the abrupt area change model is used to calculate the valve form losses.

3.5.6.3 Inertial Valve. This valve models the motion of the valve flapper assembly in an inertial-type check valve. The abrupt area change model is used to calculate kinetic form losses, assuming that the area between the flapper and the valve seat behaves as an orifice whose area changes in time as a function of the inertial valve geometry.

The motion of the flapper about the shaft axis is given by Newton's second law (angular version) as

$$\tau = I \alpha \quad (3-447)$$

where the external torques acting on the valve disk are given by

$$\tau = -W L \sin(\theta + \phi) - A_D L(\Delta P + P_{BP} + G_{head}) \quad (3-448)$$

where ΔP is the pressure drop across the valve, and α is the angular acceleration.

Substituting Equation (3-447) into Equation (3-448) yields

$$I \alpha = -W L \sin \theta - \pi R^2 L(\Delta P + P_{BP} + G_{head}) \quad (3-449)$$

where ϕ has been dropped by assuming that the valve is a horizontal pipe. Equation (3-449) is then written in finite-difference form as

$$\alpha^n = \frac{1}{I} - W L \sin \theta^n - \pi R^2 L(\Delta P^n + P_{BP} + G_{head}) \quad (3-450)$$

where the superscript, n , indicates the time level, $t + n \Delta t$. Integrating Equation (3-450) with respect to time yields the angular velocity

$$\omega^{n+1} = \omega^n + \alpha^n \Delta t \quad (3-451)$$

Similarly, integrating Equation (3-451) gives the angular position

$$\theta^{n+1} = \theta^n + \omega^{n+1} \Delta t \quad . \quad (3-452)$$

The throat flow area for the valve is set by the following function^{3-94,95}

$$A_{\text{throat}} = \begin{cases} 2\pi R^2 \tan\theta^{n+1} & \theta \leq 26.565^\circ \\ \pi R^2 & \theta > 26.565^\circ \end{cases} \quad . \quad (3-453)$$

Several options are allowed with the use of this valve, such as specifying minimum and maximum flapper angular positions when the valve is closed, specifying latch or no latch options, and specifying leakage.

3.5.6.4 Motor Valve. This valve model has the capability of controlling the junction flow area between two control volumes as a function of time. The operation of the valve is controlled by two trips; one for opening the valve and a second for closing the valve. A constant rate parameter controls the speed at which valve area changes. The motor valve area variation can also be specified using a general table. When the general table is specified, the constant rate parameter controls the valve stem position and the general table relates the stem position to the valve flow area. Conversely, when the general table is not specified, the constant rate parameter controls the rate of change in valve area.

The abrupt area change model is used to calculate kinetic form losses with respect to the valve area. However, if the normalized valve flow area has a value less than 1.0^{-10} , the valve is assumed to be closed.

A second option allowed for the motor valve is the specification of valve flow coefficients, C_v . These coefficients may be specified using a general table of C_v versus normalized stem position and the smooth junction option must be specified. The conversion of C_v to an energy loss coefficient, K , is done in the numerical scheme using the formula

$$K = 2 \frac{A_{\text{valve}}^2}{C_v^2 \rho_0} \quad (3-454)$$

where

ρ_0 = density of water at 288.71 K (630.0°F).

Provisions also exist for applying multipliers to both stem position and C_v .

3.5.6.5 Servo Valve. The servo valve operation is similar to that for the motor valve. However, the valve area or stem position is controlled by a control variable rather than by a specified rate parameter. The servo valve also has the same options as the motor valve.

3.5.6.6 Relief Valve. For thermal-hydraulic analysis of overpressure transients, it is necessary to simulate the effects of relief valves. In particular, it is desirable to model the valve dynamic behavior, including simulation of valve flutter and hysteresis effects.

To assist in understanding the relief valve model, three schematics of a typical relief valve are shown in Figures 3-33, 3-34, and 3-35. The three schematics represent the valve in the closed (Figure 3-33), partially open (Figure 3-34), and fully open (Figure 3-35) modes, respectively. In the schematics, the seven main components of a relief valve are shown, which are the valve housing, inlet, outlet, piston, rod assembly, spring, bellows, and valve adjusting ring assembly.

The numerical model of the valve simply approximates the fluid forces acting on the valve piston and the valve reaction to these forces. The model of the fluid forces is based on a quasi-steady-state form of the impulse momentum principle, and the valve reaction force is based on Newton's Second Law of motion.

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Figure 3-33. Schematic of a typical relief valve in the closed position.

Figure 3-34. Schematic of a typical relief valve in the partially open position.

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Figure 3-35. Schematic of a typical relief valve in the fully open position.

A qualitative understanding of the operation of the relief valve can be gained by referring again to Figures 3-33, 3-34, and 3-35. If the valve inlet pressure is low the valve is closed, as shown in Figure 3-33. As the inlet pressure increases, the valve piston will remain closed until the force of the upstream pressure on the valve exceeds the set point forces. The set point forces are the combined forces of the piston and rod assembly weight, the valve spring, the atmospheric pressure inside the bellows, and the downstream back pressure around the outside of the bellows. Once the set point forces are exceeded, the valve piston will begin to lift. Upon opening, the upstream fluid will begin to expand through the opening into the valve ring region. This initial expansion occurs through the angle α_0 , and the flow changes direction through an average angle θ_0 , as shown in Figure 3-33. As the flow accelerates, the momentum effects of the expansion and change in flow direction exert a thrust on the valve piston, causing the valve to open further. As the valve partially opens, the angle of expansion decreases to α_1 and the change in flow direction increases to θ_1 , as shown in Figure 3-34. This effect, in turn, further increases the thrust on the valve piston, causing it to fully open, as shown in Figure 3-35. As these processes occur, the valve reaction forces and fluid momentum forces vary in such a manner that the valve will not close until the upstream pressure decreases significantly below the valve set point pressure. In this respect, a hysteresis effect is observed that is characteristic of relief valves.

The relief valve model consists of a set of equations designed to approximate the behavior described above. In implementing the model, the dynamic behavior of the fluid is calculated at each time step by the SCDAP/RELAP5 hydrodynamic solution scheme. The resultant phasic velocities and thermodynamic properties are then used to solve a quasi-steady-equation approximating the fluid forces on the valve piston. The valve dynamic reaction forces are then calculated, and the new time valve piston speed and position are estimated.

The relief valve model is formulated, applying D'Alembert's principle in which the forces acting on the face of the valve piston are balanced, for which the valve reaction forces can be written as

$$(\text{reaction forces}) = F_R = m_v a_{v,x} + B (v_{v,x} - v_{\text{housing}}) + K_s x \quad (3-455)$$

where

m_v = mass of the valve mechanism that is in motion (i.e. the valve piston, rod assembly combined with the spring and bellows)

$a_{v,x}$ = valve assembly acceleration in the x direction

B = damping coefficient

$v_{v,x}$ = velocity of the valve mechanism in the x direction

v_{housing} = 0 = velocity of the valve housing

K_s = spring constant

x = piston position (i.e., x coordinate).

The positive x direction is assumed to be in the direction of fluid flow at the valve inlet. The fluid forces can be formulated by summing the forces acting over the surfaces of the fluid flow channel such that

$$(\text{fluid forces}) = F_F = (P_i A_D)_x - (P_a A_{Ba})_x - (P_o A_{Bo}) - (P_e A_e)_x - F_R \quad (3-456)$$

where

F_R = reaction forces

P_i = valve inlet pressure

A_D = valve piston face area exposed to the inlet flow stream

P_a = atmospheric pressure inside the bellows

A_{Ba} = valve piston area inside the bellows

P_o = valve back pressure outside the bellows

A_{Bo} = valve piston area outside the bellows

A_e = valve ring exit area

P_e = valve ring exit pressure

and where the subscript x denotes that the force component is in the x direction. Since the fluid is flowing through a channel that both expands and changes direction, the fluid undergoes a change in momentum expressed by the impulse momentum principle as

$$F_f = \Delta (mv) = \dot{m}_f (v_{e,x} - v_{i,x}) \quad (3-457)$$

where

$\dot{m}_f$ = mass flow rate of the fluid through the valve

$v_{e,x}$ = fluid velocity exiting through the rings

$v_{i,x}$ = fluid velocity entering the valve inlet.

Hence, balancing the forces by combining Equations (3-455) through (3-457) gives

$$m_v a_{v,x} + B v_{v,x} + K_s x = - (P_a A_{Ba}) - (P_o A_{Bo}) - (P_e A_e) \cos \theta - \dot{m}_f (v_e \cos \theta - v_i) + P_i A_D \quad (3-458)$$

The valve acceleration can be expressed in terms of the valve velocity as

$$a_{v,x} = \frac{dv_{v,x}}{dt} + g \quad (3-459)$$

where g is the acceleration of gravity.

Combining Equations (3-458) and (3-459), treating the velocity damping term and spring force position terms implicitly, and integrating over the time step gives

$$m_v (v_{v,x}^{n+1} - v_{v,x}^n) + B v_{v,x}^{n+1} dt + K_s x^{n+1} dt + m_v g dt = [(P_i^n A_D) - (P_a A_{Ba}) - (P_o^n A_{B0}) - (P_e^n A_e) \cos \theta_e^n - \dot{m}_F^n (v_e \cos \theta_e^n - v_i)] dt \quad (3-460)$$

where the superscripts n and $n+1$ represent the old and new time terms, respectively.

The position term, x^{n+1} , can be written in terms of the valve velocity by considering that

$$v_{v,x} = \frac{dx}{dt} \quad (3-461)$$

If Equation (3-461) is integrated over the time step, then

$$x^{n+1} = x^n + v_{v,x}^{n+1} dt \quad (3-462)$$

If the valve set point pressure is equated to $K_s x_0$, then combining Equations (3-460 and (3-462) and both adding and subtracting the term $K_s x_0$ gives the numerical form of the relief valve model, for which

$$m_v (v_{v,x}^{n+1} - v_{v,x}^n) + [(B + K_s dt) v_{v,x}^{n+1} + K_s (x^n - x_0) + m_v g] dt$$

$$\begin{aligned}
&= \theta K_s x_o dt + [(P_i^n A_D) - (P_a A_{Ba}) - (P_o^n A_{Bo}) - (P_e^n A_e) \cos \theta_e^n \\
&\quad - \dot{m}_F^n (v_e^n \cos \theta_e^n - v_i^n) dt
\end{aligned}
\tag{3-463}$$

where the sign of the gravity term, g , is dependent on the valve orientation. For example, if the valve is oriented upward (i.e.: $+x$ is upward), then the gravity term is expressed as $g = -|g|$.

In the numerical scheme, Equation (3-463) is solved for the new time valve piston velocity, v_v^{n+1} , in terms of the current time terms with superscript, n . The terms required to model the valve geometry and the valve damping, spring, and back pressure forces are input to the code as described in Volume III, Appendix A, of this report.

The characteristic relief valve hysteresis effects are inherent in the formulation of Equation (3-463). For example, if the valve is closed, then all velocity terms are zero and $x = x_o$. Therefore, acceleration of the valve piston in the positive x direction cannot occur until the upstream force $P_i A_D$ exceeds the spring set point and valve weight. Once the valve opens and the fluid accelerates, the forces due to the change in fluid momentum aid in holding the valve open. Therefore, the valve cannot close until the combined fluid pressure and momentum terms decrease below the set point forces. Hence, the desired hysteresis is incorporated in the model.

3.5.7 Accumulator

An accumulator model is included that features mechanistic relationships for the hydrodynamics, heat transfer from the tank wall and water surface, condensation in the vapor dome, and vaporization from the water surface to the vapor dome.

3.5.7.1 Hydrodynamic Model. An accumulator is modeled in SCDAP/RELAP5 as a lumped-parameter component. This model was chosen for two reasons; the spatial gradients in the accumulator tank are expected to be small, and special treatment of the equation of state can be used.

The accumulator model and associated notations are shown in Figure 3-36. The basic model assumptions are:

- o Heat transfer from the accumulator walls and heat and mass transfer from the liquid are modeled using natural convection correlations, assuming similarity between heat and mass transfer from the liquid surface.
- o The gas in the gas dome is modeled as a closed expanding system composed of an ideal gas with constant specific heat. The steam in the dome exists at a very low partial pressure; hence, its effect on the nitrogen state is neglected. However, energy transport to the gas dome as a result of vaporization/condensation is included.
- o Because of the high heat capacity and large mass of water below the interface, the water is modeled as an isothermal system.
- o The model for liquid flow includes inertia, wall friction, form loss, and gravity effects.

Using these assumptions, the basic equations governing the thermal-hydraulics of the tank and discharge line are as follows:

For conservation of mass:

Nitrogen:

$$M_n = \text{constant} = \rho_n V_v \quad (3-464)$$

where

M_n and ρ_n = gas mass and gas density, respectively

V_v = gas dome volume

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Figure 3-36. Typical accumulator.

For conservation of energy:

Nitrogen

$$M_n \left(\frac{\partial U_n}{\partial t} \right) = - P_D \left(\frac{\partial V_v}{\partial t} \right) + \dot{Q}_D \quad (3-465)$$

where

U_n = nitrogen internal energy

P_D = vapor dome pressure

$\dot{Q}_D$ = heat transfer rate to the gas dome.

Wall

$$M_{wall} C_{v_{wall}} \frac{\partial T_{wall}}{\partial t} = - \dot{Q}_{wall} \quad (3-466)$$

where

M_{wall} = metal mass in the tank wall

$C_{v_{wall}}$ = metal specific heat

T_{wall} = mean metal temperature

$\dot{Q}_{wall}$ = heat transfer rate to the wall.

For momentum^a,

a. Equation (3-467) is the combined tank and discharge line momentum equation. The wall drag coefficient, F , is given as $1/2 \rho_f \lambda_{wf} L_L / D A_L v$, where D = surge line diameter and λ_{wf} is the Darcy friction factor given by Equation (3-269).

$$\rho A \left(L \frac{\partial v}{\partial t} + \frac{1}{2} v^2 \right) + Fv = - A \frac{\partial P}{\partial x} + \Delta P_z \quad (3-467)$$

where

A = flow channel cross-sectional area

v = velocity

F = frictional loss coefficient

ΔP_z = elevation pressure differential

For the gas state relationships,

$$P_D V_v = M_n R_n T_D \quad (3-468)$$

$$U_n = M_n C_{v_n} T_D \quad (3-469)$$

Using Equation (3-469), the nitrogen energy equation [Equation (3-477)], can be rewritten as

$$M_n C_{v_n} \frac{dT_D}{dt} = - P_D v A_L + \dot{Q}_D \quad (3-470)$$

Differentiating Equation (3-468), eliminating the constant term $M_n R_n$, and substituting the result into Equation (3-470) yields

$$P_D \left(1 + \frac{R_n}{C_{v_n}} \right) \frac{dV_v}{dt} + V_v \frac{dP_D}{dt} = \frac{R_n}{C_{v_n}} \dot{Q}_D \quad (3-471)$$

Equations (3-467), (3-470), and (3-471) comprise the system of three differential equations used in the accumulator hydrodynamic model. They are used to numerically advance T_D , V_v , and P_D in time.

3.5.7.2 Heat Transfer to the Gas Dome. In the accumulator, energy transport by heat transfer is modeled to the gas dome using a typical convective transport equation of the form

$$Q_i = h_i A_i (T_i - T_d) \quad (3-472)$$

where

subscript i = thermal transport interface
 h_i = convective transport coefficient
 A_i = interface surface area
 $T_i - T_d$ = interface to gas dome temperature difference.

It should be noted that heat and mass transfer in the accumulator surge line are neglected.

Two turbulent natural convection heat transfer models are used and combined by superposition. First, heat transfer with the cylindrical walls of the tank is considered, using a turbulent natural convection correlation³⁻⁹⁶ for heat transfer within a vertical cylinder with closed ends for which

$$h_1 = 0.1 \frac{k_d}{\frac{1}{2} D_{TK}} (Gr Pr)^{\frac{1}{3}} \frac{L}{\delta} \quad (3-473)$$

and

$$A_1 = \pi D_{TK} L \quad (3-474)$$

where

h_1 = gas dome to cylinder heat transfer coefficient

L = gas dome cylinder length

δ = gas dome characteristic diameter

k_d = gas thermal conductivity

$\frac{1}{2} D_{TK}$ = integration interval normal to the surface of the cylinder

Gr = gas dome Grashof number

Pr = gas dome Prandtl number.

Second, heat transfer with the disk shaped ends of the cylinder is considered, where the top disk is the metal top of the tank and the bottom disk is the liquid-gas interface. For this model, a turbulent natural convection correlation³⁻⁹⁶ is used for heat transfer between two horizontal disks separated vertically where, for each disk,

$$h_2 = 0.15 \frac{k_d}{L} (Gr \ Pr)^{\frac{1}{3}} \frac{L}{\delta} \quad (3-475)$$

and

$$A_2 = \frac{\pi D_{TK}^2}{4} \quad (3-476)$$

In the correlations given by Equations (3-473) and (3-476), the product of the Grashof and Prandtl numbers represents the convective thermal circulation in the gas dome, where the Grashof number represents the circulation and the Prandtl number represents the thermal diffusion. Only the Grashof number is a function of the gas dome dimensions and temperature difference for which

$$Gr = \frac{g\beta_d |T_i - T_d| \delta^3}{\nu_i^2} \quad (3-477)$$

where

g = acceleration due to gravity

β_d = gas isobaric coefficient of thermal expansion

$T_i - T_d$ = magnitude of the interface, gas dome difference

ν_i = gas kinematic viscosity

δ = characteristic overall diameter of the gas dome.

If the Prandtl number is written in terms of the gas dome thermal diffusivity, then

$$Pr = \frac{\mu_d}{\rho_d \alpha_d} \quad (3-478)$$

where

ρ_d = gas density

α_d = thermal diffusivity.

The characteristic diameter is defined in terms of the typical volume-to-surface-area ratio as

$$\delta = \frac{4 V_d}{A_i} \quad (3-479)$$

where A_i is the combined gas dome cylinder, disk top, and bottom surface areas.

3.5.7.3 Mass Transfer to the Gas Dome. When the accumulator is in its stagnant initial condition, the gas dome and liquid are in thermal equilibrium and the gas dome is at essentially 100% humidity. However, as the accumulator blows down, the gas dome expands and cools, while the liquid remains essentially isothermal. As a result, there is simultaneous vaporization at the liquid-gas interface and condensation in the gas dome.

At the liquid-gas interface, as vaporization occurs the vapor diffuses across the temperature gradient into the gas dome. Assuming that the process can be approximated by a quasi-steady formulation, then for diffusion in a stagnant gas the mass transfer for the process can be written as

$$\dot{M}_{\text{vap}} = - \zeta A_i \frac{dC}{dx} \quad (3-480)$$

where

$\dot{M}_{\text{vap}}$ = rate of vapor diffusion

ζ = diffusion coefficient

A_i = surface area of the liquid-gas interface

$\frac{dC}{dx}$ = vapor concentration gradient.

The concentration can be expressed in terms of partial pressure such that

$$C = \frac{P_v}{P_d} \rho_g \quad (3-481)$$

where

C = vapor concentration

P_v = local vapor partial pressure

ρ_g = vapor density (saturated vapor at P_v).

Hence, at the dome pressure, the concentration gradient can be written as

$$\frac{dC}{dx} = \frac{1}{P_d} \frac{dP_v \rho_g}{dx} \quad (3-482)$$

Combining Equations (3-480) and (3-482) and integrating gives

$$\dot{M}_{\text{vap}} L_d = - \frac{\zeta A_i}{P_d} \left(P_v \int_{x=0}^{x=L_d} d\rho_g + \bar{\rho} \int_{x=0}^{x=L_d} dP_v \right) \quad (3-483)$$

where the integration is performed by parts.

Both of the differential terms $d\rho_g$ and dP_v can be written in terms of temperature differentials if 100% relative humidity is assumed so that

$$P_v = P^S(T_g) \quad (3-484)$$

where

$P^S(T_g)$ = saturation pressure at the temperature T_g .

Hence, the density differential can be expanded as

$$d\rho_g = \left[\left(\frac{\partial \rho_g}{\partial P_g} \right)_{T_g} \frac{dP_g}{dT} + \left(\frac{\partial \rho_g}{\partial T} \right)_{P_g} \right] dT \quad (3-485)$$

where

$$\left(\frac{\partial \rho_g}{\partial P_g} \right)_T = \kappa_g \rho_g \quad (3-486)$$

$$\left(\frac{\partial \rho_g}{\partial T} \right)_{P_g} = - \beta_g \rho_g \quad (3-487)$$

Combining Equations (3-485), (3-486), and (3-487) and substituting Clapeyron's equation for the dP_g/dT term gives

$$d\rho_g = \bar{\rho}_g \kappa_g \left(\frac{h_{fg}}{T_g^s V_{fg}} \right) - \beta_g dT \quad (3-488)$$

where Clapeyron's equation is

$$dP^S = \frac{h_{fg}}{T_g^s V_{fg}} dT \quad (3-489)$$

and the term $(h_{fg}/T_g^s V_{fg})$ is treated as a constant. Combining Equations (3-484), (3-488), and (3-489), the diffusion equation can be rewritten as

$$\dot{M}_{vap} = \frac{\zeta}{l_d} \frac{A_i}{P_d} \left\{ \bar{P}_g \bar{\rho}_g \left[\kappa_g \left(\frac{h_{fg}}{T_g^s V_{fg}} \right) - \beta_g \right] + \bar{\rho}_g \left(\frac{h_{fg}}{T_g^s V_{fg}} \right) \right\} (T_f - T_w) \quad (3-490)$$

where the dome average terms are evaluated at the dome average temperature, $T_g = T_d$, and where T_w is the tank top wall temperature.

Equation (3-490) can be made analogous to a convective equation by expressing the mass transfer coefficient as

$$h_{2s} = \frac{\zeta}{L_d} \quad (3-491)$$

where h_{2s} is the mass transfer coefficient in a stagnant gas. Then, by applying Reynolds analogy, a turbulent natural convection mass transfer coefficient can be derived in terms of the heat transfer coefficient, h_2 , from Equation (3-485) such that

$$h_{2s} = h_2 \left(\frac{\zeta}{k_d} \right) \frac{\alpha_d}{\zeta}^{1/3} \quad (3-492)$$

Equation (3-492) can then be substituted in place of (ζ/L) in Equation (3-491) such that

$$\begin{aligned} \dot{M}_{\text{vap}} = h_2 \left(\frac{\zeta}{k_d} \right) \left(\frac{\alpha_d}{\zeta} \right)^{1/3} & \left\{ \left(\frac{A_i}{\bar{p}_d} \right) \bar{p}_g \bar{\rho}_g \left[k_g \frac{h_{fg}}{T_d V_{fg}} - \beta_g \right] \right. \\ & \left. + \bar{\rho}_g \left(\frac{h_{fg}}{T_g V_{fg}} \right) \right\} (T_f - T_w) \end{aligned} \quad (3-493)$$

which gives the rate at which water vapor is transported into the accumulator gas dome by turbulent diffusion.

Since the energy transported to the gas dome by the vaporization process must come from the liquid and since the energy per unit mass required for vaporization is h_{fg} , then the rate of energy transport to the gas dome by vaporization is

$$\dot{Q}_{\text{vap}} = \Gamma_{\text{vap}} (h_{fg})_{T_f} = \dot{M}_{\text{vap}} (h_g)_{T_f} \quad (3-494)$$

where Γ_{vap} is the rate of vaporization at the liquid gas interface.

In the gas dome, as the accumulator blows down, the gas cools and condensation by turbulent diffusion occurs. The rate of condensation may be approximated by assuming that the gas dome remains at 100% humidity and considering simple humidity relationships. The humidity ratio can be written as

$$w = \frac{M_g}{M_n} = \frac{N_g P_g}{N_n P_D} \quad (3-495)$$

where

M_g, M_n = vapor, gas masses, respectively

N_g, N_n = vapor, gas molecular weights, respectively

P_g = vapor partial pressure.

Taking the derivative of Equation (3-495) gives

$$\frac{dM_g}{dt} = \frac{1}{P_D} M_n \frac{N_g}{N_n} \frac{dP_g}{dt} - M_g \frac{dP_D}{dt} \quad (3-496)$$

From Gibb's equation, the relationship between the vapor and liquid condensate in the dome is

$$V_{g_{P_g, T_D}} \frac{dP_g}{dT_D} - S_{g_{P_g, T_D}} = V_{f_{P_D, T_D}} \frac{dP_D}{dT_D} - S_{f_{P_D, T_D}} \quad (3-497)$$

and substituting the relationship

$$\frac{dP}{dt} = \frac{dP}{dT} \frac{dT}{dt} \quad (3-498)$$

into Equation (3-497) and rearranging gives

$$\frac{dP_g}{dt} = \frac{V_{f_{P_D, T_D}}}{V_{g_{P_g, T_D}}} \frac{dP_D}{dt} - \frac{h_{g_{P_g, T_D}} - h_{f_{P_D, T_D}}}{T_D} \frac{dT_D}{dt} \quad (3-499)$$

Combining Equations (3-496) and (3-495) with Equations (3-470) and (3-471) gives

$$\begin{aligned} \frac{dM_g}{dt} = & \frac{1}{P_D} \left(M_a \frac{N_g}{N_a} - M_g \right) \frac{V_{f_{P_D, T_D}}}{V_{g_{P_g, T_D}}} \frac{1}{V_v} \left[\dot{Q}_D \frac{R_n}{C_v} - P_D \left(1 + \frac{R_n}{C_v} \right) A_1 V \right] \\ & + \frac{1}{P_D} \frac{N_g}{N_a} \left(\frac{h_{g_{P_g, T_D}} - h_{f_{P_D, T_D}}}{T_D} \right) \frac{1}{C_v} \dot{Q}_D - P_D A_1 V \end{aligned} \quad (3-500)$$

and the rate of condensate formation is given as

$$\dot{M}_c = - \frac{dM_g}{dt} + \dot{M}_{vap} \quad (3-501)$$

The energy transported by the condensate to the interface can be expressed as

$$\dot{Q}_{m_c} = \dot{m}_c h_{f_{T_D}} \quad (3-502)$$

Also, since the condensation is taking place in the gas dome, the energy given up by the condensation process is given up to the gas dome at the rate expressed as

$$\dot{Q}_{M_c} = \dot{M}_c h_{fg_{T_D}} \quad (3-503)$$

Finally, since it is assumed that the condensate is transported to the interface at the condensation rate,

$$\dot{m}_c = \dot{M}_c \quad (3-504)$$

and the net energy given up to the gas dome by the condensation process can be expressed as

$$\dot{Q}_c = \dot{Q}_{M_c} - \dot{Q}_{m_c} = \dot{m}_c (h_{fgT_D} - h_{fT_D}) \quad (3-505)$$

3.5.7.4 Energy Transported to the Gas Dome by Combined Heat and Mass Transfer. The total energy transported to the gas dome can be rewritten by combining Equations (3-472), (3-473), (3-475), (3-494), and (3-505) and summing to give

$$\begin{aligned} \dot{Q}_D = & (h_1 A_1 + h_2 A_2) (T_w - T_d) + h_2 A_2 (T_f - T_d) + \dot{M}_{vap} h_{gT_f} \\ & + \dot{m}_c (h_{fgT_D} - h_{fT_D}) \quad (3-506) \end{aligned}$$

3.5.7.5 Numerical Implementation. The numerical scheme used for the accumulator model includes special features for coupling the solution scheme to the main code in such a way that it is time step independent. This scheme is semi-implicit, and special considerations are employed to preserve the nitrogen energy and mass.

The numerical scheme uses finite-difference techniques to solve the differential equations. The momentum equation is formulated by integrating Equation (3-467) over space and writing the time variation in difference form as

$$\begin{aligned}
& \rho_f \left(L_{fL} + L_{fTK} \right) \left(\frac{A_L}{A_{TK}} \right) + F_f \Delta t + \left[\rho_g \left(L_{gL} + L_{gTK} \right) \left(\frac{A_L}{A_{TK}} \right) + F_g \Delta t \right] v_{fL}^{n+1} \\
& = - \left(p^{n+1} - p_D^{n+1} \right) \Delta t + \Delta P_z \Delta t + \left[\rho_f \left(L_{fL} + L_{fTK} \right) \frac{A_L}{A_{TK}} \right. \\
& \quad \left. + \rho_g \left(L_{gL} + L_{gTK} \right) \left(\frac{A_L}{A_{TK}} \right) \right] v_{fL}^n - \text{CONVF} - \text{CONVG}
\end{aligned} \tag{3-507}$$

where

p^{n+1} = pressure downstream from the accumulator junction.

The inertia term is represented by

$$\rho_f \left(L_{fL} + L_{fTK} \right) \left(\frac{A_L}{A_{TK}} \right) + \rho_g \left(L_{gL} + L_{gTK} \right) \left(\frac{A_L}{A_{TK}} \right) \tag{3-508}$$

where L_{fL} , L_{fTK} , L_{gL} and L_{gTK} are the lengths of the liquid and gas in the surge line and tank, respectively. These terms are computed at each time step and hence vary explicitly with time, having the effect that as the accumulator blows down, the inertia term changes from a liquid-dominant to a vapor-dominant term. The liquid and gas friction terms, respectively, are formulated as

$$F_f = \frac{\rho_f}{2} \left(\lambda \frac{L_{fL}}{D_L} + K_L \frac{L_{fL}}{L_L} \right) v_{fL}^n, \tag{3-509}$$

for the liquid, and

$$F_g = \frac{\rho_g}{2} \left(\lambda \frac{L_{gL}}{D_L} + K_L \frac{L_{gL}}{L_L} \right) v_{gL}^n \tag{3-510}$$

for the vapor, where friction is neglected in the tank and the line friction factor is assumed to be the constant turbulent-turbulent Darcy friction factor given as

$$\lambda = \left| 1.74 - 2 \log \frac{2\epsilon}{D} \right|^{-2} . \quad (3-511)$$

The loss factor term, K_L , is assumed to be distributed over the surge line length, L_L . The term D_L is the surge line hydraulic diameter, and ϵ is the surge line wall roughness. The elevation head term, ΔP_z , is formulated as

$$\Delta P_z = - \frac{g\Delta z_{TK} \left(\rho_f L_{f_{TK}} + \frac{1}{2} \rho_g L_{g_{TK}} \right)}{L_{TK}} - \frac{g\Delta z_L \left(\rho_f L_{f_L} + \rho_g L_{g_L} \right)}{L_L} \quad (3-512)$$

where Δz_{TK} and Δz_L are the tank and surge line elevation changes, respectively, and g is the gravitational acceleration. The liquid and vapor momentum flux terms, CONV_F and CONV_G, respectively are formulated in linear implicit form as

$$\text{CONV}_F = \frac{1}{2} \rho_f \left[1 - \left(\frac{A_L}{A_{TK}} \right) \right]^2 \Delta t v_{f_L}^{n^2} \quad (3-513)$$

if there is liquid in the tank,

$$\text{CONV}_F = 0.0 \quad (3-514)$$

where there is no liquid in the tank,

$$\text{CONV}_G = \frac{1}{2} \rho_g \left[1 - \left(\frac{A_L}{A_{TK}} \right) \right]^2 \Delta t v_{g_L}^{n^2} \quad (3-515)$$

if there is vapor in the surge line, and, finally

$$\text{CONVG} = 0.0$$

(3-516)

where there is no vapor in the surge line. By formulation in this manner, the momentum equation is solved over the pressure gradient from the centroid of the gas dome to the accumulator junction. However, the momentum of the fluid downstream from the accumulator junction is not included. Also, since fluxing of the gas through the junction is not allowed, we have

$$v_{g_L}^{n, n+1} = v_{f_L}^{n, n+1} \quad (3-517)$$

until the accumulator empties of liquid. The effect of this formulation is that as the accumulator blows down, the liquid-gas interface moves out of the accumulator tank and surge line. Thus, the centroid of the gas dome moves towards the centroid of the combined tank and surge line.

The pressure solution is obtained by combining Equations (3-465) and (3-469) and multiplying by R_n/C_{v_n} , which results in

$$M_n R_n \frac{dT}{dt} = - \frac{R_n P_D}{C_{v_n}} \frac{dV_v}{dt} + \frac{R_n}{C_{v_n}} \dot{Q}_D \quad (3-518)$$

where $\dot{Q}_D$ is given by Equation (3-506). Equations (3-468) and (3-518) are then combined, resulting in

$$P_D \left(1 + \frac{R_n}{C_{v_n}} \right) \frac{dV_v}{dt} + V_v \frac{dP_D}{dt} = \frac{R_n}{C_{v_n}} \dot{Q}_D \quad (3-519)$$

Since the liquid is incompressible,

$$\frac{dV_v}{dt} = - \frac{dV_f}{dt} = A_L v_{f_L} \quad ; \quad (3-520)$$

and substitution in Equation (3-519) and expanding in nonconservative finite difference form gives

$$P_D^n \left(1 + \frac{R_n}{C_{v_n}} \right) A_L \Delta t v_{f_L}^{n+1} + v_v^n (P_D^{n+1} - P_D^n) = \frac{R_n}{C_{v_n}} \dot{Q}_D^n \Delta t \quad (3-521)$$

The energy equation may then be solved directly for the new time gas temperature by combining Equations (3-468), (3-471), and (3-521) and integrating, which gives

$$T_D^{n+1} = T_D^n e^{\left(\frac{R_n}{C_{v_n}} \ln \frac{v_v^n}{v_v^{n+1}} + \Delta t \frac{\dot{Q}_D^n}{P_D^n v_v^n} \right)} \quad (3-522)$$

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4. HEAT STRUCTURE MODELS

4.1 Heat Conduction Numerical Technique

Heat structures provided in SCDAP/RELAP5 permit calculation of the heat transferred across solid boundaries of hydrodynamic volumes. Modeling capabilities of heat structures are general and include fuel pins or plates with nuclear or electrical heating, heat transfer across steam generator tubes, and heat transfer from pipe and vessel walls. Heat structures are assumed to be represented by one-dimensional heat conduction in rectangular, cylindrical, or spherical geometry. Surface multipliers are used to convert the unit surface of the one-dimensional calculation to the actual surface of the heat structure. Temperature-dependent thermal conductivities and volumetric heat capacities are provided in tabular or functional form either from built-in or user-supplied data.

Finite differences are used to advance the heat conduction solutions. Each mesh interval may contain a different mesh spacing, a different material, or both. The spatial dependence of the internal heat source may vary over each mesh interval. The time-dependence of the heat source can be obtained from reactor kinetics, one of several tables of power versus time, or a control system variable. Symmetry or insulated conditions and tables of surface temperature versus time, heat transfer rate versus time, heat transfer coefficient versus time, or surface temperature are allowed for boundary conditions. For heat structure surfaces connected to hydrodynamic volumes, a heat transfer package containing correlations for convective, nucleate boiling, transition boiling, and film heat transfer from the wall to water and reverse transfer from water to wall is provided.

The following describes the numerical techniques for heat conduction. The integral form of the heat conduction equation is

$$\iiint_V \rho(\bar{T}, \bar{x}) \frac{\partial T}{\partial t}(\bar{x}, t) dV = \iint_S k(\bar{T}, \bar{x}) \bar{\nabla} T(\bar{x}, t) \cdot d\bar{s} + \iiint_V S(\bar{x}, t) dV \quad (4-1)$$

where k is the thermal conductivity, s is the surface, S is the internal heat source, t is time, T is temperature, V is volume, x represents the space coordinates, and ρ is the volumetric heat capacity. The boundary condition applied to the exterior surface has the form

$$A(T)t(t) + B(t) \frac{\partial T(t)}{\partial n} = D(t) \quad . \quad (4-2)$$

The n denotes the unit normal vector away from the boundary surface. Thus, if the desired boundary condition is that the heat transferred out of the surface equals a heat transfer coefficient, h , times the difference between the surface temperature, T , and the sink temperature, T_s , i.e.,

$$-k \frac{\partial T}{\partial n} = h(T - T_s) \quad (4-3)$$

then the correspondence between the above expression and Equation (4-2) yields

$$A = h, \quad B = k, \quad \text{and} \quad D = h(T - T_s) \quad . \quad (4-4)$$

In one-dimensional problems, boundary conditions are applied on the left and right surfaces. In steady-state problems, a valid physical problem requires that A be nonzero on at least one of the two boundary surfaces. If a transient or steady-state problem has cylindrical or spherical geometry and a zero radius for the left surface (that is, a solid cylinder or sphere), the left boundary condition is normally the symmetry condition, $\frac{\partial T}{\partial n} = 0$. Under these conditions, if B is nonzero, the numerical technique forces the symmetry boundary condition, even if it is not specified.

4.2 Mesh Point and Thermal Property Layout

Figure 4-1 illustrates the placement of mesh points at temperatures to be calculated. The mesh point spacing for a rectangular problem is taken

EC000095

Figure 4-1. Mesh point layout.

in the positive x direction. For cylindrical and spherical problems, the mesh point spacing is in the positive radial direction. Mesh points are placed on the external boundaries of the problem, at the interfaces between different materials, and at desired intervals between the interfaces, boundaries, or both.

Figure 4-2 represents three typical mesh points. The subscripts are space indexes indicating the mesh point number; and l and r (if present) designate quantities to the left and right, respectively, of the mesh point. The δ 's indicate mesh point spacings that are not necessarily equal. Between mesh points, the thermal properties, k and ρ , and the source term, S , are assumed spatially constant; but k_{lm} is not necessarily equal to k_{rm} and similarly for ρ and S .

To obtain the spatial-difference approximation for the m -th interior mesh point, Equation (4-1) is applied to the volume and surfaces indicated by the dashed line shown in Figure 4-2. For the spatial-difference approximation at the boundaries, Equations (4-1) and (4-2) are used to define the gradient along the exterior surfaces and applied to the volumes and surfaces indicated by the dashed lines shown in Figure 4-3. If the coefficient of the gradient in the boundary equation is zero, the surface temperature is given directly from Equation (4-2). Since the code is one-dimensional, the dimensions of the volume for other than the x or r coordinate are set to one. For rectangular geometry, the volume is a rectangular solid. For cylindrical geometry, the volume is a cylindrical annulus; and for spherical geometry, the volume is a spherical shell.

The spatial finite-difference approximations use exact expressions for the space and volume factors and simple differences for the gradient terms.

To condense the expressions defining the numerical approximations and to avoid writing expressions unique to each geometry, the following quantities are defined.

For rectangular geometry,

EC000096

Figure 4-2. Typical mesh points.

EC000097

Figure 4-3. Boundary mesh points.

$$\delta_{lm}^s = \frac{1}{\delta_{lm}} , \quad \delta_{rm}^s = \frac{1}{\delta_{rm}} ,$$

$$\delta_{lm}^v = \frac{\delta_{lm}}{2} , \quad \delta_{rm}^v = \frac{\delta_{rm}}{2} , \text{ and}$$

$$\delta_m^b = 1 . \quad (4-5)$$

For cylindrical geometry,

$$\delta_{lm}^v = 2\pi \frac{\delta_{lm}}{2} \left(x_m - \frac{\delta_{lm}}{4} \right) , \quad \delta_{rm}^v = 2\pi \frac{\delta_{rm}}{2} \left(x_m + \frac{\delta_{rm}}{4} \right) ,$$

$$\delta_{lm}^s = \frac{2\pi}{\delta_{lm}} \left(x_m - \frac{\delta_{lm}}{2} \right) , \quad \delta_{rm}^s = \frac{2\pi}{\delta_{rm}} \left(x_m + \frac{\delta_{rm}}{2} \right) ,$$

and

$$\delta_m^b = 2\pi x_m . \quad (4-6)$$

For spherical geometry,

$$\delta_{lm}^v = \frac{4}{3}\pi \left[x_m^3 - \left(x_m - \frac{\delta_{lm}}{2} \right)^3 \right] , \quad \delta_{rm}^v = \frac{4}{3}\pi \left[\left(x_m + \frac{\delta_{rm}}{4} \right)^3 - x_m^3 \right] ,$$

$$\delta_{lm}^s = \frac{4\pi}{\delta_{lm}} \left(x_m - \frac{\delta_{lm}}{2} \right)^2 , \quad \delta_{rm}^s = \frac{4\pi}{\delta_{rm}} \left(x_m + \frac{\delta_{rm}}{2} \right)^2 ,$$

and

$$\delta_m^b = 4\pi x_m^2 . \quad (4-7)$$

For all geometries,

$$G_m = \rho_{lm} \delta_{lm}^v + \rho_{rm} \delta_{rm}^v \quad (4-8)$$

The superscripts, v and s, refer to volume and surface-gradient weights. The δ_m^b is a surface weight used at exterior boundaries and in heat transfer rate equations.

4.3 Difference Approximation at Internal Mesh Points

Using a forward difference for the time derivative, the first term of Equation (4-1) for the volume of Figure 3-31 is approximated by

$$\iiint_V \rho(\bar{l}, \bar{x}) \frac{\partial T}{\partial t}(\bar{x}, t) d\bar{v} \approx \left(T_m^{n+1} - T_m^n \right) \frac{G_m}{\Delta t} \quad (4-9)$$

The superscript n refers to time; thus, T_m^n indicates the temperature at mesh point m at time t^n , and T_m^{n+1} indicates the temperature at mesh point m at time $t^{n+1} = t^n + \Delta t$. The second term of Equation (4-1) for the surfaces of Figure 3-31 is approximated by

$$\iint_S k(\bar{l}, \bar{x}) \bar{\nabla} T(\bar{x}, t) \cdot d\bar{s} \approx (T_{m-1} - T_m) k_{lm} \delta_{lm}^s + (T_{m+1} - T_m) k_{rm} \delta_{rm}^s \quad (4-10)$$

Note that the above expression includes the standard interface conditions of continuity of temperature and heat flow. The surface integral of Equation (4-1) is usually evaluated by integrating only along the exterior surfaces of the volume indicated by the dashed line in Figure 3-31. If, however, the volume is divided into two sub-volumes by the interface line and the surface integrals of these sub-volumes are added, the surface integrals along the common interface cancel because of the continuity of heat flow. The continuity of temperature is implied by use of a single-valued temperature at the interface.

A contact-resistance interface condition cannot be specified directly since the temperature, instead of being continuous at the interface, is given by $q = h_c \Delta T$, where q is the heat transfer rate across the interface, h_c is the contact conductivity, and ΔT is the temperature change across the interface. This condition can be specified by defining a small mesh interval with thermal properties of $k = h_c \delta$ and $\rho = 0$. The size of the mesh interval, δ , is arbitrary except in cylindrical or spherical geometry, where the surface and volume weights are dependent on the radius. This mesh interval is usually chosen very small with respect to the dimensions of the problem.

The space and time-dependence of the source term in Equation (4-1) are assumed to be separable functions

$$S(x,t) = P_f P(t) Q(x) \quad (4-11)$$

where P_f is the factor that relates the reactor power (or power from a table) to the heat generation rate for a particular heat structure; $P(t)$ is the time varying function and may be reactor power, power from a table, or a control variable; and $Q(x)$ is the space-dependent function. The value of $Q(x)$ is assumed constant over a mesh interval, but each interval can have a different value. The third term of Equation (4-1) is then approximated as

$$\iiint_V S(\bar{x},t) dV \approx \left(Q_{lm} \delta_{lm}^V + Q_{rm} \delta_{rm}^V \right) P_f P(t) \quad (4-12)$$

Gathering the approximations of terms in Equation (4-1), the basic difference equation for the m -th mesh point is

$$\begin{aligned} \frac{(T_m^{n+1} - T_m^n) G_m}{\Delta t} = & -(T_m - T_{m-1}) k_{lm} \delta_{lm}^S + (T_{m+1} - T_m) k_{rm} \delta_{rm}^S \\ & + Q_{lm} \delta_{lm}^V + Q_{rm} \delta_{rm}^V P_f P(t) \quad (4-13) \end{aligned}$$

Using the symbol, ζ_m , to represent the right side, Equation (4-13) can be written as

$$\frac{(T_m^{n+1} - T_m^n) G_m}{\Delta t} = \zeta_m \quad (4-14)$$

Thus far, the time superscripts for G_m and ζ_m have been omitted, and the procedure for approximating the temperature-dependence of the thermal properties has not been mentioned. The procedures for temperature-dependent thermal properties are discussed later. However, superscripts for thermal properties are written here even though their significance is not explained until later. For steady state, the difference approximation becomes

$$\zeta_m = 0 \quad (4-15)$$

and no time superscripts are needed. For the time-dependent case, an equation of the type

$$\frac{(T_m^{n+1} - T_m^n) G_m}{\Delta t} = w \zeta_m^{n+1} + (1 - w) \zeta_m^n \quad (4-16)$$

is an explicit formula if w is zero and is an implicit formula when w is nonzero. SCDAP/RELAP5 uses the implicit formulation with $w = 1/2$.

Writing Equation (4-16) in full, the difference approximation for the m -th interior mesh point for transient and steady-state cases is

$$a_m^n T_{m-1}^{n+1} + b_m^n T_m^{n+1} + c_m^n T_{m+1}^{n+1} = d_m \quad (4-17)$$

$$a_m^n = - \frac{k_{lm}^n \delta_{lm}^s \Delta t}{\sigma + 1} \quad (4-18)$$

$$b_m^n = \sigma G_m^n - a_m^n - c_m^n \quad (4-19)$$

$$c_m^n = - \frac{k_{rm}^n \delta_{rm}^s \Delta t}{\sigma + 1} \quad (4-20)$$

$$d_m^n = \sigma a_m^n T_{m-1}^n + \sigma \left(G_m^n + a_m^n + c_m^n \right) T_m^n - \sigma c_m^n T_{m+1}^n \\ + \Delta t P_f \left(\frac{p^{n+1}}{\sigma + 1} + \sigma p^n \right) Q_{lm} \delta_{lm}^v + Q_{rm} \delta_{rm}^v ; \quad (4-21)$$

σ is 1 for transient cases, and σ is 0 and Δt is 1.0 for steady-state cases. Individual subroutines are used for steady-state and transient cases, and σ and Δt do not appear in the steady-state coding.

4.4 Difference Approximation at Boundaries

To obtain the difference approximations for the mesh points at the boundaries, Equation (4-1) is applied to the volumes of Figure 4-3 with Equation (4-2) used to define the gradient at the surface. The second term of Equation (4-1) at $x = x_1$ is approximated by

$$\iint_S k(T, \bar{x}) \nabla T(\bar{x}, t) \cdot d\bar{s} = - \frac{k_{r1}}{B_1} (A_1 T_1 - D_1) \delta_1^b + k_{r1} (T_2 - T_1) \delta_{r1}^s . \quad (4-22)$$

The complete basic expression for the left boundary mesh point becomes

$$- \frac{(T_1^{n+1} - T_1^n)}{\Delta t} \rho_{r1} \delta_{r1}^v = - \frac{k_{r1}}{B_1} (A_1 T_1 - D_1) \delta_1^b \\ + k_{r1} (T_2 - T_1) \delta_{r1}^s + Q_{r1} \delta_{r1}^v P_f P(t) . \quad (4-23)$$

If B in the boundary condition equation is zero, the above equation is not used, since the boundary condition determines the temperature. Also in that case, a divide by zero would be indicated if Equation (4-23) were used. Approximations for the boundary at $x = x_m$ are derived in a similar fashion. These equations for the boundary mesh points are converted to the implicit formulas in the same manner as for the interior mesh points, except that the surface temperature appearing in the boundary condition is evaluated completely at the $n+1$ time level. Thus, for the left boundary

$$b_1^n T_1^{n+1} + c_1^n T_2^{n+1} = d_1 \quad (4-24)$$

$$b_1^n = \sigma \rho_{r1}^n \delta_{r1}^v + \frac{k_{r1}^n A_1^n \delta_1^b \Delta t}{B_1^n} - c_1^n \quad (4-25)$$

$$c_1^n = \frac{k_{r1}^n \delta_{r1}^s \Delta t}{\sigma + 1} \quad (4-26)$$

$$d_1 = -\sigma c_1^n T_2^n + \sigma \rho_{r1}^n \delta_{r1}^v + c_1^n T_1^n + \frac{k_{r1}^n \delta_1^b D_1^n \Delta t}{B_1^n} + P_f \frac{(\sigma P^n + P^{n+1}) Q_{r1} \delta_{r1} \Delta t}{\sigma + 1} \quad (4-27)$$

In the coding, a variable, HTBCCO, is defined as $C_1^n = A_1^n T_1^n - D_1^n$. Substituting this relation into Equation (4-27) gives

$$d_1 = \sigma c_1^n T_2^n + \left(\sigma \rho_{r1}^n \delta_{r1}^v + \sigma c_1^n + \frac{k_{r1}^n \delta_1^b A_1^n \Delta t}{B_1^n} \right) T_1^n - \frac{k_{r1}^n \delta_1^b C_1^n \Delta t}{B_1^n} + \frac{P_f (\sigma P^n + P^{n+1}) Q_{r1} \delta_{r1}^v \Delta t}{\sigma + 1} \quad (4-28)$$

For the right boundary,

$$a_M^n T_{M-1}^{n+1} + b_M^n T_M^{n+1} = d_M \quad (4-29)$$

$$a_M^n = \frac{-k_{LM}^n \delta_{LM}^S \Delta t}{\sigma + 1} \quad (4-30)$$

$$b_M^n = \sigma \rho_{LM}^n \delta_{LM}^V + \frac{k_{LM}^n A_M^n \delta_M^b \Delta t}{B_M^n} - \sigma a_M^n \quad (4-31)$$

$$d_M = -\sigma a_M^n T_{M-1}^n + \sigma \left(\rho_{LM}^n \delta_{LM}^V + a_M^n \right) T_M^n + \frac{k_{LM}^n \delta_M^b D_M^n \Delta t}{B_M^n} + P_f \frac{(\sigma P^n + P^{n+1}) Q_{LM} \delta_{LM}^V \Delta t}{\sigma + 1} \quad (4-32)$$

In the coding, a variable, HIBCCN, is defined as $C_M^n = A_M^n T_M^n - D_M^n$. Substituting this relation into Equation (4-32) gives:

$$d_M = -\sigma a_M^n T_{M-1}^n + \sigma \rho_{LM}^n \delta_{LM}^V + a_M^n + \frac{k_{LM}^n \delta_M^b A_M^n \Delta t}{B_M^n} T_M^n - \frac{k_{LM}^n \delta_M^b C_M^n \Delta t}{B_M^n} + \frac{P_f (\sigma P^n + P^{n+1}) Q_{LM} \delta_{LM}^V \Delta t}{\sigma + 1} \quad (4-33)$$

4.5 Solution of Simultaneous Equations

The difference approximations for the mesh points [Equations (4-17), (4-24), and (4-29)] lead to a tridiagonal set of M equations. The coefficient matrix is symmetric unless the boundary condition specifies the

surface temperature. In that case, the elements, c_1 and a_M , are 0 and destroy the symmetry for the first and last row. The solution to the above equations is obtained by

$$1. \text{ Form } E_1 = \frac{c_1}{b_1} \text{ and } F_1 = \frac{d_1}{b_1} \quad (4-34)$$

$$2. \text{ Form } E_j = \frac{c_j}{b_j - a_j E_{j-1}} \text{ and } F_j = \frac{d_j - a_j F_{j-1}}{b_j - a_j E_{j-1}}$$

(4-35)

for $j = 2, 3, \dots, M-1$

$$3. \text{ Form } T_M^{n+1} = \frac{d_M - a_M F_{M-1}}{b_M - a_M E_{M-1}} \quad (4-36)$$

$$4. \text{ Form } T_j^{n+1} = -E_j T_{j+1}^{n+1} + F_j$$

(4-37)

for $j = M-1, M-2, \dots, 3, 2, 1$.

These procedures can be derived by applying the rules for Gaussian elimination. This method of solution introduces little roundoff error if the off-diagonal elements are negative and the diagonal is greater than the sum of the magnitudes of the off-diagonal elements. From the form of the difference equations, these conditions are satisfied for any values of the mesh point spacing, time step, and thermal properties.

4.6 Thermal Properties, Boundary Condition Parameters, and Iteration Procedures

The thermal conductivity, k , and the volumetric heat capacity, ρ , are considered functions of temperature and space. These thermal properties are obtained for each interval by using the average of the mesh point temperatures bounding the interval

$$k_{lm} = k \left(\frac{T_{r,m-1} + T_{l,m}}{2} \right) = k_{r,m-1} \quad (4-38)$$

$$k_{rm} = k \left(\frac{T_{r,m} + T_{l,m+1}}{2} \right) = k_{l,m+1} \quad (4-39)$$

The quantity, ρ , is treated in the same manner. The boundary condition parameters, A, B, and D, are considered functions of temperature and time. In steady-state problems, no superscripts would be required for the thermal parameters, k , ρ , A, B, and D. Accordingly, in Equations (4-21), (4-24), and (4-25), those quantities written with superscripts n or $n+1/2$ are ignored, since they are multiplied by $\sigma = 0$, and only quantities with superscript $n+1$ are used. If these quantities are not temperature-dependent, the solution of Equations (4-21), (4-24), and (4-25) will immediately give steady-state temperatures. When these parameters are temperature-dependent, iterations are used to resolve the difficulty of obtaining thermal parameters as a function of temperature when the temperatures are unknown.

In transient problems, the thermal properties, k , ρ , A, B, and D, with superscript n are evaluated as a function of the temperatures, T^n , at the beginning of a time step. Since these are either initial temperatures or results of the last time-advancement, the corresponding thermal parameters can be determined. Those thermal parameters with superscript $n+1$ are evaluated as a function of the temperatures, T^{n+1} , at the end of the time step. Since these temperatures are not available, the initial estimate of the thermal parameters is obtained using $k^{n+1} = k^n$ and similarly for ρ , A, B, and D. The superscript $n+1/2$ indicates an average of the quantities with superscript n and $n+1$, or

$$\rho^{n+1/2} = \frac{\rho^{n+1} + \rho^n}{2} \quad (4-40)$$

If thermal parameters and boundary conditions are constant or do not vary greatly during a time step, the temperatures obtained from the solution of

Equations (4-21), (4-24), and (4-25) with $k^{n+1} = k^n$, etc., are satisfactory. This is presently assumed in SCDAP/RELAP5.

4.7 Difference Approximation for Boundary Conditions

The development of the difference equations uses a general form for the boundary conditions, but SCDAP/RELAP5 uses only the following conditions,

$$-k \frac{\partial T}{\partial x} = 0 \quad (4-41)$$

$$-k \frac{\partial T}{\partial x} = q_T(t) \quad (4-42)$$

$$-k \frac{\partial T}{\partial x} = H(T - T_B) \quad (4-43)$$

$$T = T_T(t) \quad (4-44)$$

where q_T and T_T are tabular functions of time. For the first three conditions, the heat transfer rate is given directly by the boundary conditions once the surface temperature has been calculated. For the temperature boundary condition, the heat transfer rate is obtained from the difference equation. The expression for the right boundary is

$$\begin{aligned} q_M^{n+1} \delta_M^b = & \frac{k_{LM}^n}{\sigma + 1} (T_{M-1}^{n+1} - T_M^{n+1}) \delta_{LM}^s + \frac{\sigma k_{LM}^n}{\sigma + 1} (T_M^n - T_{M-1}^n) \delta_{LM}^s \\ & + P_f \frac{(\sigma P^n + P^{n+1})}{\sigma + 1} Q_{LM} \delta_{LM}^v - \frac{\sigma \rho_{LM}^n}{\Delta t} (T_M^{n+1} - T_M^n) \delta_{LM}^v . \end{aligned} \quad (4-45)$$

4.8 Two-Dimensional Conduction Solution/Reflood

A two-dimensional conduction scheme is used in the reflood model for cylindrical or rectangular heat structures. Figure 4.4 shows an elemental cell around the mesh point. For a cylindrical geometry, the volume elements are

$$V_1 = \pi \delta_t \delta_l (r_i - \delta_l/4)/2 \quad (4-46)$$

$$V_2 = \pi \delta_t \delta_r (r_i + \delta_r/4)/2 \quad (4-47)$$

$$V_3 = \pi \delta_b \delta_l (r_i - \delta_l/4)/2 \quad (4-48)$$

$$V_4 = \pi \delta_b \delta_r (r_i + \delta_r/4)/2 \quad (4-49)$$

and the surface elements are

$$A_1 = \pi \delta_l (r_i - \delta_l/4) \quad (4-50)$$

$$A_2 = \pi \delta_r (r_i + \delta_r/4) \quad (4-51)$$

$$A_3 = \pi \delta_t (r_i + \delta_r/2) \quad (4-52)$$

$$A_4 = \pi \delta_b (r_i + \delta_r/2) \quad (4-53)$$

$$A_5 = A_2 \quad (4-54)$$

$$A_6 = A_1 \quad (4-55)$$

$$A_7 = \pi \delta_b (r_i - \delta_l/2) \quad (4-56)$$

$$A_8 = \pi \delta_t (r_i - \delta_l/2) \quad (4-57)$$

Integration of the heat conduction Equation (4-21) over the elemental cell yields the following form of finite difference equation

EC000098

Figure 4-4. Volume and surface elements around a mesh point (i, j) .

$$\begin{aligned}
G_{ij} \left(T_{i,j}^{n+1} - T_{i,j}^n \right) \Delta t = & a_{ij}^L T_{i-1,j} + a_{ij}^R T_{i+1,j} \\
& + a_{ij}^T T_{i,j+1} + a_{ij}^B T_{i,j-1} - \left(a_{ij}^L \right. \\
& \left. + a_{ij}^R + a_{ij}^B + a_{ij}^T \right) T_{ij} + S_{ij} .
\end{aligned} \tag{4-58}$$

By defining the material properties, ρ_{ij} and k_{ij} , at the center of the r -direction interval between mesh points (ij) and $(i+1,j)$, the coefficients G_{ij} , a_{ij}^R and a_{ij}^T of Equation (4-58) can be written as

$$G_{ij} = \rho_{i-1,j} (V_1 + V_3) + \rho_{ij} (V_2 + V_4) \tag{4-59}$$

$$a_{ij}^R = K_{ij} (A_3 + A_4) / \delta_r \tag{4-60}$$

$$a_{ij}^T = \left[(k_{ij} + k_{i,j+1}) A_2 / 2 + (k_{i-1,j} + k_{i-1,j+1}) A_1 / 2 \right] / \delta_t . \tag{4-61}$$

The other two coefficients, a_{ij}^L and a_{ij}^B , are obtained by the symmetry relations

$$a_{ij}^L = a_{i-1,j}^R \tag{4-62}$$

$$a_{ij}^B = a_{i,j-1}^T . \tag{4-63}$$

The space and time dependence of the source term, S , described in Equation (4-11) are extended to two-dimensional cases as

$$S = P_R P(t) Q(r,z) \tag{4-64}$$

with the assumption that Q is independent of z within a heat structure. Accordingly, the heat source term S_{ij} of Equation (4-58) is

$$S_{ij} = P_R P(t) (Q_L^T v_1 + Q_L^B v_3 + Q_r^T v_2 + Q_r^B v_4) \quad (4-65)$$

Here, $Q_L^T = Q_L^B$ and $Q_r^T = Q_r^B$ if the entire cell is within the same heat structure.

Equation (4-58) is written, of course, for an interior point (ij). For a point on the boundary, some of the coefficients a_{ij}^L , a_{ij}^R , a_{ij}^B , and a_{ij}^T should vanish. For example, at the bottom corner, a_{ij}^L and a_{ij}^B are zero. It is also obvious that some of the terms in Equations (4-61) and (4-64) disappear. Furthermore, the boundary condition must be added. To be consistent with the one-dimensional heat conduction scheme, an assumption is made that no heat is fluxed across the top and bottom ends. For the right and left boundaries, the boundary condition can be represented by one of the general forms described in Equations (4-41) through (4-44). The boundary condition specifying the surface temperature as a function of time, Equation (4-55), has been dropped in the two-dimensional scheme for computational efficiency.

The difference Equation (4-58) is solved using the alternative-direction implicit (ADI) method. The scheme is represented by two steps as follows:

1. Column Inversion:

$$\begin{aligned} (T_{ij}^{n+1/2} - T_{ij}^n) G_{ij} / (\Delta t/2) = & a_{ij}^L T_{i-1,j}^n \\ & + a_{ij}^R T_{i+1,j}^n + a_{ij}^B T_{i,j-1}^{n+1/2} + a_{ij}^T T_{i,j+1}^{n+1/2} \\ & - (a_{ij}^L + a_{ij}^R) T_{ij}^n - (a_{ij}^T + a_{ij}^B) T_{ij}^{n+1/2} + S_{ij} \quad (4-66) \end{aligned}$$

2. Row Inversion:

$$\begin{aligned}
 (T_{ij}^{n+1} - T_{ij}^{n+1/2}) G_{ij} / (\Delta t / 2) = & a_{ij}^L T_{i-1,j}^{n+1} + a_{ij}^R T_{i+1,j}^{n+1} \\
 & + a_{ij}^B T_{i,j-1}^{n+1/2} + a_{ij}^T T_{i,j+1}^{n+1/2} - (a_{ij}^L + a_{ij}^R) T_{ij}^{n+1} \\
 & - (a_{ij}^T + a_{ij}^B) T_{ij}^{n+1/2} + S_{ij} .
 \end{aligned} \tag{4-67}$$

Here the superscripts n , $n+1/2$, and $n+1$ denote the values at times t , $t+\Delta t/2$, and $t+\Delta t$, respectively.

The tridiagonal system of equations at each stage of ADI is solved by either a fully vectorized 2D odd-even reduction scheme or a vectorized Gaussian elimination method. The odd-even reduction scheme operates on vectors of length $m = nax \cdot nr1$, $m/2$, $m/4$, . . . until the vector length is either $2 \cdot nax$ or $3 \cdot nax$, if the ADI iteration is in the radial direction, $2 \cdot nr1$ or $3 \cdot nr1$ if the ADI iteration is in the axial direction. Here, nax and $nr1$ are the number of axial and radial nodes, respectively. This requires that $nax = 2 \cdot 2^p$ or $3 \cdot 2^p$, where p is a positive integer, if ADI is in the axial direction or $nr1 = 2 \cdot 2^p$ or $3 \cdot 2^p$ if ADI is in the radial direction. If these conditions are not satisfied, then a vectorized Gaussian elimination method is used. In addition, if nax exceeds 20 and if the code detects strong diagonal dominance for the tridiagonal matrix, then iterative methods are used when the ADI iteration is in the axial direction. Because odd-even reduction is capable of greatly increasing the diagonal dominance of a strongly diagonal dominant matrix, the iterations typically converge in one to three iterations.⁴⁻¹ It is found that the adoption of these methods can reduce the run time of the entire code by 20% to 30% over the old version when nonvectorized Gaussian elimination methods are used.

4.9 Fine Mesh-Rezoning Scheme

A fine mesh-rezoning scheme is implemented to efficiently use the two-dimensional conduction solution for reflood calculations. The scheme is similar to the one used in COBRA-TF⁴⁻² and is intended to resolve the large axial variation of wall temperatures and heat fluxes. The number of axial nodes in the heat structures is varied in such a way that the fine nodes exist only in the nucleate boiling and transition boiling regions.

A heat-structure geometry, which is composed of 1 to 99 heat structures as specified by users, is selected as an elementary unit for the reflood model. Figure 4-5 shows a typical heat-structure geometry with one fluid control volume connected to each heat structure. The dots are radial mesh points. At the initiation of the reflood model, each heat structure is subdivided into two axial intervals (Figure 4-6). A two-dimensional array of mesh points is thus formed. Thereafter, the number of axial intervals may be doubled, halved, or unchanged at each time step according to a set of rules to be discussed in the next paragraph. Figure 4-6 shows an example of a heat structure going through a cycle of axial nodalization variation.

The number of axial mesh intervals in a heat structure depends on the heat transfer regimes in the heat structures. At each time step, all heat structures in a heat-structure geometry are searched to find the positions of T_{CHF} , the wall temperature where the critical heat flux occurs, T_Q , the quench or rewetting temperature, and T_{IB} , the wall temperature at the incipience of boiling (see Section 3.3.4). Let us assume that T_{IB} , T_{CHF} , and T_Q are at the i -, j - and k -th heat structures and $k \geq j \geq i$. Also, let N be the number of maximum axial mesh intervals specified by the user and α_g be the void fraction in the connected control volume. The number of axial mesh intervals in a heat structure is determined according to the following rules:

- o For $\alpha_g > 0.999$ or $\alpha_g = 0$, the number is halved but not less than 2.

EC000099

Figure 4-5. An elementary heat structure unit for reflood.

EC000100

Figure 4-6. An example of the fine mesh-rezoning process.

- o For the $(k+1)$ -th heat structure, the number is doubled but not $>N/2$.
- o For the $(i-1)$ -th heat structure, the number is halved but not $<N/2$.
- o The number is doubled up to N for the heat structures between $\max(j+1, k)$ and $\min(j-1, i)$ and in the region of maximum wall temperature gradient.
- o For all other heat structures, the number is unchanged.

4.10 Gap Conductance Model

The SCDAP/RELAP5 dynamic gap conductance model defines an effective gap conductivity based on a simplified deformation model generated from FRAP-T6.⁴⁻³ The model employs the following assumptions: First, the fuel-to-cladding radiation heat transfer, which only contributes significantly to the gap conductivity under the conditions of cladding ballooning, is neglected. This is appropriate, since cladding ballooning is not included in this simple model. Second, the minimum gap size is limited such that the maximum effective gap conductivity is about the same order as that of metals. Third, the direct contact of the fuel pellet and the cladding is not explicitly considered.

The gap conductance through the gas is inversely proportional to the size of the gap. Since the longitudinal axis of the fuel pellets is usually offset from the longitudinal axis of the cladding, the width of the fuel-cladding gap varies with circumferential position. This variation causes the conductance through the gas in the fuel-cladding gap to vary with circumferential position. The circumferential variation of the conductance is taken into account by dividing the gap into several equal length segments, as shown in Figure 4-7. The conductance for each segment is calculated and then an average conductance, h_g , is computed in the FRAP-T6 model, by the equation

Figure 4-7. Segmentation at the fuel-cladding gap.

$$h_g = \frac{k_g}{N} \sum_{n=1}^N 1/[t_n + 3.2 (R_F + R_C) + (g_1 + g_2)] \quad (4-68)$$

where

h_g = conductance through the gas in the gap ($W/m^2 \cdot K$)

n = number of a circumferential segment

N = total number of circumferential segments = 8

k_g = thermal conductivity of gas ($W/m \cdot K$)

t_n = width of fuel-cladding gap at the midpoint of the n -th circumferential segment (m)

R_F = surface roughness of the fuel (m)

R_C = surface roughness of the cladding (m)

g_1, g_2 = temperature jump distance terms for fuel and cladding.

The width of the fuel-cladding gap at any given circumferential segment is calculated by the equation

$$t_n = t_g + [-1 + (2n-1)/N] t_o \quad (4-69)$$

where

t_g = circumferentially averaged fuel-cladding gap width (m)

t_o = as-fabricated fuel-cladding gap width (m).

The value of t_n in Equation (4-69) is limited between zero and $2t_g$.

The temperature jump distance terms account for the temperature discontinuity caused by incomplete thermal accommodation of gas molecules to the surface temperature. The terms also account for the inability of gas molecules leaving the fuel and cladding surfaces to completely exchange their energy with neighboring gas molecules, which produces a nonlinear temperature gradient near the fuel and cladding surfaces. The terms are calculated by

$$g_1 + g_2 = 0.024688 \left(k_g T_g^{1/2} P_g \sum_i f_i a_i M_i^{-1/2} \right) \quad (4-70)$$

where

T_g = temperature of gas in the fuel-cladding gap (K)

P_g = gas pressure (Pa)

f_i = mole fractions of i-th component of gas

a_i = accommodation coefficient of the i-th component of gas

M_i = molecular weight of the i-th component of gas.

The accommodation coefficients for helium and xenon are obtained by using curve fits to the data of Ullman⁴⁻⁴:

$$a_{He} = 0.425 - 2.3 \times 10^{-4} T_g \quad (\text{helium}) \quad (4-71)$$

$$a_{Xe} = 0.740 - 2.5 \times 10^{-4} T_g \quad (\text{xenon}) \quad (4-72)$$

If T_g is >1000 K, T_g is set to 1000 K. The accommodation coefficients for other gases are determined by interpolation and written as

$$a_i = a_{He} + \frac{(M_i - M_{He})}{(M_{Xe} - M_{He})} (a_{Xe} - a_{He}) . \quad (4-73)$$

The circumferential averaged width of the fuel cladding gap, t_g , in Equation (4-69) is determined by the expression

$$t_g = t_o - u_F + u_C \quad (4-74)$$

where

u_F = radial displacement of the fuel pellet surface (m),

u_C = radial displacement of cladding inner surface (m).

The radial displacements, u_F and u_C , are primarily due to thermal expansion.

The radial displacement, of the fuel pellet surface, u_F , is calculated by the equation

$$u_F = u_{TF} + u_r + u_s \quad (4-75)$$

where

u_{TF} = radial displacement due to thermal expansion (m)

u_r = radial displacement due to uniform fuel relocation (m)

u_s = radial displacement due to fission gas induced fuel swelling and densification (m).

In the SCDAP/RELAP5 model, the variable u_r is assumed to be zero. The value of the variable u_s is supplied by the user. The fuel thermal expansion is obtained from the equation

$$u_{TF} = \sum_{n=2}^N (r_n - r_{n-1}) \epsilon_{TF} (T_{n+1/2}) \quad (4-76)$$

where

n = radial mesh point number

N = total number of mesh points in the fuel

r_n = radius of radial mesh point n

ϵ_{TF} = function defining thermal expansion of fuel as a function of temperature

$T_{n+1/2}$ = average fuel temperature at the center of the node between mesh points n and $n+1$.

The radial displacement of the inner surface of the cladding is calculated by

$$u_c = u_{TC} + u_{cc} + u_e \quad (4-77)$$

where

u_{TC} = radial displacement due to thermal expansion (m)

u_{cc} = radial displacement due to cladding creepdown (m)

u_e = radial displacement due to elastic deformation (m).

The value of u_{cc} must be supplied by the user. For beginning-of-life fuel rods, u_{cc} is equal to zero. For fuel rods with a significant amount of burnup, a FRAPCON-2⁴⁻⁵ analysis is required to determine the value of u_{cc} . The thermal expansion, u_{TC} , is obtained from

$$u_{TC} = r_{cm} \epsilon_{TC} (T_c) \quad (4-78)$$

where

r_{cm} = radius of midplane of cladding (m)

ϵ_{TC} = function defining thermal expansion of cladding as a function of temperature

T_c = temperature of cladding at midplane (K).

The elastic deformation, u_e , is calculated by

$$u_e = r_{cm} (\sigma_h - \nu \sigma_z) / E \quad (4-79)$$

where

E = Young's modulus for the cladding (Pa)

σ_h = cladding hoop stress (Pa)

σ_z = cladding axial stress (Pa)

ν = Poisson's ratio for the cladding.

The cladding hoop and axial stress are given by

$$\sigma_h = (P_g r_i - P_f r_o) / (r_o - r_i) \quad (4-80)$$

$$\sigma_z = \left(P_g r_i^2 - P_f r_o^2 \right) / \left(r_o^2 - r_i^2 \right) \quad (4-81)$$

where

P_f = coolant pressure (Pa)

r_i = inner radius of cladding (m)

r_o = outer radius of cladding (m).

The Poisson's ratio used is

$$\nu = 0.3 \quad (4-82)$$

The internal gas pressure P_g is determined in FRAP-T6⁴⁻³ by a detailed plenum model. Since a plenum model is not included in the simplified approach, a static ideal gas approximation for a fixed plenum volume is used to calculate P_g , i.e.,

$$P_g = P_{g,i} (T_f/T_{f,i}) \quad (4-83)$$

where

$P_{g,i}$ = initial gas pressure in the gap (Pa)

$T_{f,i}$ = initial coolant temperature at the top of the core (K)

T_f = current coolant temperature at the top of the core (K).

The initial internal gas pressure must be supplied by the user.

The volumetric heat capacity and thermal conductivity of the fuel rod materials, except for the thermal conductivity of the gap gas, must be supplied by the user. For the computation of the gas thermal conductivity, the user is required to provide the gas composition in terms of the mole fractions of seven common gases included in the model. The properties for determining material thermal expansion and elastic deformation are calculated from permanent data within the code, and no user input is

needed. The user, however, should be aware that these properties are computed under the assumption that the fuel material is uranium oxide and the cladding material is zircaloy. The properties of UO_2 and zircaloy along with gas conductivity are taken from MATPRO-11 (Revision 2)⁴⁻⁶ and are described below.

The conductivity as a function of temperature for a pure noble or diatomic gas is calculated using

$$k_g = A T_g^B \quad (4-84)$$

The constants A and B for seven common gases are given in Table 4-1. The thermal conductivity of a gas mixture is calculated from the expression

$$k_g = \sum_{i=1}^N k_i X_i / \left(X_i + \sum_{j=1}^N \Phi_{ij} X_j \right) \quad (4-85)$$

where

$$\Phi_{ij} = \left[1 + (k_i/k_j)^{1/2} (M_i/M_j)^{1/4} \right]^2 [8 (1 + M_i/M_j)]^{1/2} \quad (4-86)$$

and

N = number of components in the mixture

M_i = molecular weight of component i

X_i = mole fraction of the component i

k_i = thermal conductivity of the component i (W/m·K).

TABLE 4-1. CONSTANTS USED IN GAS THERMAL CONDUCTIVITY CORRELATION

Gas	Constant	
	A	B
Helium	2.639×10^{-3}	0.7085
Argon	2.986×10^{-4}	0.7224
Krypton	8.247×10^{-5}	0.8363
Xenon	4.351×10^{-5}	0.8685
H ₂	1.097×10^{-3}	0.8785
N ₂	5.314×10^{-4}	0.6898
O ₂	1.853×10^{-4}	0.8729

The strain function, ϵ_{TF} in Equation (4-76), of the UO_2 fuel due to thermal expansion is described by

$$\epsilon_{TF} = 1.0 \times 10^{-5} T - 3.0 \times 10^{-3} + 4.0 \times 10^{-2} \exp(-6.9 \times 10^{-20}/k_B T) \quad (4-87)$$

where

T = fuel pellet temperature

k_B = Boltzmann constant (1.38×10^{-23} J/K).

The radial strain function, ϵ_{TC} in Equation (4-78), for the cladding thermal expansion is given by

$$\epsilon_{TC} = 1.5985 \times 10^{-3} + 6.721 \times 10^{-6} T \quad (4-88)$$

for $T < 1073.15$ K (α phase) and

$$\epsilon_{TC} = -4.150 \times 10^{-3} + 9.7 \times 10^{-6} T \quad (4-89)$$

for $T > 1273.15$ K (β phase), where T = cladding temperature (K). In the α -to- β phase transition zone (1073.15 K $< T < 1273.15$ K), a table lookup is used. Some selected values are listed in table 4-2.

Young's modulus, E , and shear modulus, G , for zircaloy cladding are approximated by neglecting the effects of oxidation, cold work, and irradiation. Young's modulus is given by

$$E = 1.088 \times 10^{11} - 5.475 \times 10^7 T \quad (4-90)$$

for $T < 1090$ K (α -phase) and

$$E = 9.21 \times 10^{10} - 4.05 \times 10^7 T \quad (4-91)$$

TABLE 4-2. RADIAL THERMAL STRAIN OF ZIRCALOY FOR 1083 K < T < 1273 K

Temperature (K)	ϵ_{TC}
1073.0	5.22×10^{-3}
1093.0	5.25×10^{-3}
1103.0	5.28×10^{-3}
1123.0	5.24×10^{-3}
1143.0	5.15×10^{-3}
1183.0	4.45×10^{-3}
1223.0	2.97×10^{-3}
1273.0	2.90×10^{-3}

for $T > 1240$ K (β -phase), where T is the cladding temperature (K). In the α -to- β phase transfer zone, $1090 \text{ K} \leq T \leq 1240 \text{ K}$, Young's modulus is given by

$$E = 4.912 \times 10^{10} - 4.827 \times 10^7 (T - 1090) \quad . \quad (4-92)$$

4.11 References

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- 4-3. L. J. Siefken et al., FRAP-T6: A Computer Code for the Transient Analysis of Oxide Fuel Rods, EGG-CDAP-5410, April 1981.
- 4-4. A. Ullman, R. Acharya and D. R. Olander, "Thermal Accommodation Coefficients of Inert Gases on Stainless Steel and UO_2 ," Journal of Nuclear Materials 51, 1974, pp. 277-279 .
- 4-5. G. A. Berna et al., FRAPCON-2 Developmental Assessment, NUREG/CR-1949, PNL-3849, July 1981.
- 4-6. D. L. Hagrman, G. A. Reyman, and R. E. Mason, MATPRO-Version 11 (Revision 2), A Handbook of Materials Properties for Use in the Analysis of Light Water Reactor Fuel Rod Behavior, NUREG/CR-0479, TREE-1280, Revision 2, August 1981.

5. CONTROL SYSTEM

The control system provides the capability to evaluate simultaneous algebraic and ordinary differential equations. The capability is primarily intended to simulate control systems typically used in hydrodynamic systems, but it can also model other phenomena described by algebraic and ordinary differential equations. (Note: The reader is referred to Section 8.4.5 for a description of specialized controllers for use in steady-state initialization.) Another use is to define auxiliary output quantities, such as differential pressures, so they can be printed in major and minor edits and be plotted.

The control system consists of several types of control components. Each component defines a control variable as a specific function of time-advanced quantities. The time-advanced quantities include: hydrodynamic volume, junction, pump, valve, heat structure, reactor kinetics, trip quantities, and the control variables themselves (including the control variable being defined). This permits control variables to be developed from components that perform simple, basic operations.

In the following equations that define the control components and associated numerical techniques, Y_i is the control variable defined by the i -th control component, A_j , R , and S are real constants input by the user, I is an integer constant input by the user, V_j is a quantity advanced in time by SCDAP/RELAP5 and can include Y_i , t is time, and s is the Laplace transform variable. Superscripts involving the index n denote time levels. The name in parentheses to the right of the definition is used in input data to specify the component.

5.1 Arithmetic Control Components

Constant

$$Y_i = S \quad (\text{CONSTANT}) \quad (5-1)$$

Addition-Subtraction

$$Y_i = S(A_0 + A_1 V_1 + A_2 V_2 + \dots) \quad (\text{SUM}) \quad (5-2)$$

Multiplication

$$Y_i = S V_1 V_2 \dots \quad (\text{MULT}) \quad (5-3)$$

Division

$$Y_i = \frac{S}{V_1} \text{ or } Y_i = \frac{S V_2}{V_1} \quad (\text{DIV}) \quad (5-4)$$

Exponentiation

$$Y_i = S V_1^I \quad (\text{POWERI}) \quad (5-5)$$

$$Y_i = S V_1^R \quad (\text{POWERR}) \quad (5-6)$$

$$Y_i = S V_1^{V_2} \quad (\text{POWERX}) \quad (5-7)$$

Table Lookup Function

$$Y_i = S F(V_1) \quad (\text{FUNCTION}) \quad (5-8)$$

where F is a function defined by table lookup and interpolation.

Standard Functions

$$Y_i = S F(V_1, V_2, V_3, \dots) \quad (\text{STDFUNCTN}) \quad (5-9)$$

where F can be $|V_1|$, $\exp(V_1)$, $\ln(V_1)$, $\sin(V_1)$, $\cos(V_1)$, $\tan(V_1)$, $\tan^{-1}(V_1)$, $(V_1)^{1/2}$, $\text{MAX}(V_1, V_2, V_3, \dots)$, and $\text{MIN}(V_1, V_2, V_3, \dots)$. Only MAX and MIN may have multiple arguments and must have at least two arguments.

Delay

$$Y_i = SV_1(t - t_d) \quad (\text{DELAY}) \quad (5-10)$$

where t_d is the delay time. A user input, h, determines the length of the table used to store past values of V_1 . The maximum number of time-function pairs is h+2. The delay table time increment is t_d/h . The delayed function is obtained by linear interpolation using the stored past history. As time is advanced, new time values are added to the table. Once the table fills, new values replace values that are older than the delay time.

Unit Trip

$$Y_i = SU(\pm t_r) \quad (\text{TRIPUNIT}) \quad (5-11)$$

Trip Delay

$$Y_i = ST_r(t_r) \quad (\text{TRIPDLAY}) \quad (5-12)$$

In the above two trip-related components, t_r is a trip number and, if negative, indicates that the complement of the trip is to be used; U is 0.0 or 1.0, depending on trip t_r (or its complement if t_r is negative) being false or true; and T_r is -1.0 if the trip is false and the time the trip was last set true if the trip is true.

No numerical approximations are involved in evaluating the algebraic components. Evaluation is by simply performing the indicated operations. In the sequence of operations that perform a time advancement of the trip, heat conduction, hydrodynamic, reactor kinetic, and control systems of

SCDAP/RELAP5, the control system is processed last. Thus, the end of time step $(n+1)$ values for trip variables t_r and all V_i variables except control variables Y_i are available. The control components are evaluated in component number order. As the first control variable Y_i is being evaluated, only old time values are available for all control component variables. Once Y_i is evaluated, the new time value is available for the remaining control variable evaluations of Y_j . In general, while Y_i is being evaluated, new time values are available for Y_k , $k < i$, and only old time values are available for Y_k , $k \geq i$.

In the example,

$$Y_{10}^{n+1} = A_0 + A_1 T^{n+1} + A_2 P^{n+1} + A_3 Y_8^{n+1} + A_4 Y_{10}^n + A_5 Y_{15}^n, \quad (5-13)$$

T and P , which represent a temperature and pressure from the heat structure or hydrodynamic systems, are new time values. The value Y_8 is also a new time value because it was advanced before control component 10, and Y_{10} and Y_{15} are old time values.

Initialization of the algebraic control components is very similar to a time advancement. At the start of control component initialization, all other time-advanced quantities have been initialized. Control component input includes an initial value and a flag that indicates if initialization is to be performed. The initialization proceeds in the order of component numbers. The initial value entered becomes the initial value if no initialization is specified. If initialization is specified, it is simply the specified computation using the available data. If component i references Y_k , $k < i$, the initialized value of Y_k is used; if $k \geq i$, the entered initial value is used.

5.2 Integration Control Component

The integration component evaluates

$$Y_i = S \int_{t_1}^t V_1 dt \quad (\text{INTEGRAL}) \quad (5-14)$$

where t_1 is the simulation time when the component is added to the system, and the initial value at t_1 is the input item regardless of the initialization flag.

The integral is advanced by trapezoidal approximation,

$$Y_i^{n+1} = Y_i^n + S[V_1^n + V_1^{n+1}] \frac{\Delta t}{2} . \quad (5-15)$$

Both new time (n+1) and old time (n) values are available for V_1 except when it is a control variable Y_k , $k \geq i$. For the case when $V_1 = Y_k$, $k \geq i$, the V_1^n and V_1^{n+1} are instead V_1^{n-1} and V_1^n . Use of the integral component when old time values will be used should be avoided. Consider the example

$$a = P_1 - P_2 - BV - kd \quad (5-16)$$

$$V = a \Delta t \quad (5-17)$$

$$d = V \Delta t . \quad (5-18)$$

This acceleration-velocity-distance system cannot be advanced without use of old values. As a general rule, it is considered better to use the old value in the algebraic expression and not in the integral expressions.

Thus, using $Y_1 = a$, $Y_2 = V$, $Y_3 = d$

$$Y_1 = P_1 - P_2 - BY_2 - kY_3 \quad (5-19)$$

$$Y_2 = \text{INTEGRAL}(Y_1) \quad (5-20)$$

$$Y_3 = \text{INTEGRAL } (Y_2) \quad . \quad (5-21)$$

5.3 Differentiation Control Components

Two components provide for differentiation

$$Y_i = \frac{dV_1}{dt} \quad . \quad (5-22)$$

One component evaluates the derivative by the inverse of the integration technique,

$$Y_i = \frac{2S}{\Delta t} (V_1^{n+1} - V_1^n) - Y_i^n \quad . \quad (\text{DIFFERN1}) \quad (5-23)$$

This component is not recommended, since it can be unstable, requires an accurate initial value, and does not recover from a bad initial value. Deletion of this component is being considered. The recommended derivative component uses a simple difference expression,

$$Y_i = S \frac{(V_1^{n+1} - V_1^n)}{\Delta t} \quad . \quad (\text{DIFFERND}) \quad (5-24)$$

Differentiation is a noisy process and should be avoided. Differentiation of control system variables can almost always be avoided. Filtering the result of differentiation of other variables should be considered. Similar to the case of the integral component, old time values are used when advancement of Y_i involves $V_1 = Y_k$, $k \geq i$.

5.4 Proportional-Integral Component

This component evaluates

$$Y_i = S \left[A_1 V_1 + A_2 \int_{t_1}^t V_1 dt \right] \quad (\text{PROP-INT}) \quad (5-25)$$

or, in Laplace transform notation,

$$Y_i(s) = S \left[A_1 + \frac{A_2}{s} \right] V_1(s) \quad . \quad (5-26)$$

This component is advanced in time by

$$I^{n+1} = I^n + \left(V_1^n + V_1^{n+1} \right) \frac{\Delta t}{2} \quad (5-27)$$

$$Y_i^{n+1} = S \left(A_1 V_1^{n+1} + A_2 I^{n+1} \right) \quad . \quad (5-28)$$

The comments in the previous section concerning integration with $V_1 = Y_k$ hold for this component.

If the initialization flag is off, Y° is the entered initial value and

$$I^\circ = \frac{1}{A_2} \left(\frac{Y_i^\circ}{S} - A_1 V_1^\circ \right) \quad . \quad (5-29)$$

If the initialization flag is on,

$$I^\circ = 0 \quad (5-30)$$

$$Y_i^\circ = S A_1 V_1^\circ \quad . \quad (5-31)$$

5.5 Lag Control Component

The lag component is defined in Laplace transform notation as

$$Y_i(s) = S \left(\frac{1}{1 + A_1 s} \right) V_1(s) \quad (LAG) \quad (5-32)$$

through algebraic rearrangement,

$$Y_i(s) + A_1 s Y_i(s) = S V_1(s) \quad (5-33)$$

$$\frac{Y_i(s)}{s} + A_1 Y_i(s) = \frac{S V_1(s)}{s} \quad (5-34)$$

$$Y_i(s) = \frac{S V_1(s) - Y_i(s)}{A_1 s} \quad (5-35)$$

Transforming to the time domain gives

$$Y_i = \int_0^t \frac{[S V_1 - Y_i] dt}{A_1} \quad (5-36)$$

The above expression is advanced numerically by

$$Y_i^{n+1} = Y_i^n + \left[S(V_1^n + V_1^{n+1}) - Y_i^n - Y_i^{n+1} \right] \frac{\Delta t}{2A_1} \quad (5-37)$$

or

$$Y_i^{n+1} = \frac{Y_i^n \left(1 - \frac{\Delta t}{2A_1} \right) + S \left(V_1^n + V_1^{n+1} \right) \frac{\Delta t}{2A_1}}{1 + \frac{\Delta t}{2A_1}} \quad (5-38)$$

If the initialization flag is set,

$$Y_i^o = S V_1^o \quad (5-39)$$

5.6 Lead-Lag Control Component

The lead-lag component is defined in Laplace transform notation as

$$Y_i(s) = S \left(\frac{1 + A_1 s}{1 + A_2 s} \right) V_1(s) \quad . \quad (\text{LEAD-LAG}) \quad (5-40)$$

Rearranging algebraically, this yields

$$Y_i(s) + A_2 s Y_i(s) = S V_1(s) + A_1 s S V_1(s) \quad (5-41)$$

or

$$Y_i(s) = \frac{A_1 S V_1(s)}{A_2} + \frac{S V_1(s) - Y_i(s)}{A_2 s} \quad . \quad (5-42)$$

Transforming to the time domain gives

$$Y_i = \frac{A_1 S V_1}{A_2} + \int_0^t \left(\frac{S V_1 - Y_i}{A_2} \right) dt \quad . \quad (5-43)$$

Note that the differentiation implied by the $sV_1(s)$ term has been avoided.

The above expression is advanced numerically by

$$Y_i^{n+1} = \frac{A_1}{A_2} S V_1^{n+1} + I^n + \left[S (V_1^n + V_1^{n+1}) - Y_i^n - Y_i^{n+1} \right] \frac{\Delta t}{2A_2} \quad (5-44)$$

or

$$Y_i^{n+1} = \frac{\frac{A_1}{A_2} S V_1^{n+1} + I^n + \left[S (V_1^n + V_1^{n+1}) - Y_i^n \right] \frac{\Delta t}{2A_2}}{1 + \frac{\Delta t}{2A_2}} \quad (5-45)$$

and finally

$$I_i^{n+1} = I_i^n + \left[S(V_i^n + V_i^{n+1}) - Y_i^n - Y_i^{n+1} \right] \frac{\Delta t}{2A_2} \quad (5-46)$$

If no initialization is specified, $I_i^0 = 0$ and Y_i is the entered initial value. If initialization is specified, then

$$Y_i^0 = S V_i^0, \quad I_i^0 = \left(1 - \frac{A_1}{A_2} \right) S V_i^0 \quad (5-47)$$

For both lag and lead-lag components, if $V_i = Y_k$: $k = i$ is an error; when $k < i$, old and new values are used as indicated; if $k > i$,

V_i^n and V_i^{n+1} are really Y_k^{n-1} , Y_k^n .

5.7 Shaft Component

The shaft component is a specialized control component that advances the rotational velocity,

$$\sum_i I_i \frac{d\omega}{dt} = \sum_i \tau_i - \sum_i f_i \omega + \tau_c \quad (\text{SHAFT}) \quad (5-48)$$

where I_i is the moment of inertia from component i , τ_i is the torque from component i , f_i is the friction from component i , and τ_c is an optional torque from a control component. The summations are over the pump, generator, motor, or turbine components that might be connected to the shaft and the shaft itself. The shaft and each associated component contains its own model, data, and storage for inertia, friction, and torque and has storage for its rotational velocity. Each associated component also has a disconnect trip number. If zero (no trip), the component is always connected to the shaft. If a trip is specified, the component is connected when false and disconnected when true. Any disconnected component is advanced separately and thus can have a different rotational velocity than the shaft. All connected components have the same rotational velocity.

The shaft equation is advanced explicitly by

$$\sum_i I_i^n \frac{(\omega^{n+1} - \omega^n)}{\Delta t} = \sum_i \tau_i^n - \sum_i f_i^n \omega^n + \tau_c \quad . \quad (5-49)$$

Inertias, torques, and friction are evaluated using old time information. The torque from the control system, τ_c , would be in terms of new time values for quantities other than control variables and would use new or old time values for control variables, depending on their component numbers relative to the shaft component number. Except when a generator component is involved, the shaft component calculations consist of solving Equation (5-49) for ω^{n+1} separately for each component disconnected from the shaft (if any) and for the shaft and the connected components as one system. For separated components, the new rotational velocity is stored with the component data, and the summations are only over terms within the component. For the shaft and the connected components, the summations are over the shaft and the connected components; and the new rotational velocity is stored as the shaft's and each connected component's rotational velocity. A tripped generator, attached or connected, is treated as described above. An untripped generator rotates at the input synchronous speed; and, if connected to the shaft, the shaft and all connected components are forced to the synchronous speed.

6. TRIP SYSTEM

The trip system consists of the evaluation of logical statements. Each trip statement is a simple logical statement which has a true or false result and an associated variable, TIMEOF. The TIMEOF variable is -1.0 whenever the trip is false and contains the time the trip was last set true whenever the trip is true. This variable allows for time delays and unit step functions based on events during the transient.

Within the structure of SCDAP/RELAP5, the trip system is considered to be only the evaluation of the logical statements. The decision of what action is needed based on trip status resides within other models. For example, valve models are provided that open or close the valve based on trip values; pump models test trip status to determine whether a pump electrical breaker has tripped.

Two types of trip statements are provided--variable and logical trips. Since logical trips involve variable trips and other logical trips, complex logical expressions can be constructed from simple logical statements. Both types of trips can be latched or unlatched. A latched trip, once set true, is no longer tested and remains true for the remainder of the problem or until reset at a restart. An unlatched trip is evaluated every time step.

6.1 Variable Trips

A variable trip evaluates the statement

$$T_{ri} = V_1 \text{ OP } (V_2 + C) \quad . \quad (6-1)$$

The value T_{ri} is the i -th trip variable that may be true or false. Values V_1 and V_2 are quantities from the heat structures, hydrodynamics, reactor kinetics, control systems, or may be a TIMEOF quantity. C is a constant; OP is one of the arithmetic relational operations: (EQ) is equal; (NE) is not equal; (GT) is greater than; (GE) is greater than or equal; (LT) is less than; (LE) is less than or equal.

Trips are evaluated at the beginning of the overall SCDAP/RELAP5 time advancement and are evaluated in numerical order. Except for TIMEOF variables, all other V quantities have beginning of time step values; and the results of the trip evaluation are independent of the evaluation order. But when a variable trip statement references TIMEOF (T_{rk}), the new value of TIMEOF is used if $k < i$.

6.2 Logical Trips

A logical trip evaluates

$$T_{ri} = \pm T_{rj} \text{ OP } \pm T_{rl} \quad . \quad (6-2)$$

The values T_{rj} and T_{rl} are variable or logical trips; and the minus sign, if present, denotes the complement of the trip value. The value OP is one of the logical operations AND, OR (inclusive or), or XOR (exclusive or).

Logical trips are evaluated following the evaluation of variable trips and are evaluated in numerical order. When T_{rj} (or T_{rl}) is a variable trip, new trip values are used; when T_{rj} is a logical trip used in logical trip expression i , new values are used when $j < i$, and old values are used when $j \geq i$.

7. REACTOR KINETICS MODELS

The reactor kinetics capability can be used to compute the power behavior in a nuclear reactor when running RELAP5 models without the SCDAP core behavior models. The power is computed using the space-independent or point kinetics approximation that assumes that power can be separated into space and time functions. This approximation is adequate for cases in which the space distribution remains nearly constant.

The reactor kinetics model computes both the immediate fission power and the power from decay of fission fragments. The immediate power is that released at the time of fission and includes power from fission fragment kinetic energy and neutron moderation. Decay power is generated as the fission products undergo radioactive decay. The user can select the decay power model based on either an ANS Standard⁷⁻¹ proposed in 1973 or on the 1979 ANS Standard for Decay Heat Power in Light Water Reactors.⁷⁻²

7.1 Reactor Kinetics Equations

The point kinetics equations are

$$\frac{d\phi(t)}{dt} = \frac{[\rho(t) - \beta] \phi(t)}{\Lambda} + \sum_{i=1}^N \lambda_i C_i(t) + S \quad (7-1)$$

$$-\frac{dC_i(t)}{dt} = -\frac{\beta f_i}{\Lambda} \phi(t) - \lambda_i C_i(t) \quad i = 1, 2, \dots, N \quad (7-2)$$

$$\psi(t) = \Sigma_f \phi(t) \quad (7-3)$$

$$P_f(t) = Q_f \psi(t) , \quad (7-4)$$

where

t	=	time
ϕ	=	neutron flux
C_i	=	number of delayed neutron precursors of group i
β	=	effective delayed neutron fraction
Λ	=	prompt neutron generation time
ρ	=	reactivity (only the time dependence has been indicated; however, the reactivity is dependent on other variables)
f_i	=	fraction of delayed neutrons of group i
λ_i	=	decay constant of group i
S	=	source
ψ	=	fission rate in #/s
Σ_f	=	fission cross section
P_f	=	immediate fission power in MeV/s
Q_f	=	immediate fission energy per fission in MeV.

7.2 Fission Fragment Decay Model

The 1979 standard expresses the power $P_\alpha(t)$ in MeV/s as a function of time t resulting from one fission of isotope α at $t = 0$ as

$$P_\alpha(t) = \sum_{j=1}^{N_\alpha} a_{\alpha j} \exp(-\lambda_{\alpha j} t) \quad . \quad (7-5)$$

Data are presented for three isotopes, ^{235}U , ^{238}U , and ^{239}Pu . The parameters a and λ were obtained by fitting to fission decay power data. The fitting for each isotope used 23 groups ($N_\alpha = 23$). The above expression is an impulse response to one fission and can be extended to an arbitrary fission rate $\psi_\alpha(t)$ through the convolution integral

$$P_\alpha(t) = \sum_j^{N_\alpha} a_{\alpha j} \exp(-\lambda_{\alpha j} t) * \psi_\alpha(t) \quad (7-6)$$

where the convolution operation is defined by

$$A(t) * B(t) = \int_0^t A(t - \tau) B(\tau) d\tau = \int_0^t A(\tau) B(t - \tau) d\tau . \quad (7-7)$$

Since numerical evaluation of convolution integrals is cumbersome, a set of differential equations equivalent to the convolution integral is derived.

Assume that the power from each group is from radioactive decay of a fission fragment i . Then

$$P_{\alpha j}(t) = \lambda_{\alpha j} \gamma_{\alpha j} = a_{\alpha j} \exp(-\lambda_{\alpha j} t) . \quad (7-8)$$

For simplification in the following derivation, the α and j subscripts are dropped and the following expressions represent an equation for one group for one isotope. From Equation (7-8), we have

$$\gamma(t) = \frac{a}{\lambda} \exp(-\lambda t) . \quad (7-9)$$

Laplace transforming Equation (7-8), gives

$$\gamma(s) = \frac{a}{\gamma(s) + \lambda} \quad (7-10)$$

Rearranging Equation (7-10) gives

$$s\gamma(s) = \frac{a}{\lambda} - \lambda\gamma(s) \quad (7-11)$$

Transforming to real time yields

$$\frac{d\gamma(t)}{dt} = \frac{a}{\lambda} \delta(0) - \lambda\gamma(t) \quad (7-12)$$

where $\delta(0)$ is the impulse function. Applying a time-dependent fission rate $\psi(t)$ in place of the single fission (impulse response), Equation (7-11) and (7-12) become

$$s\gamma(s) = \frac{a}{\lambda} \psi(s) - \lambda\gamma(s) \quad (7-13)$$

$$\frac{d\gamma(t)}{dt} = \frac{a}{\lambda} \psi(t) - \lambda\gamma(t) \quad (7-14)$$

Solution of Equation (7-13) or (7-14) (remembering that $P = \lambda\gamma$) for an impulse yields Equation (7-5) and a similar expression in the standard. Solution of Equation (7-13) or (7-14) for an arbitrary fission source yields Equation (7-7). When specifying

$$\psi(t) = 1, 0 \leq t \leq T$$

$$= 0, t > T, \quad (7-15)$$

Equations (7-13) and (7-14) yield another solution given in the standard. (Note that the standard defines t as starting at 0 after fissioning for 1 seconds.)

A physical model can be attached to the terms in Equation (7-14). The first term on the right represents production of the isotope during fission; the last term is the loss of the isotope due to decay. A more mechanistic model would provide for production of one isotope due to the decay of another (see Section 7.3).

The 1979 ANS standard for decay power can be implemented by advancing the differential equations, which become

$$\frac{d\gamma_{\alpha j}(t)}{dt} = \frac{F_Y a_{\alpha j}}{\lambda_{\alpha j}} F_{\alpha} \psi(t) - \lambda_{\alpha j} \gamma_{\alpha j}(t)$$

$$j = 1, 2, \dots, N_{\alpha}$$

$$\alpha = 1, 2, 3 \quad (7-16)$$

$$P_Y(t) = \sum_{\alpha=1}^3 \sum_{j=1}^{N_{\alpha}} \lambda_{\alpha j} \gamma_{\alpha j}(t) \quad (7-17)$$

where ψ is the fission rate from all isotopes, F_{α} is the fraction of fissions from isotope α , and P_Y is the decay power. Summation of F_{α} over α is 1.0. The value F_Y is a input factor to allow easy specification of a conservative calculation. It is usually 1.0 for best-estimate calculations, and 1.2 was recommended for a conservative calculation with the 1973 data. The 1979 data should allow consistent use of 1.0 for F_Y .

The 1973 proposed standard as implemented in RELAP5/MOD1 used one isotope and prescribed data for 11 groups. The 1979 standard lists data for three isotopes, ^{235}U , ^{238}U , and ^{239}Pu , and uses 23 groups for each isotope. A user option also allows only the 1979 standard data for ^{235}U to be used. The data for both standards are built into the code as default data, but the user may enter different data.

7.3 Actinide Decay Model

The actinide model describes the production of ^{239}U , ^{239}Np , and ^{239}Pu from neutron capture by ^{238}U .

$$\frac{d\gamma_u(t)}{dt} = F_u \psi(t) - \lambda_u \gamma_u(t) \quad (7-18)$$

$$\frac{d\gamma_N(t)}{dt} = \lambda_u \gamma_u(t) - \lambda_N \gamma_N(t) \quad (7-19)$$

$$P_\alpha = \eta_u \lambda_u \gamma_u + \eta_N \lambda_N \gamma_N \quad (7-20)$$

The quantity F_u is user-specified and is the number of atoms of ^{239}U produced by neutron capture in ^{238}U per fission from all isotopes. A conservative factor if desired should be factored into F_u . The λ and η values can be user-specified, or default values equal to those stated in the standard can be used.

The first equation describes the rate of change of atoms of ^{239}U . The first term on the right represents the production of ^{239}U ; the last term is the loss of ^{239}U due to beta decay. The second equation describes the rate of change of ^{239}Np . The production of Np is from the beta decay of ^{239}U , and ^{239}Pu is formed from the decay of ^{239}Np . Solution of the actinide equations, Equations (7-18) and (7-19), for the fission source given in Equation (7-15) yields the result quoted in the 1979 standard.

7.4 Transformation of Equations for Solution

The differential equations to be advanced in time are Equation (7-1), (7-2), (7-16), (7-18), and (7-19). (The equations are ordered in storage as listed for programming convenience and to enhance vectorization.) Multiplying by Σ_f and X , the conversion from MeV/s to watts, as needed, the equations become,

$$\frac{d}{dt} [X \psi(t)] = \frac{[\rho(t) - \beta]}{\Lambda} X \psi(t) + \sum_{i=1}^N \lambda_i X \sum_f C_i(t) \quad (7-21)$$

$$\frac{d}{dt} [X \sum_f C_i(t)] = \frac{\beta f_i X \psi(t)}{\Lambda} - \lambda_i X \sum_f C_i(t)$$

$$i = 1, 2, \dots, N \quad (7-22)$$

$$\frac{d}{dt} [X \gamma_{\alpha j}(t)] = \frac{F_{\gamma_{\alpha j}} F_{\alpha} X}{\lambda_{\alpha j}} \psi(t) - \lambda_{\alpha j} X \gamma_{\alpha j}(t)$$

$$j = 1, 2, \dots, N_{\alpha}$$

$$\alpha = 1, 2, 3 \quad (7-23)$$

$$\frac{d}{dt} [X \gamma_u(t)] = F_u X \psi(t) - \lambda_u X \gamma_u(t) \quad (7-24)$$

$$\frac{d}{dt} [X \gamma_N(t)] = \lambda_u X \gamma_u(t) - \lambda_N X \gamma_N(t) \quad (7-25)$$

The total power, P_T , is the sum of immediate fission power, fission product decay, and actinide decay, and now in units of watts is

$$P_T(t) = Q_F X \psi(t) + \sum_{a=1}^3 \sum_{j=1}^{N_a} \lambda_{aj} X \gamma_{aj}(t) + \eta_u g_u X q_u(t)$$

$$+ \eta_N \gamma_N X \lambda_N(t) \quad (7-26)$$

For solution convenience, the following substitutions are made:

$$\rho(t) = \beta r(t) \quad (7-27)$$

$$X \psi(t) = \psi'(t) \quad (7-28)$$

$$X \frac{\Lambda S}{\beta} = S' \quad (7-29)$$

$$X \sum_f C_i(t) = \frac{\beta f_i W_i(t)}{\Lambda \lambda_i} \quad (7-30)$$

$$X \gamma_{\alpha j}(t) = \frac{F_Y a_{\alpha j} F_{\alpha}}{\lambda_{\alpha j}^2} Z_{\alpha j}(t) \quad (7-31)$$

$$X \gamma_u(t) = \frac{F_u}{\lambda_u} Z_u(t) \quad (7-32)$$

$$X q_N(t) = Z_N(t) \quad (7-33)$$

The equations to be advanced are now

$$\frac{d\psi'}{dt}(t) = \frac{\beta}{\Lambda} [r(t) - 1] \psi'(t) + \sum_{i=1}^N f_i W_i(t) + S' \quad (7-34)$$

$$\frac{d}{dt} W_i(t) = \lambda_i \psi'(t) - \lambda_i W_i(t) \quad i = 1, 2, \dots, N \quad (7-35)$$

$$\frac{d}{dt} Z_u(t) = \lambda_u \psi'(t) - \lambda_u Z_u(t) \quad (7-36)$$

$$\frac{d}{dt} Z_N(t) = F_u Z_u(t) - \lambda_N Z_N(t) \quad (7-37)$$

$$P_1(t) = Q_f \psi'(t) + \sum_{\alpha=1}^3 \sum_{j=1}^{N_{\alpha}} \frac{F_Y a_{\alpha j} F_{\alpha} Z_{\alpha j}(t)}{q_{\alpha j}}$$

$$+ F_u \eta_u Z_u(t) + \eta_N \lambda_N Z_N(t) \quad . \quad (7-38)$$

These equations are advanced using the modified Runge-Kutta method¹⁶⁸ described in Section 5.7.

7.5 Initialization

Two initialization options are provided. In both options, the fission rate and delayed neutrons are in steady state or equilibrium conditions, that is, their time derivatives are zero. With $r(0)$ an input quantity,

$$W_i(0) = \psi(0) \quad i = 1, 2, \dots, N \quad (7-39)$$

$$S' = -r(0) \psi(0) \quad . \quad (7-40)$$

The first option assumes that the fission product decay and actinides are also in equilibrium. This is equivalent to assuming that the reactor has been operating at a constant total power for an infinite period of time. The initial conditions are

$$Z_{aj}(0) = \psi(0) \quad j = 1, 2, 3, \dots, N_a$$

$$a = 1, 2, 3 \quad (7-41)$$

$$Z_u(0) = \psi(0) \quad (7-42)$$

$$Z_N(0) = \frac{F_u}{q_u} \psi(0) \quad (7-43)$$

$$P_T(0) = Q \psi(0) \quad (7-44)$$

$$Q = Q_f + \sum_{\alpha=1}^3 \sum_{j=1}^{N_\alpha} \frac{F_{q_{\alpha j}}}{\lambda_{\alpha j}} + F_u \eta_u + F_u \eta_N \quad . \quad (7-45)$$

The quantity Q , which is the total energy in MeV generated per fission, is either an input value or can be defaulted to 200 MeV. The quantity Q_f is defined from Equation (7-45) and the user-specified or defaulted data, even if the second initialization option is used. The total power is an input quantity, and the source ψ is computed from Equation (7-44).

The second option uses a power history to determine the initial values of the fission product and actinide quantities. The power history consists of one or more periods of constant total power. For each period, the input consists of the total power, the time duration at that power, and, in the case of three isotopes, the fraction of power from each isotope. The fission product and actinide differential equations, Equations (7-35), (7-36), and (7-37) are advanced in time starting with initial values of zero. The fission rate, ψ , is defined from Equation (7-38). The fission rate is reset to zero whenever a negative value is computed. This would occur whenever the user-entered total power is less than the current fission product and actinide decay power. Thus, for shutdown periods, the user may conveniently enter zero total power even though significant decay power remains. The fission product and actinide values at the end of the power history become the initial values for the transient. The initial fission rate is computed from Equation (7-38), using the total reactor power at the start of the transient (which may be different from the last power history value). If this fission rate is negative or zero, it is reset such that the immediate fission power is 10^{-12} times the decay power.

The differential equations for the power history calculation are advanced using the same numerical technique as for the transient advancement except for a simplified time step control. Time step control consists of starting the advancement of each history period with a time step of 1 s. The time step is doubled after each advancement. When the next advancement would exceed the time duration, the last advancement is with the remaining time. This scheme was selected since, with each different power value, the solution moves toward a new equilibrium condition asymptotically; and the most rapid change is at the beginning of a power change.

7.6 Reactivity Feedback

One of two models can be selected for reactivity feedback. The separable model defines reactivity as

$$r(t) = r_0 - r_B + \sum_i^{n_s} r_{si}(t) + \sum_i^{n_c} v_{ci} + \sum_i^{n_\rho} \left\{ w_{\rho i} R_\rho [\rho_i(t)] + a_{wi} T_{wi}(t) \right\} + \sum_i^{n_F} \left\{ w_{Fi} R_F [T_{Fi}(t)] + a_{Fi} T_{Fi}(t) \right\} \quad (7-46)$$

The quantity r_0 is an input quantity and represents the reactivity corresponding to assumed steady-state reactor power at $t = 0$. The quantity r_B is the bias reactivity and is calculated during input processing such that $r(0) = r_0$. This bias reactivity is printed in the input level printout. Should the user check the bias reactivity computation using Equation (7-46), the temperature used in the $a_{wi} T_{wi}(t)$, and $a_{Fi} T_{Fi}(t)$ terms should use absolute temperature (i.e., Kelvin in SI units and Rankine in British units). The temperature used in the table lookup term $w_{Fi} R_F [T_{Fi}(t)]$, however, should still use Kelvin in SI units and Fahrenheit in British units.

The quantities r_{si} are obtained from input tables defining n_s reactivity curves as a function of time. The quantities v_{ci} are n_c control variables that can be user-defined as reactivity contributions. R_ρ is a table defining reactivity as a function of the current density of water $\rho_i(t)$ in the hydrodynamic volume i ; $w_{\rho i}$ is the density weighting factor for volume i ; T_{wi} is the spatial density averaged temperature of volume i ; a_{wi} is the temperature coefficient (not including density changes) for volume i ; and n_ρ is the number of hydrodynamic volumes in the reactor core. The value R_F is a table defining reactivity as a function of the average fuel temperature T_{Fi} in

a heat structure; w_{fi} and a_{fi} are the fuel temperature weighting factor and the fuel temperature coefficient, respectively; and n_f is the number of heat structures in the reactor core.

This model assumes nonlinear feedback effects from moderator density and fuel temperature changes and linear feedback from moderator temperature changes. It is called the separable model because each effect is assumed to be independent of the other effects. Boron feedback is not provided, but a user-defined boron feedback can be implemented with the control system.

The separable model can be used if boron changes are quite small and the reactor is near critical about only one state point.

A postulated BWR A1WS accident is an example where the reactor could be nearly critical for two different state points. One point is at normal power operating conditions--high moderator and fuel temperatures, highly voided, and no boron. During accident recovery, the reactor might approach a critical condition with relatively cold moderator and fuel temperatures, with no voids, but with some boron concentration. The reactivity could be nearly critical for both states, but the contributions from the different feedback effects are vastly different. The assumptions of no interactions among the different feedback mechanisms, especially boron, cannot be justified. The tabular model defines reactivity as

$$r(t) = r_0 - r_B + \sum_i^{n_s} r_{si} + \sum_i^{n_c} v_{ci} + R[\bar{\rho}(t), \bar{T}_w(t), \bar{T}_f(t), \bar{B}(t)] \quad (7-47)$$

$$\bar{\rho}(t) = \sum_i^n w_{\rho i} \rho_i(t) \quad (7-48)$$

$$\bar{T}_W(t) = \sum_i^{n_p} W_{pi} T_{Wi}(t) \quad (7-49)$$

$$\bar{B}(t) = \sum_i^{n_p} W_{pi} B_i(t) \quad (7-50)$$

$$\bar{T}_F(t) = \sum_i^{n_f} W_{Fi} T_{Fi}(t) \quad (7-51)$$

where B is boron density. The average quantities are obtained with the use of one weighting factor for each hydrodynamic volume and each heat structure contributing to reactivity feedback. The reactivity function R is defined by a table input by the user. In the TABLE4 option (see Section 11.1 of Volume III of this report), the table is four-dimensional; the TABLE3 option assumes no boron dependence and the table is then three-dimensional.

The tabular model overcomes the objections of the separable model, since all feedback mechanisms can be nonlinear and interactions among the mechanisms are included. The penalty for the expanded modeling capability greatly increases the input data requirements.

The reactivity function R is evaluated by a direct extension of the one-dimensional table lookup and linear interpolation scheme to multiple dimensions. One-dimensional table lookup and interpolation of the function $V = F(W)$ uses an ordered set of N_w independent variable values W_i , with the corresponding values of the dependent variable V_i , to determine the value of V corresponding to a search argument W . The independent variable is searched such that W_i and W_{i+1} bracket W ; an equation for a straight line is fitted to the points W_i, V_i , and W_{i+1}, V_{i+1} ; and the straight line equation is evaluated for the given W .

Using subscripts 0 and 1 for bracketing independent values and corresponding dependent values and defining $w = (W - W_0)/(W_1 - W_0)$ so that w varies from 0 through 1 as W varies from W_0 through W_1 , the interpolation equations are

$$V = \sum_{i=0}^1 a_i w^i \quad (7-52)$$

$$a_0 = V_0 \quad (7-53)$$

$$a_1 = V_1 - V_0 \quad (7-54)$$

For two-dimensional interpolation of $V = F(W,X)$, two sets of independent variables are used: N_w values of W_i and N_x values of X_j . A total of $N_w N_x$ dependent values of V_{ij} are entered, one value for each combination of variables from the two sets of independent variables. Graphically, the two sets of independent variables form a rectangular grid when the W_i and X_j variables are plotted on horizontal and vertical coordinates, respectively. The dependent variables are entered corresponding to the intersections of the mesh lines. The search for bracketing values in each independent set locates a mesh rectangle, and the dependent values at the four corners are used to form an interpolation equation which is the product of two straight line functions, one for each independent variable. Using 0 and 1 subscripts for the bracketing values,

$$V = \sum_{i=0}^1 \sum_{j=0}^1 a_{ij} w^i x^j \quad (7-55)$$

$$x = \frac{x - X_0}{X_1 - X_0} \quad (7-56)$$

$$a_{00} = V_{00} \quad (7-57)$$

$$a_{01} = V_{01} - V_{00} \quad (7-58)$$

$$a_{10} = V_{10} - V_{00} \quad (7-59)$$

$$a_{11} = V_{11} - V_{01} - V_{10} + V_{00} \quad (7-60)$$

This process is simply extended to three and four dimensions. Three sets of independent variables define a three-dimensional rectangular grid; and eight dependent quantities corresponding to the corners of a rectangular solid are used to define the interpolation equation, which is the product of three straight line functions. In four dimensions, four sets of independent variables are defined; and 16 dependent values are used to define the interpolation equations, which is the product of four straight line functions.

For three-dimensional interpolation,

$$V = F(W, X, Y) \quad (7-61)$$

$$y = \frac{y - Y_0}{Y_1 - Y_0} \quad (7-62)$$

$$V = \sum_{i=0}^1 \sum_{j=0}^1 \sum_{k=0}^1 a_{ijk} w^i x^j y^k \quad (7-63)$$

$$a_{000} = V_{000} \quad (7-64)$$

$$a_{001} = V_{001} - V_{000} \quad (7-65)$$

$$a_{010} = V_{010} - V_{000} \quad (7-66)$$

$$a_{100} = V_{100} - V_{000} \quad (7-67)$$

$$a_{011} = V_{011} - V_{001} - V_{010} + V_{000} \quad (7-68)$$

$$a_{101} = V_{101} - V_{001} - V_{100} + V_{000} \quad (7-69)$$

$$a_{110} = V_{110} - V_{010} - V_{100} + V_{000} \quad (7-70)$$

$$a_{111} = V_{111} - V_{011} - V_{101} - V_{110} + V_{001} + V_{010} + V_{100} - V_{000} \quad (7-71)$$

For four-dimensional interpolation,

$$V = F(W, X, Y, Z) \quad (7-72)$$

$$z = \frac{Z - Z_0}{Z_1 - Z_0} \quad (7-73)$$

$$V = \sum_{i=0}^1 \sum_{j=0}^1 \sum_{k=0}^1 \sum_{l=0}^1 a_{ijkl} w^i x^j y^k z^l \quad (7-74)$$

$$a_{0000} = V_{0000} \quad (7-75)$$

$$a_{0001} = V_{0001} - V_{0000} \quad (7-76)$$

$$a_{0010} = V_{0010} - V_{0000} \quad (7-77)$$

$$a_{0100} = V_{0100} - V_{0000} \quad (7-78)$$

$$a_{1000} = V_{1000} - V_{0000} \quad (7-79)$$

$$a_{0011} = V_{0011} - V_{0001} - V_{0010} + V_{0000} \quad (7-80)$$

$$a_{0101} = V_{0101} - V_{0001} - V_{0100} + V_{0000} \quad (7-81)$$

$$a_{0110} = V_{0110} - V_{0010} - V_{0100} + V_{0000} \quad (7-82)$$

$$a_{1001} = V_{1001} - V_{0001} - V_{1000} + V_{0000} \quad (7-83)$$

$$a_{1010} = V_{1010} - V_{0010} - V_{1000} + V_{0000} \quad (7-84)$$

$$a_{1100} = V_{1100} - V_{0100} - V_{1000} + V_{0000} \quad (7-85)$$

$$a_{0111} = V_{0111} - V_{0011} - V_{0101} + V_{0110} + V_{001} + V_{0010} \\ + V_{0100} - V_{0000} \quad (7-86)$$

$$a_{1011} = V_{1011} - V_{0011} - V_{1001} + V_{1010} + V_{0001} + V_{0010} \\ + V_{1000} - V_{0000} \quad (7-87)$$

$$a_{1101} = V_{1101} - V_{0101} - V_{1001} + V_{1100} + V_{0001} + V_{0100} \\ + V_{1000} - V_{0000} \quad (7-88)$$

$$a_{1110} = V_{1110} - V_{0110} - V_{1010} + V_{1100} + V_{0010} + V_{0100} \\ + V_{1000} - V_{0000} \quad (7-89)$$

$$a_{1111} = V_{1111} - V_{0111} - V_{1011} - V_{1101} - V_{1110} + V_{0011} \\ + V_{0101} + V_{0110} + V_{1101} + V_{1001} + V_{1010} + V_{1100} \\ - V_{0001} - V_{0010} - V_{0100} - V_{1000} + V_{0000} \quad (7-90)$$

The interpolating equations define a continuous function, that is, there is no discontinuity in the dependent quantity, as any one or combination of dependent variables pass to the next bracketing pair of values.

Using N_W , N_X , N_Y , and N_Z as the number of values in the four sets of independent variables, the number of data points for a three-dimensional table is $N_W N_X N_Y$ and is $N_W N_X N_Y N_Z$ for a four-dimensional table. Using only four values for each independent variable, a four-dimensional table requires 256 data points.

7.7 Reactor Kinetics Numerical Procedures

The reactor kinetics equations are advanced in time using the modified Runge-Kutta Method of Cohen.⁷⁻³ A first-order differential equation is written as

$$\dot{n}(t) = \alpha n(t) + R(n,t) \quad (7-91)$$

where α is constant over the time step, and $R(n,t)$ contains the remaining terms of the differential equation, including the nonconstant portion of any coefficient of $n(t)$. If the coefficient of $n(t)$ is $\beta(n,t)$, α would be $\beta[n(0),0]$; and $R(n,t)$ would contain a term of the form $\beta[n(t),t] - \alpha n(t)$. Multiplying Equation (7-91) by an integrating factor and integrating gives

$$n(t) = n(0) e^{\alpha t} + \int_0^t e^{\alpha(t-\lambda)} R(n,\lambda) d\lambda \quad (7-92)$$

Since

$$n(0) e^{\alpha t} = n(0) + \int_0^t \alpha n(0) e^{\alpha(t-\lambda)} d\lambda, \quad (7-93)$$

$$n(t) = n(0) + \int_0^t [\alpha n(0) + R(n,\lambda)] e^{\alpha(t-\lambda)} d\lambda \quad (7-94)$$

Letting $\lambda = ut$, then $d\lambda = tdu$, and

$$n(t) = n(0) + t \int_0^1 [\alpha n(0) + R(n,u)] e^{\alpha t(1-u)} du \quad (7-95)$$

The numerical technique for advancing the solution over the time step consists of making approximations to the behavior of $R(n,u)$ over the time step. For convenience in the following expressions, the following function is defined:

$$C_m(x) = \int_0^1 u^{m-1} e^{x(1-u)} du \quad (7-96)$$

Stage 1:

Assume $R(n,\lambda) = R[n(0),0] = R_0$, and write $n(0)$ as n_0 ; then compute $n(\frac{h}{2})$,

$$n_1 = n(\frac{h}{2}) = n_0 + \frac{h}{2} (\alpha n_0 + R_0) C_1 \left(\alpha \frac{h}{2} \right) \quad (7-97)$$

Stage 2:

Assume straight-line variation of $R(n,\lambda)$ between R_0 and $R_1 = R(n_1, \frac{h}{2})$, and compute $n(\frac{h}{2})$,

$$R(n,\lambda) = R_0 + \frac{2(R_1 - R_0)\lambda}{h} \quad (7-98)$$

$$R(n,\lambda) = R_0 + (R_1 - R_0) u \quad (\text{using } \lambda = u \frac{h}{2}) \quad (7-99)$$

$$n_2 = n(\frac{h}{2}) = n_1 + \frac{h}{2} (R_1 - R_0) C_2 \left(\alpha \frac{h}{2} \right) \quad (7-100)$$

Stage 3:

Assume straight-line variation of $R(n, \lambda)$ between R_0 and $R_2 = R(n_2, \frac{h}{2})$, and compute $n(h)$,

$$R(n, \lambda) = R_0 + \frac{2(R_2 - R_0)g}{h} \quad (7-101)$$

$$R(n, u) = R_0 + 2(R_2 - R_0) \quad (\text{using } g = uh) \quad (7-102)$$

$$n_3 = n(h) = n_0 + h(\alpha n_0 + R_0) C_1(\alpha h) + 2h(R_2 - R_0) C_2(\alpha h) . \quad (7-103)$$

Stage 4:

Assume quadratic through points R_0 , R_2 , and $R_3 = R(n_3, h)$; then compute $n(h)$,

$$R(n, u) = (2R_0 - 4R_2 + 2R_3) u^2 + (-3R_0 + 4R_2 - R_3) u + R_0 \quad (7-104)$$

$$n_4 = n(h) = n_3 + h (R_4 - R_3) [2C_3(\alpha h) - C_2(\alpha h)] . \quad (7-105)$$

Stage 5:

Assume quadratic through points R_0 , R_2 , and $R_4 = R(n_4, h)$; then compute $n(h)$

$$n_5 = n(h) = n_4 + h (R_4 - R_3) [2C_3(\alpha h) - C_2(\alpha h)] . \quad (7-106)$$

Third-, fourth-, and fifth-order approximations are obtained by terminating the process at the end of the third, fourth, and fifth stages, respectively. SCDAP/RELAP5 uses only the fifth order approximation.

By direct integration, the function, $C_1(x)$, is given by

$$C_1(x) = \frac{e^x - 1}{x} . \quad (7-107)$$

Using integration by parts, a recursion relation for $C_m(x)$ is

$$C_{m+1}(x) = \frac{mC_m(x) - 1}{x} . \quad (7-108)$$

During machine calculations of the $C_m(x)$ functions for $x \leq 1$, excessive loss of significance occurs. For this range, $C_3(x)$ is computed from its MacClaurin series expansion

$$C_3(x) = 2 \left[\frac{1}{3!} + \frac{x}{4!} + \frac{x^2}{5!} + \frac{x^3}{6!} + \frac{x^4}{7!} + \frac{x^5}{8!} + \frac{x^6}{9!} + \frac{x^7}{10!} \right] . \quad (7-109)$$

C_2 and C_1 are evaluated by solving Equation (7-108) for $C_m(x)$.

During the advancement in time of the solution, the time increment is automatically increased or decreased to maintain a specified degree of accuracy. After the calculations for a reactor kinetics time-advancement, an empirical formula is used to estimate the error. If the error is excessive, the time increment is halved; and the advancement calculation is redone. If the error is sufficiently small, the time interval is doubled for the next time step. If the estimated error is between limits, the same interval is used for the next time advancement. These procedures for time step control, taken from the AIREK⁷⁻⁴ code, are as follows:

$$\omega_1 = \frac{\dot{\Phi}(0)}{\Phi(0)} \quad (7-110)$$

$$\omega_3 = \frac{\dot{\Phi}(h)}{\Phi(h)} \quad (7-111)$$

$$\omega \text{ is defined by } \Phi(h) = \Phi(0)e^{-\omega h} \quad (7-112)$$

$$Q = \frac{h C_2(\alpha h)}{1 + C_1(\alpha h)} [\omega_1 - 2\omega_2 + \omega_3] \quad . \quad (7-113)$$

The α in Equation (7-113) is that of the neutron flux equation [Equation (7-23)]. The quantity, δ , is defined as the maximum (taken over all differential equations) of the quantity,

$$\frac{n_1 - n_0}{n_1} \quad .$$

The Q_L and Q_H appearing below are 0.0001 and 0.001, respectively.

1. If $\delta < 2^{-15}$ and $Q \geq Q_L$, the program continues with the same time step.
2. If $\delta < 2^{-15}$ and $Q < Q_L$, the program doubles the time step for the next advancement.
3. If $\delta \geq 2^{-15}$ and
 - a. $Q < Q_L$, the time step is doubled for the next advancement.
 - b. $Q \leq Q_H$, the same time step is used for the next advancement.
 - c. $Q > Q_H$, the time advancement is recalculated with half the time step.
4. The time advancement is also recomputed with the time step halved if
 - a. αh of any equation > 88.0 .

b. negative or zero power is computed.

If the coefficient of the neutron flux in Equation (7-23) is negative, a subtraction is involved in determination of the derivative and a loss of significant figures can occur. If this coefficient is negative, a check is made of the number of bits lost in the subtraction. If more than nine bits are lost, the value of neutron flux computed by the current stage of the advancement procedure is discarded; instead, neutron flux is determined from the expression obtained by setting the neutron flux derivative to zero,

$$D(t) = \frac{-\sum_{i=1}^I f_i W_i(t) - \frac{SA}{b}}{r(t) - 1} \quad . \quad (7-114)$$

The transfer of information between the reactor kinetics calculation and the other SCDAP/RELAP5 calculations is explicit. Hydrodynamic and heat conduction/transfer calculations precede reactor kinetics, and the control system calculation follows reactor kinetics. The reactor power used in hydrodynamics and heat conduction is the value at the beginning of the time step. The reactivity used as an end-of-time step value in the kinetics advancement uses end-of-time step values from hydrodynamics and heat conduction and beginning-of-time step values from the control system.

The reactor kinetics equations are advanced at the same time step rate as the hydrodynamics, and reactivity is assumed to vary linearly between time step values. The maximum time step for the reactor kinetics advancement is the hydrodynamic time step. That time step is reduced, if necessary, as described above.

7.8 References

- 7-1. American Nuclear Society Proposed Standard ANS 5.1, Decay Energy Release Rates Following Shutdown of Uranium-Fueled Thermal Reactors, October 1971, revised October 1973.
- 7-2. American National Standard for Decay Heat Power in Light Water Reactors, ANSI/ANS-5.1-1979.

7-3. E. R. Cohen, "Some Topics in Reactor Kinetics," A/CONF, 15, 1958,
p. 629.

7-4. A. Schwartz, Generalized Reactor Kinetics Code AIREK II,
NAA-SR-Memo-4980, 1960.

8. SPECIAL TECHNIQUES

The semi-implicit and nearly implicit solution methods are mass and energy conservative. The mass from the state relationship is compared to the mass from the continuity equation, and the difference is a measure of the truncation error inherent in the numerical solution. This is the main method used to control the time step and thus control the truncation error, even though mass and energy are preserved in the solution scheme.

Special methods are provided in the code for use in obtaining initial conditions. These methods are based on the transient solution algorithm but make use of an accelerated thermal transient solution technique in order to shorten the computer time required to achieve steady state.

8.1 Time Step Control

A variety of checks on solution acceptability are used to control the time step. These include material Courant limit checks, mass error checks, material properties out of defined ranges, water property errors, excessive extrapolation of state properties in the meta-stable regimes, or change in heat slab temperature of more than 50 K.

The material Courant limit check is made before a hydrodynamic advancement takes place. Thus, it may reduce the time step, but it does not cause a time step to be repeated. All of the other checks may cause all or part of the time advancement to be repeated at a smaller time step. The material Courant limit is evaluated for each hydrodynamic volume using the volume mass average velocity i.e.,

$$(\Delta t_c)_i = [\Delta x \max(\alpha_f^n, \alpha_g^n) / \max(|\alpha_f^n v_f^n|, |\alpha_g^n v_g^n|)]_i \quad (8-1)$$
$$i = 1, 2, \dots, N$$

The N volumes are sequentially divided into five subsets, i.e., (1, 6, 11, ...) volumes belong to the first subset, (2, 7, 12, ...) volumes belong to

the second subset, etc. The minimum Courant limits for each of the five subsets are rearranged in ascending order, i.e.,

$$\Delta t_c^1 \leq \Delta t_c^2 \leq \Delta t_c^3 \leq \Delta t_c^4 \leq \Delta t_c^5 . \quad (8-2)$$

Obviously, Δt_c^1 is the Courant limit for the entire system. This is the number printed at each major edit under "CRNT. DT = ." For the semi-implicit scheme, Δt_c^2 is used for limiting time step size. Thus, partial violation of the material Courant limit is allowed for this scheme. There is no user input option to select the degree of partial Courant limit violation. For the nearly implicit scheme, five times Δt_c^2 is used for limiting the time step size for the transient mode; and 10 times Δt_c^2 is used for limiting the time step size for the steady-state mode.

The mass error check is made after the time step solution is nearly complete. Thus, if excessive mass error is detected, then the time step is repeated at a reduced interval. Two types of mass error measures are computed. The first one is designed to check the validity of density linearization and is defined as

$$\epsilon_m = \max (|\rho_{mi} - \rho_i| / \rho_i , i = 1, 2, \dots, N) \quad (8-3)$$

where ρ_m is the total density of the i-th volume obtained from the mass continuity equation, and ρ_i is the total density of the i-th volume computed from the state relationship. The second one is a measure of overall system mass error and is given by

$$\epsilon_{rms} = 2 \sum_{i=1}^N [V_i (\rho_i - \rho_{mi})]^2 / \sum_{i=1}^N (V_i \rho_i)^2 . \quad (8-4)$$

If either ϵ_m or ϵ_{rms} is $> 8 \times 10^{-3}$, the time step is rejected and repeated with one half of the time step size. Otherwise, the time step is accepted; and the next time step size is doubled if both ϵ_m and ϵ_{rms} are $< 8 \times 10^{-4}$.

At any point in the solution flow, if a material property is found to lie outside the defined range, then the time step is halved and repeated. This process will proceed until the user-specified minimum time step is reached. If the minimum time step is reached without obtaining a valid solution, then the code calculation is terminated; and the last time step is repeated with a diagnostic dump printed. A program stop is encountered at completion of the step. This same procedure is applied for all property or extrapolation failures.

8.2 Mass/Energy Mitigation

The semi-implicit numerical scheme described in Sections 3.1.4 and 3.1.6 has two calculations of the new time variables α_g , U_g , U_f , and X_n . These variables are first calculated in connection with a linearization of all the product terms involved in the time derivatives and are referred to as tentative new time variables [see Equations (3-65) through (3-69)]. They are denoted by a tilde in Sections 3.1.4 and 3.1.6. This first calculation uses a numerically conservative form for all flux calculations of mass and energy; but, because the products in the time derivatives are linearized, the quantities $\alpha_g \rho_g$, $\alpha_f \rho_f$, $\alpha_g \rho_g U_g$, $\alpha_f \rho_f U_f$, and $\alpha_g \rho_g X_n$ are not numerically conserved. These tentative new time values are only used to evaluate the interphase heat and mass transfer terms to be used in the second evaluation of the basic equations. In this second evaluation of the basic equations [see Equations (3-83), (3-85), (3-86), (3-88), and (3-89)], the products appearing in the time derivatives are not linearized. This second step also uses the numerically conservative form for the flux terms. Hence, the final end of time step values have been calculated using an accurate, numerically conservative form of differencing.

The truncation errors in the linearization procedure may produce errors in the solution of pressure, phasic energies, and void fraction. Since the state is computed from these basic variables, the resultant density may have some error. This error is used in the time step control presented in Section 8.1. Furthermore, the convective terms in the field

equations are computed with donored properties determined by the directions of phasic velocities. There are chances that the final velocities may differ in directions from the explicit velocities used to define the donored properties. This may result in mass/energy errors due to incorrect properties used in the numerical scheme. The scheme used to handle this situation will next be presented.

The term velocity flip-flop refers to the situation in which the final velocities and the explicit velocities differ in sign. In the SCDAP/RELAP5 numerical scheme, the pressures and final velocities are calculated using the donor properties based on the explicit velocities (see Section 3.1.). The velocity flip-flop implies that inconsistent donor properties were used for the pressure computation and the final mass/energy computation. This may result in bad velocity and energy solutions and large mass errors.

Let $\bar{\alpha}_{fj}$, $\bar{\rho}_{fj}$, $\bar{U}_{fj}$, $\bar{\alpha}_{gj}$, $\bar{\rho}_{gj}$, $\bar{U}_{gj}$ be the junction liquid fraction, liquid density, liquid energy, void fraction, vapor density, and vapor energy respectively, based on the explicit velocities and

$\tilde{\alpha}_{fj}$, $\tilde{\rho}_{fj}$, $\tilde{U}_{fj}$, $\tilde{\alpha}_{gj}$, $\tilde{\rho}_{gj}$, and $\tilde{U}_{gj}$ be the same variables based on the final velocities. A velocity flip-flop has occurred when one of the junctions in a system satisfies the following condition:

$$\left| \bar{\alpha}_{fj} \bar{\rho}_{fj} \bar{U}_{fj} + \bar{\alpha}_{gj} \bar{\rho}_{gj} \bar{U}_{gj} - \tilde{\alpha}_{fj} \tilde{\rho}_{fj} \tilde{U}_{fj} - \tilde{\alpha}_{gj} \tilde{\rho}_{gj} \tilde{U}_{gj} \right| > 0.20 (\bar{\alpha}_{fj} \bar{\rho}_{fj} \bar{U}_{fj} + \bar{\alpha}_{gj} \bar{\rho}_{gj} \bar{U}_{gj}) \quad (8-5)$$

Under such circumstances, the pressures and final velocities are recalculated using the donor properties of the previously calculated final velocities. The solution is then accepted if no velocity flip-flop exists between the previous final velocities and new final velocities. Otherwise, the time step size is reduced.

8.3 Steady State

A steady-state initialization capability is included in SCDAP/RELAP5. With this capability, the transient solution algorithm is continually monitored to determine the achievement of a steady state. During this process, convergence criteria are calculated and used in the steady-state testing scheme. These convergence criteria are related to an overall calculational precision. This overall precision is the result of combining both the precision of the transient solution algorithm and the standard tolerance of the thermodynamic state algorithm. The following discussion describes the fundamental concepts of tests to detect steady state during transient calculations.

8.3.1 Fundamental Concepts for Detecting Hydrodynamic Steady State During Transient Calculations

The fundamental concept of steady state is that the state of a system being modeled does not change with respect to time. In the hydrodynamic solution scheme, three terms can be monitored whose variation in time include the variation of all of the other terms. These three terms are the thermodynamic density, internal energy, and pressure. Furthermore, these three terms can be combined into a single term, enthalpy. Hence, monitoring the time variation of enthalpy is equivalent to monitoring the time variation of all of the other variables in the solution scheme. For each volume cell in the system model, the enthalpy can be written as

$$V_i \rho_i^n h_i^n = V_i (\rho_i^n U_i^n + P_i^n) \quad (8-6)$$

where subscript i denotes the i -th volume element; superscript n denotes the solution time, t^n ; h_i is the volume element enthalpy in units of energy per unit mass; V_i is the element volume that is constant; and ρ_i , U_i , and P_i are the thermodynamic density, internal energy and pressure, respectively, of the substance within the volume. Since volume is constant, Equation (8-6) can be simplified as

$$\rho_i^n h_i^n = \rho_i^n u_i^n + p_i^n \quad (8-7)$$

The rate of variation with respect to time of Equation (8-7) can be expressed numerically as

$$\left(\frac{d\rho h}{dt}\right)_i^n \sim \frac{\rho_i^{n+1} u_i^{n+1} + p_i^{n+1} - \rho_i^n u_i^n + p_i^n}{\Delta t^n} \quad (8-8)$$

where superscript n and n+1 denote the old and new time values, respectively. Absolute hydrodynamic steady state occurs when Equation (8-8) is zero for each of the volume elements in the modeled system.

In order to simplify the task of detecting steady state, a system mean enthalpy can be expressed as

$$\overline{\rho h}^n = \frac{\sum_{i=1}^{NVOLS} V_i (\rho_i^n u_i^n + p_i^n)}{\sum_{i=1}^{NVOLS} V_i} \quad (8-9)$$

A system mean rate of change can also be formulated as

$$\overline{\frac{d\rho h}{dt}}^n = \frac{1}{\Delta t^n} \frac{\sum_{i=1}^{NVOLS} V_i \left[(\rho_i^{n+1} u_i^{n+1} + p_i^{n+1}) - (\rho_i^n u_i^n + p_i^n) \right]}{\sum_{i=1}^{NVOLS} V_i} \quad (8-10)$$

However, since the rate of change in any volume element can be positive or negative, these terms would tend to cancel. Hence, a better formulation for the mean rate of change is as a mean square summation that can be written as

$$\left(\frac{d\rho h}{dt}\right)^2 = \frac{1}{(\Delta t^n)^2} \frac{\sum_{i=1}^{NVOLS} v_i^2 \left[(\rho_i^{n+1} u_i^{n+1} + p_i^{n+1}) - (\rho_i^n u_i^n + p_i^n) \right]^2}{\sum_{i=1}^{NVOLS} v_i^2} \quad (8-11)$$

During the course of the problem solution, Equation (8-11) can be used to monitor the system approach to steady state because, as each volume element approaches steady state, its rate of change goes to zero and drops out of the summation. The detection of absolute steady state is therefore relatively simple, since the calculations need only be monitored until Equation (8-11) becomes zero. However, another property of Equation (8-11) is that it will fluctuate wildly, varying between small and large magnitudes. These fluctuations decrease in magnitude as the calculations proceed toward steady state. Hence, Equation (8-11) is not a well-behaved function, and it is therefore difficult to monitor its behavior. However, a well-behaved function can be curve-fitted to the results of Equation (8-11) over reasonable time intervals. An exponential function is of this type; and if

$$\left(\frac{d\rho h}{dt}\right)^2 \sim y = e^{\alpha} + \beta t^n + \gamma t^{n^2} + \phi t^{n^3}, \quad t_0 \leq t^n \leq t, \quad (8-12)$$

the coefficients α , β , γ , and ϕ may be computed by the method of least squares over any reasonable time interval greater than four time steps. Equation (8-12) has the property that it can increase to large values at small values of time and then decrease to small values as time increases and the system approaches steady state. Equation (8-12) represents the time-smoothed root mean square (RMS) rate of change in system enthalpy.

Because the user must provide boundary conditions, controls, or trips to guide the transient solution to steady state, it may not be possible to achieve an absolute steady state. For example, a steam generator water

level control may be modeled so that the water level oscillates between high and low set points. In addition, since numerical schemes are inexact, it may only be possible to calculate absolute steady state within a small limit of precision. For this kind of fluctuating average steady state, the RMS ($d\rho h/dt$) will approach a constant, positive, non-zero value. As a result, an additional method must be used to detect an average steady state over limited time intervals.

If the system $\overline{\rho h}^n$ is varying with time over the interval

$$t_1 \leq t^n \leq t_2, \quad (8-13)$$

its variation can be expressed approximately in the form of a straight line such that

$$H^n = b + at^n \sim \overline{\rho h}^n. \quad (8-14)$$

If the system is approaching an absolute steady state, then the line rate of change will be zero and Equation (8-14) will give the system time average ρh such that

$$\overline{\rho h}^{t_1 t_2} = b, \quad t_1 \leq t^n \leq t_2 \quad (8-15)$$

where the superscript $t_1 \text{---} t_2$ denotes a time average over the interval $t_1 \leq t^n \leq t_2$.

The second testing method consists of monitoring the system ρh^n at the completion of each successful time step and, at reasonable time intervals, solving, for the straight line coefficients a and b using the method of least squares.

In performing the method of least squares, the mean system enthalpy is computed at the successful completion of each time step in the interval

$$t_1 \leq t^n \leq t_2, \quad (8-16)$$

and an equation expressing the sum of the squares of the differences between ρh^n and Equation (8-14) can be written as

$$\xi_{\rho h}^2 \left|_{t_1}^{t_2} = \sum_{n=n_1}^{n_2} (\bar{\rho h}^n - b - at^n)^2. \quad (8-17)$$

The coefficients a and b can then be calculated by the method of least squares.

A measure of the RMS fluctuation of ρh^n with respect to the line of Equation (8-14) can also be computed using the mean square form of Equation (8-17) where

$$\left|_{t_1}^{t_2} \frac{1}{(f_{\rho h}^2)_{\text{RMS}}} = \left[\frac{1}{(n_2 - n_1)} \xi_{\rho h}^2 \left|_{t_1}^{t_2} \right]^{1/2}. \quad (8-18)$$

The RMS fluctuation then represents a measure of the typical difference between the mean system enthalpy and the line of Equation (8-14). However, the coefficients a and b cannot be calculated with any better precision than the overall precision of the solution scheme for the entire system.

8.3.2 Calculational Precision and the Steady-State Convergence Criteria

In the SCDAP/RELAP5 solution scheme, at the successful completion of calculations over a time step, three fundamental variables are computed for each volume element in the system modeled. These variables are:

1. ρ_{mi}^{n+1} , the thermodynamic density of the volume substance, where subscript m denotes the solution by conservation of mass.

2. U_i^{n+1} , the thermodynamic internal energy of the volume substance resulting from conservation of energy.
3. P_i^{n+1} , the thermodynamic pressure of the volume substance resulting from the combined solution conserving momentum, mass, and energy.

The superscript $n+1$ denotes the new time solution at time $t^{n+1} = t^n + \Delta t^n$. Only three of these variables are required to define the thermodynamic state of the volume substance.

The thermodynamic pressure, phasic internal energies, and vapor volume fraction are used to compute the state using a set of properties tables. In the resulting calculations, a thermodynamic density ρ^{n+1} is calculated corresponding to the solution results. If the pressure and overall internal energy are preserved, then the precision of the calculations can be defined as

$$\epsilon_{\rho,i}^{n+1} = \rho_i^{n+1} - \rho_{mi}^{n+1} \quad (8-19)$$

for each volume element in the system. If the calculations were exact, then Equation (8-19) would be zero. However, the properties tables are limited in precision to a tolerance of ± 1 in the fifth significant figure. In statistical terminology, the mean expected precision would be approximately ± 5 in the sixth significant figure. If the mean expected precision is considered to be a standard precision, an approximate expression can be written in terms of the properties table density as

$$\epsilon_{std,\rho,i}^{n+1} \sim \pm(5 \times 10^{-6}) \rho_i^{n+1} \quad (8-20)$$

which is approximately ± 5 in the density sixth significant figure and which represents the best expected precision for the calculational scheme.

In the steady-state testing scheme, the precision of the volume enthalpy can be written as

$$\epsilon_{\rho h, i}^{n+1} = \left(\rho_i^{n+1} U_i^{n+1} + P_i^{n+1} \right) - \left(\rho_{mi}^{n+1} U_i^{n+1} + P_i^{n+1} \right) \quad (8-21)$$

or

$$\epsilon_{\rho h, i}^{n+1} = \left(\rho_i^{n+1} - \rho_{mi}^{n+1} \right) U_i^{n+1} \quad (8-22)$$

Similarly, the precision of the rate of change in volume enthalpy can be written as

$$\begin{aligned} \epsilon_{\left(\frac{d\rho h}{dt} \right), i}^{n+1} = \frac{1}{\Delta t^n} \left\{ \left[\left(\rho_i^{n+1} U_i^{n+1} + P_i^{n+1} \right) - \left(\rho_i^n U_i^n + P_i^n \right) \right] \right. \\ \left. - \left[\left(\rho_{mi}^{n+1} U_i^{n+1} + P_i^{n+1} \right) - \left(\rho_{mi}^n U_i^n + P_i^n \right) \right] \right\} \quad (8-23) \end{aligned}$$

which simplifies to

$$\epsilon_{\left(\frac{d\rho h}{dt} \right), i}^{n+1} = \frac{1}{\Delta t^n} \epsilon_{\rho h, i}^{n+1} \quad (8-24)$$

For the entire system at the current time step, a statistical precision can be defined where

$$\epsilon_{\rho h}^{n+1} = \left\{ \frac{\sum_{i=1}^{NVOLS} v_i^2 \left[\left(\rho_i^{n+1} - \rho_{mi}^{n+1} \right) U_i^{n+1} \right]^2}{\sum_{i=1}^{NVOLS} v_i^2} \right\}^{1/2} \quad (8-25)$$

for the system mean enthalpy and where

$$\epsilon_{\left(\frac{d\rho h}{dt}\right)}^{n+1} = \left[\frac{1}{(\Delta t^n)^2} \bar{\epsilon}_{\rho h}^2 \right]^{1/2} \quad (8-26)$$

for the system rate of change in enthalpy.

Simple mean differences for the entire system can also be written as

$$\bar{\delta}_{\rho h}^{n+1} = \frac{\sum_{i=1}^{NVOLS} v_i (\rho_i^{n+1} - \rho_{mi}^{n+1}) U_i^{n+1}}{\sum_{i=1}^{NVOLS} v_i} \quad (8-27)$$

for the system mean enthalpy and as

$$\bar{\delta}_{\left(\frac{d\rho h}{dt}\right)}^{n+1} = \frac{1}{\Delta t^n} \bar{\delta}_{\rho h}^{n+1} \quad (8-28)$$

for the system rate of change in enthalpy.

The relationship between the mean difference and precision terms defines the uncertainty characteristics of the overall solution scheme. From Equations (8-25) through (8-28), it is obvious that

$$-\epsilon_{\eta} \leq \delta_{\eta} \leq \epsilon_{\eta} \quad (8-29)$$

where subscript η denotes the particular term, ρh or $d(\rho h/dt)$, being considered. In particular, if ϵ_{η} is small, it can be concluded that calculations are made with a high degree of precision throughout the entire system modeled. If the mean difference term is such that

$$\delta_{\eta} \sim 0, \quad (8-30)$$

then the overall system solution is said to be unbiased. This means that the overall system mass, energy, and momentum are precisely conserved. However, if

$$\delta_{\eta} \sim \epsilon_{\eta} , \quad (8-31)$$

then the overall system solution is said to be biased. This means that if Equation (8-43) is true and

$$\delta_{\eta} < 0 , \quad (8-32)$$

then the overall system solution behaves as if it were losing mass, energy, or momentum. If

$$\delta_{\eta} > 0 , \quad (8-33)$$

then the system solution behaves as if it were gaining mass, energy, or momentum. In SCDAP/RELAP5, the size of the calculational time steps are controlled to maintain a high degree of precision which, in turn, limits the system bias. However, the characteristics just described can have an effect in determining time average steady state.

Since the time average straight line test defined by Equation (8-14) is conducted over a time interval, time average precision and mean difference terms must be calculated over the same time interval using the relationships

$$\frac{t_1 - t_2}{\epsilon_{ph}} = \frac{\sum_{n=n1}^{n2} \Delta t^n (\epsilon_{ph}^n)^2}{\sum_{n=n1}^{n2} \Delta t^n} \quad (8-34)$$

$$t_1 \frac{t_2}{\epsilon^2 \frac{d\rho_h}{dt}} = \frac{\sum_{n=n1}^{n2} \Delta t^n \left(\epsilon^2 \frac{d\rho_h}{dt} \right)^n}{\sum_{n=n1}^{n2} \Delta t^n} \quad (8-35)$$

$$t_1 \frac{t_2}{\delta_{\rho_h}} = \frac{\sum_{n=n1}^{n2} \Delta t^n \delta_{\rho_h}^n}{\sum_{n=n1}^{n2} \Delta t^n} \quad (8-36)$$

$$t_1 \frac{t_2}{\delta \left(\frac{d\rho_h}{dt} \right)} = \frac{\sum_{n=n1}^{n2} \Delta t^n \left(\delta \frac{d\rho_h}{dt} \right)^n}{\sum_{n=n1}^{n2} \Delta t^n} \quad (8-37)$$

where superscript $t_1 \frac{t_2}{\delta}$ denotes a time average over the time interval and the summation terms $n1$ and $n2$ denote the number of time steps taken over the interval from t_1 to t_2 , respectively.

Equations (8-34) through (8-37) represent the precision of the actual calculations relative to the thermodynamic state algorithm. These equations have the characteristic that if the system approaches absolute steady state, both Equations (8-34) and (8-35) will become very small. Since the properties tables are limited in precision, it is useless in a practical sense to continue calculations if absolute steady state is achieved with a precision better than that for the properties tables. This criteria can be defined by considering equations similar to Equations (8-34) and (8-35) but written in terms of the properties tables standard precision. These equations can be derived by simply substituting Equation (8-35) for the density difference term in the equations leading to Equations (8-34) and (8-35).

The steady-state convergence criteria can then be defined by combining the calculational and standard precisions such that

$$\frac{t_1 - t_2}{\epsilon_{c, \rho h}} = \left\{ \frac{1}{2} \left[\left(\frac{t_1 - t_2}{\epsilon_{std, \rho h}} \right)^2 + \left(\frac{t_1 - t_2}{\epsilon_{\rho h}} \right)^2 \right] \right\}^{1/2} \quad (8-38)$$

for the system mean enthalpy, and

$$\frac{t_1 - t_2}{\epsilon_{c, (\frac{d\rho h}{dt})}} = \left\{ \frac{1}{2} \left[\left(\frac{t_1 - t_2}{\epsilon_{std, (\frac{d\rho h}{dt})}} \right)^2 + \left(\frac{t_1 - t_2}{\epsilon_{(\frac{d\rho h}{dt})}} \right)^2 \right] \right\}^{1/2} \quad (8-39)$$

for the system rate of change in enthalpy.

Equations (8-38) and (8-39) represent the steady-state convergence criteria. It can be said that, within the limits of calculational and properties precision, time average steady state is achieved when the mean rate of change in system enthalpy is within the limits of

$$-\frac{t_1 - t_2}{\epsilon_{c, \frac{d\rho h}{dt}}} \leq a \leq + \frac{t_1 - t_2}{\epsilon_{c, \frac{d\rho h}{dt}}} \quad (8-40)$$

where "a" is the mean rate of change in system enthalpy given by Equation (8-14). If Equation (8-40) is true and if Equation (8-12) is such that

$$y \leq \frac{t_1 - t_2}{\epsilon_{c, \frac{d\rho h}{dt}}}, \quad (8-41)$$

then absolute steady state is achieved. If Equation (8-40) is true and

$$y > \frac{t_1 - t_2}{\epsilon_{c, \frac{d\rho h}{dt}}}, \quad (8-42)$$

then the system is fluctuating and time average steady state is achieved.

8.3.3 Steady-State Testing Scheme, Time Interval Control, and Output

In the steady-state testing scheme, the concepts discussed for detecting steady state are used, and calculations are performed over time intervals composed of a number of time steps. Because the nature of each problem is different, a systematic method of varying the test time intervals is performed.

These tests are performed in two parts. First, the system model overall state and rate of change in state are monitored by evaluating Equations (8-6) through (8-11) and including these results in the least-square terms for Equation (8-12). At time intervals computed internally, Equation (8-12) is evaluated; and the current system rate of change is determined. If the rate of change in state is increasing, then a divergent condition is indicated. If the rate of change in state is decreasing or zero, then a convergent condition is indicated. Second, if a convergent condition is indicated, then calculations are performed to determine the system average state and average rate of change in state over the internally computed time intervals. These time averages are formed by obtaining successive overlapping least-square solutions for Equation (8-13). These successive time average values are compared, and the achievement or nonachievement of a time average steady state is determined. In performing these tests, the calculational precision is accounted for by using Equations (8-19) through (8-42).

In the steady-state scheme, each time a solution for Equation (8-12) is obtained, the overall-state and steady-state convergence test results are printed. This printout is composed of current time results and time smoothed results integrated over the test time interval. The current time results are (a) the state and rates of change in state resulting from Equations (8-9), (8-10), and (8-11); (b) the current time uncertainties resulting from Equations (8-25) through (8-28); and (c) the current time mean and root mean square (RMS) mass errors. The time-smoothed results

that are printed are the current time evaluation of Equation (8-12) and the resultant coefficients of Equation (8-12) determined by the least-squares solution over the time interval from t_1 to the current time TIMEHY. The time, t_1 , corresponds to the time at the successful completion of calculations for the first time step after problem initiation. For example, if the problem is a NEW problem, then t_1 corresponds to

$$t_1 = 0 + \Delta t_1 \quad (8-43)$$

where Δt_1 is the first successful time step. If the problem is a RESTART problem, then t_1 corresponds to

$$t_1 = \text{TREST} + \Delta t \quad (8-44)$$

where TREST is the time of restart and Δt is the first successful time step after restart. If the results of the overall state tests indicate a convergent condition, then time average tests are initiated.

The time average tests consist of approximating the overall state with a set of three straight lines where each test line is fitted to the calculational results over successive test intervals. The time rates of change of these test lines are then monitored to determine time average steady state. In the testing scheme, when the time average tests are initiated, calculations continue until the successive test time interval is exceeded. At this time, the first test line, Line A, is defined and its results are printed. Calculations then continue until the next successive test time interval is exceeded. At this time, the second test line, Line B, is defined for the second test interval and the third test line, Line C, is defined for the combined first and second test intervals. The results for the three test lines are then printed, and tests are performed to determine the achievement of time average steady state. If steady state has not been achieved, then test Line A is reset to Line B and the process is repeated until steady state is achieved.

In the printed edit for time average steady state tests, the results for each of the three test lines are printed. The test line results are obtained by curve fitting Equation (8-14) over each of the line test intervals. The results printed are the endpoints of Equation (8-14) evaluated at the test interval start and end times and the time rate of change of Equation (8-14). Also printed are the time average uncertainties from Equations (8-34) through (8-37), the RMS fluctuation of system mean ρh about the line from Equation (8-18), and the mass error integrated over the line test interval.

In performing both the overall and time average sets of tests, calculations proceed through a logic scheme to perform tests that monitor the solution scheme's approach to steady state. After completing the logic scheme calculations, the steady-state conclusions and next course of action are printed. This printout is composed of statements of the mode of convergence and the state of the system in alphanumeric terms. These statements are defined as the calculations proceed through the logic scheme. To prevent excessive printout during the overall state convergence tests, the first test for overall convergence is not performed until the completion of ten successful time steps. At this time, a current test time interval is initialized as $\Delta t_c = \text{TIMEHY} - t_1$. If this test indicates a divergent condition, then the test time interval is increased and the test procedure is repeated. To increase the test time interval, three tests are performed. First, the current test time interval is halved and the time t_2 is estimated as

$$t_2 = \text{TIMEHY} + \frac{1}{2} \Delta t_c \quad . \quad (8-45)$$

Then Equation (8-12) is evaluated as $y(t_2)$. If $y(t_2)$ is greater than the current value of y , then the time t_2 is reset to

$$t_2 = \text{TIMEHY} + \Delta t_c \quad (8-46)$$

and Equation (8-12) is reevaluated, which results in resetting $y(t_2)$. If $y(t_2)$ is again $> y$, then the time t_2 is again reset to

$$t_2 = \text{TIMEHY} + 2\Delta t_c \quad (8-47)$$

In any case, the test time interval is expanded by either maintaining, halving, or doubling the current test time interval based on a projected estimate of the current time-smoothed convergence function. This test procedure is then successively repeated until a convergent condition is calculated.

To provide efficiency for the time average testing scheme, upon the first occurrence of an overall state convergent condition, the time average testing scheme is activated and the test time interval is redefined by estimating the time interval over which a 10% change in state will occur. This time interval is approximately

$$\Delta t_c \sim 0.1(\overline{\rho h^n})/y \quad (8-48)$$

However, to prevent excessively small or large intervals, the time interval is limited such that

$$10 \, dt \leq \Delta t_c \leq 100 \, dt \quad (8-49)$$

where dt is the current calculational time step. The calculations for the time average scheme then proceed with each successive test time interval specified 10% larger than the time interval just completed. As the calculations progress and approach steady state, the line segments approach a constant value within the steady-state convergence criteria. When this condition is met, the test time interval is doubled. If this condition is recursively maintained for two more successive test intervals, then a final steady state has been achieved and the calculations are terminated. If the line segment tests indicate the solution is diverging from steady state,

the results of the time average tests are discarded. When the conditions of Equation (8-12) again become true, the time average tests are reinitiated and the procedure is continued until steady state is achieved.

8.3.4 Heat Structure Heat Conductance Scheme for Steady State

In both the steady-state and transient solution schemes, the same transient heat transfer algorithm is used. However, in the steady-state scheme, the heat structure heat capacity data input by the user are ignored. Instead, this term is evaluated as an artificially small number such that

$$\frac{\rho C_p (\Delta x)^2}{k \Delta t_{ht}} \geq 2 \quad (8-50)$$

where ρC_p is the heat capacity term, Δx is the heat structure mesh interval, k is the heat structure thermal conductivity and Δt_{ht} is the heat transfer scheme calculational time step. Equation (8-50) corresponds to the explicit stability criteria for a transient numerical heat conduction scheme.

In a transient solution scheme, the heat capacity term is treated analogously to a thermal inertia, and its magnitude determines the characteristic response time of the conduction solution. For example, ρC_p is typically quite large, on the order of 10^5 or larger. Hence, a large value of ρC_p results in a characteristic response time much greater than the hydrodynamic response time. Indeed, hydrodynamic steady state can be approximately achieved in reasonably short calculational times before large heat structures have even begun to respond.

By making the value of the heat capacity term small, the characteristic response time is made small and on the order of or less than the hydrodynamic calculational time step. The resultant solution would therefore be equivalent to a steady-state solution that is damped and

stabilized by a small thermal inertia. Hence, fluctuations of the heat structure rate of change in state are on the order of or less than the fluctuations of its hydrodynamic boundary conditions. As a result, the heat structure solution scheme will achieve time average steady state at approximately the same time as time average hydrodynamic steady state.

8.3.5 Interrelationship of Steady-State and Transient Restart/Plot Records

During the course of the calculations, restart/plot records are written at the frequency specified by the user. When the code determines that steady state has been achieved, a restart/plot record is written unconditionally. Subsequent problems can then be run as restarts using any of these restart records. However, the code will treat the restart records differently, depending on the type of problem using the restart record.

If a transient problem is being run by restarting from a steady-state restart record or, conversely, if a steady-state problem is being run restarting from a transient restart record, the restart is treated as a new problem. In this case, only the restart record at which the problem restarts is written and used for initial conditions. The code time step counters, statistics, and problem simulation time are reset to zero, and additional restart/plot records are written as the problem progresses.

If a steady-state problem is being run restarting from a steady-state restart record or, conversely, if a transient problem is being run restarting from a transient restart record, then the restart is treated as a continuation of the problem. In the continuation case, the previous restart/plot records up to the point of restart are preserved; and additional records are written as the problem progresses.

8.4 Self-Initialization

8.4.1 General Description

Obtaining an initialized, steady-state condition for the SCDAP/RELAP5 PWR-type plant model often requires considerable time and effort on the

part of the analyst. Typically, this process involves successive calculations involving a trial-and-error approach in adjusting various input data.

To reduce the time, effort, and cost associated with this process, a self-initialization option is available. The strategy of the scheme is to automate the control aspects of the problem and to significantly reduce the computational time needed to reach a steady state. The concept retains the conventional approach of conducting a transient calculation that is driven to a desired steady-state condition.

Automation of plant model control is effected by a generic set of controllers that mimic an actual plant control system. These controllers are new control components defined by the user. Four suboptions are permitted with respect to the definition of independent and dependent plant model parameters. The choice of suboptions affords the user flexibility in meeting particular analysis objectives. Moreover, the overall scheme has been designed such that the user may invoke a standard control package or opt to custom-tailor the new control components to suit a particular plant model.

A reduction in calculational computer time to perform the initialization is accomplished by using the steady-state and nearly implicit solution scheme options (see Subsections 8.3 and 3.1.7, respectively). The steady-state option diminishes thermal capacitance terms to lower stability limits, thereby significantly reducing thermal relaxation of the model. It also monitors for a steady-state condition. The nearly implicit solution scheme permits time steps larger than those implied by the material Courant limit. The two options in combination often produce run times faster than real time, thereby conserving computer time and accelerating turnaround.

The self-initialization option is compatible with PWR-type models employing either U-tube or once-through steam generators and of single or multiple loop design.

8.4.2 Required Plant Model Characteristics

The option accommodates plant models representing all domestically produced PWR designs, i.e., those of Westinghouse, Combustion Engineering, and Babcock & Wilcox. More specifically, single-loop, two-loop, three-loop, four-loop, and 2 x 4 loop representations are accommodated, utilizing either U-tube or once-through steam generators. Other assumptions and restrictions related to the plant model are as follows:

- o The model must have at least one coolant loop consisting of a core region, pump, steam generator, and pressurizer.
- o The core power cannot be computed using the point kinetics option, but rather must be a constant boundary condition. Reactor kinetics input may be used, but no feedback may be entered so that the reactor power is constant. Reactor kinetics data with feedback can be entered at a transient restart.
- o User-specified makeup and letdown flow modeling should be suppressed during the null transient. The same applies to pressurizer heater and spray modeling. They may be introduced into the model as a renodalization at transient initiation. Volume and pressure control during the null transient must be effected through a time-dependent volume that serves to replace the pressurizer.
- o Self-initialization of the plant model encompasses the primary coolant system and steam generators under the standard approach described subsequently. That is, no provisions are included to steady state balance-of-plant components, although this is possible and is not incompatible with the self-initialization option. However, if the plant model includes a balance-of-plant representation (e.g., turbine, condensers, feedwater pumps, feedwater heaters, etc.), appropriate controllers would have to be supplied by the user to govern the operation of these components.

- o The option is executable from either a new problem data deck or the restart of an old problem.

8.4.3 Standard Suboptions

Four standard suboptions are available in terms of specifying the independent parameter data set. This flexibility allows the user to select the suboption that best suits the situation at hand. Here it should be noted that the term standard refers to the employment of the control components in a standardized way that will subsequently be described. The nature of the control components, however, allows them to be used in other ways (i.e., with respect to sensed variable and controlled variable).

It should be recognized that the state of the plant model cannot be totally dictated by the analyst, since this would represent an overspecification of the problem. Certain interdependencies are implied by the plant model geometry and the mathematical models in the code. For example, one cannot simultaneously specify the thermal power, cold leg temperature, primary coolant flow rate, secondary pressure, and coolant level. This is an overspecification, since the load rejection characteristics of the steam generator(s) have been implied by its (their) geometrical description and the heat transfer models in the code. Either the secondary pressure (and temperature) or cold leg temperature would have to be dependent in this example.

Each of the four standard suboptions has a common set of fixed parameters. These, and the remaining independent and dependent parameters for each suboption, are listed in table 8-1. These suboptions are derived from the four logical combinations that result from selecting two of four variables, allowing the other two to be dependent. These four are primary flow, RCP speed, cold leg temperature, and secondary pressure. Each of the suboptions is described below.

8.4.3.1 Suboption A. Loop flow and cold leg temperature are specified. (Note that specification of primary flow, core thermal power, and primary pressure fixes the differential temperature across the

TABLE 8-1. INDEPENDENT/DEPENDENT DATA SET SUBOPTIONS

Always fixed:

Core thermal power
Pressurizer pressure
Feedwater temperature
Secondary coolant level

<u>Suboption</u>	<u>Independent</u>	<u>Dependent</u>
A	Loop flow Cold leg temperature	RCP speed Secondary pressure Secondary flow
B	RCP speed Cold leg temperature	Loop flow Secondary pressure Secondary flow
C	Loop flow Secondary pressure	RCP speed Cold leg temperature Secondary flow
D	RCP speed Secondary pressure	Loop flow Cold leg temperature Secondary flow

vessel.^a) This suboption requires that the pump speed, secondary pressure, and secondary feedwater flow be dependent variables.

The pump speed (N) is determined based on loop flow ($\dot{m}$), loop pressure drop (Δp), and the pump characteristics, as determined from pump model input. That is,

$$N = f(\dot{m}, \Delta p) \quad . \quad (8-51)$$

Here it should be noted that the resulting pump speed may be different than an observed value (in the case of an experimental facility) or the synchronous speed (in the case of a full-scale plant). This merely implies that a mismatch is present in the input data. For example, the user-specified geometry and/or loss coefficients for the PCS may be inaccurate, and/or the pump model may be inaccurate. The analyst must resolve such inconsistencies on his own. The code will not alter either the pump model or loss coefficients to arrive at a flow/speed combination that matches facility data.

Analogously, specifying the cold leg temperature (along with power and loop flow) requires that the secondary pressure and flow must be dependent. The secondary pressure dictates the secondary sink temperature and, therefore, the primary-to-secondary heat transfer potential and cold leg temperature. Here again, it should be noted that the resulting secondary pressure may not match that observed in the plant or test facility. This may mean one of two things. Either the plant model representation of the steam generator is inadequate (e.g., inaccurately modeled, improperly nodalized, etc.), or the physical models in the code are imprecise. For example, the failure to match a measured value of secondary pressure might be due to the fact that the tube fouling was not accounted for in the input model.

a. This takes into account the total pump power and heat losses as well.

8.4.3.2 Suboption B. RCP speed and cold leg temperature are specified, while loop flow, secondary pressure, and secondary flow are dependent. This suboption is similar to suboption A except that the roles of RCP speed and loop flow as dependent and independent variables are reversed. This suboption would be desirable when modeling a plant for which no data exist but the synchronous pump speed is known.

8.4.3.3 Suboption C. Loop flow and secondary pressure are specified, while RCP speed, cold leg temperature, and secondary flow are dependent. This suboption is desirable when secondary pressure matching (to data) would play an important role in the transient.

8.4.3.4 Suboption D. RCP speed and secondary pressure are specified, while loop flow, cold leg temperature, and secondary flow are dependent. This suboption is similar to suboption C, except that the independent/dependent roles of loop flow and pump speed are reversed.

8.4.4 Inherent Model Incompatibilities

With such generality possible in defining a plant model with SCDAP/RELAP5, it is clearly possible that a desired steady-state condition is impossible to achieve given the input data supplied. Several types of incompatibilities will be not readily apparent until a null transient is attempted. For example, the load rejection capacity of the steam generator(s) may be insufficient to transfer the total core thermal power without causing the hot leg temperature to exceed T_{SA1} . Such anomalies will be obvious as the null transient proceeds but cannot be readily identified from the input data stream.

8.4.5 Description of Standard Controllers

To effect overall control of the model during the null transient, three generic control components are available and are used to invoke any one of the four suboptions just described. These control components are identified as PUMPC1L, STEAMCTL, and FEEDCTL. For all suboptions, both

STEAMCTL and FEEDCTL are needed; whereas PUMPCTL is used only for suboptions A and C where loop flow control is desired. The following subsections describe the design and operation of the controllers.

8.4.5.1 PUMPCTL Controller. The standard equipment of the PUMPCTL component is to sense loop flow and control pump speed to achieve the desired flow rate. As is the case with the other controllers, it utilizes proportional and integral control. Through input, the user specifies (among other things) the desired flow rate, where the flow is to be sensed, and which pump is to be controlled. The mathematical expressions representing the operation of the controller are next described.

An error signal (E_1) is generated by subtracting the actual (V_2) from desired (V_1) flow rate and dividing the result by a user-supplied constant (S_1):

$$E_1 = \frac{V_1 - V_2}{S_1} \quad (8-52)$$

This error signal is used to compute a new output signal (pump speed = Y_1) for the next time advancement in accordance with the relationship:

$$Y_1^{n+1} = G_1 \left(\frac{E_1}{T_1} + \frac{\int_0^t E_1 dt}{T_2} \right) + (Y_1)_0 \quad (8-53)$$

where G_1 equals the gain, T_1 is a constant applied to the proportional part, T_2 is the time constant for the integral part, and $(Y_1)_0$ is the initial (time zero) value of the pump speed.

The proportional part of the control provides the direct coupling between the error (flow) and controlled variable (speed) while the integral part introduces damping.

8.4.5.2 STEAMCTL Controller. The standard employment of the STEAMCTL component is to sense either cold leg temperature (suboptions A and B) or secondary pressure (suboptions C and D) and control steam flow (through adjustment of steam valve flow area) to achieve the desired set point. It functions in exactly the same way as the PUMPCTL component just described, except that the definition of sensed and controlled variables is changed. For the STEAMCTL component,

$$E_2 = \frac{V_3 - V_4}{S_j} \quad (8-54)$$

where V_3 is the desired temperature (or pressure), V_4 is the actual value, and S_j is a constant supplied by the user. Likewise, the output signal (normalized steam valve area) for each new advancement is given as

$$Y_2^{n+1} = G_2 \left(\frac{E_2}{T_3} + \frac{\int_0^t E_2 dt}{T_4} \right) + (Y_2)_0 \quad (8-55)$$

where the terms are analogous to those for the PUMPCTL component.

8.4.5.3 FEEDCTL Controller. The standard employment of the FEEDCTL component is to sense steam flow and steam generator secondary coolant level (or coolant mass) and control feedwater flow (through adjustment of feedwater valve flow area) to achieve a match between feedwater flow and steam flow and to achieve the desired coolant level (or mass). It is also a proportional/integral controller but utilizes a summed error signal made up of the individual flow and level (mass) errors:

$$E_3 = \frac{V_5 - V_6}{S_k} + \frac{V_7 - V_8}{S_m} \quad (8-56)$$

where

V_5 = desired level (mass)
 V_6 = actual level (mass)
 S_k = user-supplied constant
 V_7 = actual steam flow
 V_8 = actual feedwater flow
 S_m = user-supplied constant .

The output signal (feedwater valve flow area) is computed analogously to the PUMPCTL and STEAMCTL components:

$$Y_3^{n+1} = G_3 \left(\frac{E_3}{T_5} + \frac{\int_0^t E_3 dt}{T_6} \right) + (Y_3)_0 . \quad (8-57)$$

8.4.5.4 Pressure and Volume Control. The self-initialization option requires that a constant pressure boundary condition be imposed on the primary coolant system during the null transient. The user supplies this condition by adding a time-dependent volume as a replacement for the pressurizer. This time-dependent volume should be defined as containing liquid at the desired primary system pressure and at a temperature near that estimated to be the final hot leg temperature. During the null transient, liquid will either flow into or out of the time-dependent volume to accommodate expansion and shrinkage, with no attendant change in primary pressure. When the self-initialization option is invoked, the code will check to determine if the time-dependent volume has been included.