This chapter describes the fluid field equations used by TRACE to model two-phase flow, and the numerical approximations made to solve these equations. Derivation of the equation set used in TRACE starts with single phase Navier-Stokes equations in each phase, and jump conditions between the phases. Time averaging is applied to this combination of equations, to obtain a useful set of two-fluid, two-phase conservation equations. TRACE uses this flow model in both one and three dimensions. Kocamustafaogullari (Ref. 1-1), Ishii (Ref. 1-2), and Bergles et al. (Ref. 1-3) have provided detailed derivations of the equations similar to those used in TRACE, and a more concise derivation related to the TRACE equations is available in a report by Addessio (Ref. 1-4). That this model is formally ill-posed was the subject of considerable debate many years ago and is discussed by Stewart and Wendroff (Ref. 1-5). Our experience, however, has always been that this is a moot point, since the numerical solution procedures effectively introduce minor modifications to the field equations, making them well-posed. A paper by Stewart (Ref. 1-6) confirms these observations and demonstrates clearly that with normal models for interfacial drag and reasonable finite-difference nodalizations, the problem solved numerically is well-posed.

The basic two-fluid, two-phase field equation set consists of separate mass, energy, and momentum conservations for the liquid and gas fields. This gives a starting point of six partial differential equations (PDEs) to model steam/water flows. For a wide range of reactor safety analysis, noncondensable gas may enter the system and mix with the steam. At any given location TRACE assumes that all components of the gas mixture are moving at the same velocity and are at the same temperature. As a result a single momentum equation and a single energy equation are used for the gas mixture. Relative concentrations of steam and noncondensable are determined by using separate mass equations for each component of the gas field. In a typical LOCA nitrogen will eventually enter the primary loops from the accumulators, and air from the containment. Because the properties of nitrogen and air are so similar, users normally treat both noncondensable sources as air, adding one mass equation to the set of PDEs that must be solved. However, TRACE permits users to treat nitrogen and air as two separate components of the gas field (two additional mass equations), and allows requests for more noncondensable mass equations if needed (e.g. for hydrogen).

The set of field equations can be further extended if a user chooses to follow the boron concentration in the system. An additional mass conservation equation can be activated to follow the concentration of boric acid, moving with the liquid. Total content of boric acid is assumed to be small enough that its mass is not used in the liquid momentum equation and it does not
contribute to the thermodynamic or other physical properties of the liquid. Boron tracking capabilities are extended through the use of a model for solubility of boric acid, and a simple inventory of boric acid plated out in each cell in the system. Another solute could be modeled through a user option to replace the default solubility curve.

The TRACE code, as well as most other codes like it, invokes a quasi-steady approach to the heat-transfer coupling between the wall and the fluid as well as the closure relations for interfacial and wall-to-fluid heat transfer and drag. This approach assumes detailed knowledge of the local fluid parameters and ignores time dependencies so that the time rate of change in the closure relationships becomes infinite and the time constants are zero. It has the advantages of being reasonably simple (and, therefore, generally applicable to a wide range of problems) and not requiring previous knowledge of a given transient. Where appropriate, we integrate the effects of the quasi-steady approach; however, in the interests of brevity, the description of the quasi-steady methodology presented in this chapter is somewhat limited. Appendix A contains a much more detailed discussion of the quasi-steady assumption and the averaging operators used in the code.

**Nomenclature**

Before presenting the fluid field equations, we need to define certain terminology. In our nomenclature, the term "gas" implies a general mixture of water vapor and the noncondensable gas. The subscript $g$ will denote a property or parameter applying to the gas mixture; the subscript $v$ indicates a quantity applying specifically to water vapor (referred to as simply "vapor"); and the subscript $a$ (for "air") signifies a quantity associated with mixture of one or more noncondensable gases. The term "liquid" implies pure liquid water, and the subscript $l$ denotes a quantity applying specifically to liquid water. For convenience, we define the following terms that will be used in the subsequent equations and list them alphabetically, with the Greek symbols and subscripts to follow. The following notation applies to the discussion of numerical methods. A caret ($^\hat{}$) above a variable denotes an explicit predictor value. A tilde ($^\sim$) above a variable denotes an intermediate result, and a line ($^\bar{}$) above denotes an average operation. Details of the specific average are provided in discussion of the equations in which it occurs. A horizontal arrow (or half-arrow) above a variable denotes a vector quantity (in the physical sense such that it has both a magnitude and direction).

\begin{align*}
A &= \text{flow area between mesh cells} \\
A_i &= \text{interfacial area per unit volume between the liquid and gas phases} \\
c &= \text{speed of sound} \\
C &= \text{shear coefficient} \\
E_i &= \text{rate of energy transfer per unit volume across phase interfaces} \\
e &= \text{internal energy}
\end{align*}
Field Equations

\[ f = \text{force per unit volume} \]

\[ \mathbf{g} \text{ or } \mathbf{g}' = \text{gravity vector} \]

\[ g = \text{magnitude of the gravity vector} \]

\[ h = \text{heat-transfer coefficient (HTC)} \]

\[ h_{sg} = \text{gas saturation enthalpy} \]

\[ h_{wg} = (1 - f_g) h'_{wg} , \text{the effective wall HTC to gas} \]

\[ h_{wl} = f_l h'_{wl} , \text{the effective wall HTC to liquid} \]

\[ h'_l = \text{liquid enthalpy of the bulk liquid if the liquid is vaporizing or the liquid saturation enthalpy if vapor is condensing} \]

\[ h'_v = \text{vapor enthalpy of the bulk vapor if the vapor is condensing or the vapor saturation enthalpy if liquid is vaporizing} \]

\[ K = \text{form-loss coefficient or wall friction coefficient} \]

\[ m = \text{solute concentration in the liquid (mass of solute per unit mass of liquid)} \]

\[ M_i = \text{rate of momentum transfer per unit volume across phase interfaces} \]

\[ P = \text{fluid pressure or total pressure} \]

\[ q = \text{heat-transfer rate per unit volume} \]

\[ q_d = \text{power deposited directly to the gas or liquid (without heat-conduction process)} \]

\[ q_{gl} = \text{liquid-to-gas sensible heat transfer} \]

\[ q' = \text{heat flux} \]

\[ r = \text{radius} \]

\[ R = \text{ideal gas constant (including effects of molecular weight)} \]

\[ \mathbf{R} = \text{Reynolds/viscous stress tensor} \]

\[ S = \text{factor applied to the 1D component so that its positive flow direction becomes the positive flow direction of the vessel} \]

\[ S_c = \text{plated-out solute density (mass of plated solute divided by cell volume)} \]

\[ SC = \text{product of an orifice factor} \]

\[ S_m = \text{source term in the solute-mass differential equation} \]

\[ t = \text{time} \]

\[ T = \text{temperature} \]

\[ \mathbf{T} = \text{stress tensor} \]
\( T_{sv} \) = saturation temperature corresponding to the vapor partial pressure

\( \vec{V} \) or \( \vec{V} \) = velocity vector

\( V \) = magnitude of the velocity

\( vol \) = hydrodynamic-cell volume

\( w \) = weighting factor

\( x \) = distance

\( X \) = mass fraction of an additional noncondensable gas species

\( Y \) = dummy variable

\( z \) = axial coordinate

**Greek**

\( \alpha \) = gas volume fraction

\( \beta \) = momentum-convection temporal expansion flags

\( \gamma \) = weighting factor

\( \Gamma \) = interfacial mass-transfer rate (positive from liquid to gas)

\( \Gamma^+ \) = maximum of \( \Gamma \) and 0

\( \Gamma^- \) = minimum of \( \Gamma \) and 0

\( \rho \) = density

\( \Delta P \) = pressure difference

\( \Delta r \) = radial ring increment for 3D components

\( \Delta t \) = time-step size

\( \Delta V \) = velocity change

\( \Delta x \) = cell length for 1D components

\( \Delta z \) = axial level increment for 3D components

\( \Delta \theta \) = azimuthal segment increment for 3D components

\( \delta P \) = linear Taylor series expansion term for pressure

\( \delta T \) = linear Taylor series expansion term for temperature

\( \delta \alpha \) = linear Taylor series expansion term for void fraction

\( \theta \) = inclination angle from vertical or the azimuthal coordinate
\( \phi \) = angle between the main and side tubes in a TEE component

**Subscripts**

1D = one dimensional  
3D = three dimensional  

\( \text{donor} \) = donor cell  

\( T \) = the first cell in the side leg of the TEE or the interface between the \( j^{th} \) cell of the primary and the first cell in the side leg  

\( a \) = noncondensable gas  

\( d \) = 1) generic index for \( r, \theta, \) or \( z \) or \( i, j, \) or \( k \); 2) denotes direct heating when used with energy source (q)  

\( g \) = gas mixture  

\( i \) = interfacial  

\( j \) = cell-center index  

\( j + 1 \) = downstream cell-center index  

\( j + 1/2 \) = downstream cell-edge index  

\( j - 1 \) = upstream cell-center index  

\( j - 1/2 \) = upstream cell-edge index  

\( k \) = index on additional noncondensable gas species  

\( l \) = liquid  

\( max \) = maximum  

\( min \) = minimum  

\( r \) = radial  

\( sat \) = saturation  

\( v \) = water vapor  

\( w \) = wall  

\( z \) = axial  

\( \theta \) = azimuthal

**Superscripts**

\( n \) = current-time quantity  

\( n + 1 \) = new-time quantity
Field Equations

In the discussion of the finite-difference equations, all quantities except for the velocities are centered in the hydrodynamic cell (cell-centered), and the velocities are cell-edge quantities.

**Fluid Field Equations**

Time averaging of the single phase gas and single phase liquid conservation equations combined with interface jump conditions results in a starting point summarized in Eqs. (1-1) through (1-6). In these equations an overbar represents a time average, \( \alpha \) is the probability that a point in space is occupied by gas, and \( \Gamma_i, E_i, \) and \( M_i \) represent the contribution of time averaged interface jump conditions to transfer of mass, energy and momentum respectively. In addition \( q' \) is conductive heat flux, \( q_d \) is direct heating (e.g. radioactive decay) and \( T \) is the full stress tensor. Subscripts of "g" and "l" distinguish between gas specific and liquid specific terms respectively.

**Time Averaged Mass Equations**

\[
\frac{\partial}{\partial t}[(1 - \alpha)\bar{\rho}_l] + \nabla \cdot \left[(1 - \alpha)\bar{\rho}_l \bar{V}_l\right] = -\Gamma_i
\]

(1-1)

\[
\frac{\partial (\alpha \bar{\rho}_g)}{\partial t} + \nabla \cdot \left[\alpha \bar{\rho}_g \bar{V}_g\right] = \bar{\Gamma}_i
\]

(1-2)

**Time Averaged Energy Equations**

\[
\frac{\partial}{\partial t} \left[(1 - \alpha)\bar{\rho}_l \left(\bar{e}_l + \frac{\bar{V}_{l}^2}{2}\right)\right] + \nabla \cdot \left[(1 - \alpha)\bar{\rho}_l \left(\bar{e}_l + \frac{\bar{V}_{l}^2}{2}\right) \bar{V}_l\right]
\]

\[
= -\nabla \cdot \left[(1 - \alpha)\bar{q}_{l}\right] + \nabla \cdot \left[(1 - \alpha)\bar{T}_l \cdot \bar{V}_l\right] + (1 - \alpha)\bar{\rho}_l \bar{g} \cdot \bar{V}_l - \bar{E}_i + q_{dl}
\]

(1-3)
\[
\frac{\partial \left[ \alpha \bar{\rho}_g \left( e_g + \frac{V_g^2}{2} \right) \right]}{\partial t} + \nabla \cdot \left[ \alpha \bar{\rho}_g \left( e_g + \frac{V_g^2}{2} \right) \bar{V}_g \right] = - \nabla \cdot \left[ \alpha \bar{q}_g \right] + \nabla \cdot \left[ \alpha \left( T_g \cdot \bar{V}_g \right) \right] + \alpha \bar{\rho}_g \dot{\gamma} \cdot \bar{V}_g + \bar{E}_i + \bar{q}_{dg}
\] (1-4)

**Time Averaged Momentum Equations**

\[
\frac{\partial \left[ (1 - \alpha) \bar{\rho}_l \bar{V}_i \right]}{\partial t} + \nabla \cdot \left[ (1 - \alpha) \bar{\rho}_l \bar{V}_i \bar{V}_i \right] = \nabla \cdot \left[ (1 - \alpha) \bar{T}_i \right] + (1 - \alpha) \bar{\rho}_l \dot{\gamma} \cdot \bar{M}_i
\] (1-5)

\[
\frac{\partial \left[ \alpha \bar{\rho}_g \bar{V}_g \right]}{\partial t} + \nabla \cdot \alpha \bar{\rho}_g \bar{V}_g \bar{V}_g = \nabla \cdot \left[ \alpha \bar{T}_g \right] + \alpha \bar{\rho}_g \dot{\gamma} + \bar{M}_i
\] (1-6)

The equations are consistent with Reynolds averaging and splitting the velocities into mean and fluctuating contributions will yield expressions familiar to those who work with turbulence. However, contributions from the Reynolds stress, as well as most of the terms on the right hand side of the energy and momentum equations will be modeled with engineering correlations, so the following forms of the energy and momentum equations do not include full notation from classic turbulence formulation. In the energy equation the term \(q'\) is redefined to include energy flux due to turbulent diffusion. Energy carried with mass transfer at the interface is represented by the products of mass transfer rate and appropriate stagnation enthalpy at the interface (\(\Gamma h'_{i'}\) and \(\Gamma h'_{j'}\)). Work done on the fluid is split into that due to the pressure terms in the stress tensor, and a term simply labeled "\(W\)", containing work done by shear stress and by interfacial force terms.

**Revised Time Average Energy Equations**

\[
\frac{\partial \left[ (1 - \alpha) \bar{\rho}_l \left( e_i + \frac{V_i^2}{2} \right) \right]}{\partial t} + \nabla \cdot \left[ (1 - \alpha) \bar{\rho}_l \left( \frac{P}{\bar{\rho}_l} + \frac{V_i^2}{2} \right) \bar{V}_i \right] = - \nabla \cdot \left[ (1 - \alpha) \bar{q}_i \right] + (1 - \alpha) \bar{\rho}_l \dot{\gamma} \cdot \bar{V}_i - \Gamma h'_i \bar{V}_i + W_i + q_{dl}
\] (1-7)
In the momentum equations pressure is also isolated from the stress tensor, and for purposes of this derivation the viscous shear stress terms are combined with the Reynolds stress into a single tensor $R$.

**Revised Time Average Momentum Equations**

\[
\frac{\partial}{\partial t} \left[ (1-\alpha)\bar{\rho}_i \bar{V}_i \right] + \nabla \cdot (1-\alpha)\bar{\rho}_i \bar{\nabla} \cdot \bar{V}_i = \nabla \cdot [(1-\alpha)\bar{R}_i] + (1-\alpha)\bar{\rho}_i \bar{g} - \bar{M}_i \]  

\[
\frac{\partial}{\partial t} \left[ \alpha \bar{\rho}_g \bar{V}_g \right] + \nabla \cdot \alpha \bar{\rho}_g \bar{\nabla} \cdot \bar{V}_g = \nabla \cdot [\alpha \bar{R}_g] + \alpha \bar{\rho}_g \bar{g} + \bar{M}_i \]  

At this point it is possible to move on to the finite volume conservation equations. However, the next round of approximations made in the TRACE flow model can also be illustrated by considering a volume averaged form of the above field equations. First the overbar is dropped and all variables are treated as time averages. Next the overbar is returned to the notation as a volume average of terms in the conservation equations.

**Volume Averaged Mass Equations**

\[
\frac{\partial}{\partial t} \left[ (1-\alpha)\rho_i \bar{V}_i \right] + \nabla \cdot [(1-\alpha)\rho_i \bar{V}_i] = -\bar{\Gamma} \]  

\[
\frac{\partial}{\partial t} \left[ \alpha \rho_g \bar{V}_g \right] + \nabla \cdot [\alpha \rho_g \bar{V}_g] = \bar{\Gamma} \]  

\[
\frac{\partial}{\partial t} \left[ \alpha \rho_g \bar{V}_g \right] + \nabla \cdot [\alpha \rho_g \bar{V}_g] = \bar{\Gamma} \]
Volume Averaged Energy Equations

\[
\frac{\partial}{\partial t} \left[ (1 - \alpha) \rho_i (e_i + \frac{V_i^2}{2}) \right] + \nabla \cdot \left[ (1 - \alpha) \rho_i \left( e_i + \frac{P}{\rho_i} + \frac{V_i^2}{2} \right) \hat{V}_i \right] = -\nabla \cdot \left[ (1 - \alpha) \hat{q}_i \right] + (1 - \alpha) \rho_i \hat{g} \cdot \hat{V}_i - \Gamma h'_i + W_i + q_{dl} \\
\frac{\partial}{\partial t} \left[ \alpha \rho_g (e_g + \frac{V_g^2}{2}) \right] + \nabla \cdot \left[ \alpha \rho_g \left( e_g + \frac{P}{\rho_g} + \frac{V_g^2}{2} \right) \hat{V}_g \right] = -\nabla \cdot \left[ \alpha \hat{q}_g \right] + \alpha \rho_g \hat{g} \cdot \hat{V}_g + \Gamma h'_v + W_g + q_{dg}
\]

Volume Averaged Momentum Equations

\[
\frac{\partial}{\partial t} [(1 - \alpha) \rho_i \hat{V}_i] + \nabla \cdot [(1 - \alpha) \rho_i \hat{V}_i \hat{V}_i] = \nabla \cdot [(1 - \alpha) \hat{R}_i] + (1 - \alpha) \rho_i \hat{g} \cdot \hat{M}_i \\
\frac{\partial}{\partial t} [\alpha \rho_g \hat{V}_g] + \nabla \cdot \alpha \rho_g \hat{V}_g \hat{V}_g = \nabla \cdot [\alpha \hat{R}_g] + \alpha \rho_g \hat{g} \cdot \hat{M}_i
\]

Now a series of approximations are made.

1) The volume average of a product is assumed to be equal to the product of volume averages. This is reasonable if the averaging volume is small enough, but eventually when applied within the finite volume context to reactor systems, the averaging volume will span flow channels. In this case, the approximation is good for most turbulent flows due to the flat profile across most of the flow cross-section. However, for laminar single phase flow in a circular channel cross-section, when the average of the product of two parabolic profiles is replaced by the product of the average velocities, momentum flux terms will be low by 25%. Flows with rising droplets and falling wall film or certain vertical slug flows will also present problems.
2) Only contributions from wall heat fluxes and heat fluxes at phase interfaces within the averaging volume are normally included in the volume average of the divergence of heat flux. An option exists to include the conduction heat flux within the fluid (perhaps useful for liquid metal flow), but no provision has been made for turbulent heat flux between averaging volumes. In effect, heat flux is a subgrid model. This approximation prevents accurate calculations of such phenomena as collapse of a steam bubble blocking natural circulation through a B&W candy-cane, or of the details of steam condensation at the water surface in an AP1000 core makeup tank. From a practical standpoint, lack of the volume to volume heat diffusion terms will not make a major difference in a simulation. For any normal spatial discretization the numerical diffusion (see (Ref. 1-7)) will significantly exceed the physical thermal diffusion.

3) Only contributions from the stress tensor due to shear at metal surfaces or phase interfaces within the averaging volume are considered. No contributions due to shear between flows in adjacent averaging volumes is included. Again from a practical standpoint, numerical diffusion terms exceed any physical terms dropped by this approximation. However, code users need to understand that field equations with this approximation are not capable of modeling circulation patterns within a large open region regardless of the choice of mesh size.

4) Only those portions of the work terms \( W_i \) and \( W_g \) that contribute to change in bulk kinetic energy of motion are retained. Viscous heating is ignored, except as a special model within pump components, accounting for heating of the fluid by a pump rotor through the direct heating source term \( q_{dl} \).

As a result of the first approximation, overbars are eliminated from the following equations, and a combination of time and volume average is implied for all state variables. At this point a switch is made in the definition of \( \alpha \) from a probability that a point is space is gas, to the fraction of the averaging volume occupied by gas (void fraction). Heat transferred from the interface to gas and to liquid (W/m\(^3\)) is represented by the terms \( q_{ig} \) and \( q_{il} \) respectively. Similar expressions (\( q_{wg}, q_{wl} \)) are used for heat transferred from surfaces of structures to the fluid. Expressions for all of these will come from correlations developed from steady state data, and they replace the heat transport terms in Equations (1-13) and (1-14) as shown in the following expressions

\[
-\nabla \cdot \left[ (1 - \alpha) \overrightarrow{q}_i \right] \Rightarrow q_{il} + q_{wl} \quad (1-17)
\]

\[
-\nabla \cdot \left[ \alpha \overrightarrow{q}_g \right] \Rightarrow q_{ig} + q_{wg} \quad (1-18)
\]

Under the third approximation the right hand sides of the momentum equations are changed to a simpler form:
where \( f_i \) is the force per unit volume due to shear at the phase interface, \( f_{wl} \) is the wall shear force per unit volume acting on the liquid, \( f_{wg} \) is the wall shear force per unit volume acting on the gas, and \( V_i \) is the flow velocity at the phase interface.

Given the above notation for force terms, and the fourth assumption, the energy equations can be written in the form:

\[
\frac{\partial[(1-\alpha)\rho_l \vec{V}_l]}{\partial t} + \nabla \cdot [(1-\alpha)\rho_l \vec{V}_l \vec{V}_l + (1-\alpha)\nabla P] = \vec{f}_i + \vec{f}_{wl} + (1-\alpha)\rho_l \vec{g} - \Gamma \vec{V}_i \quad (1-19)
\]

\[
\frac{\partial[\alpha \rho_g \vec{V}_g]}{\partial t} + \nabla \cdot [\alpha \rho_g \vec{V}_g \vec{V}_g + \alpha \nabla P] = \vec{f}_i + \vec{f}_{wg} + \alpha \rho_g \vec{g} + \Gamma \vec{V}_i \quad (1-20)
\]

Under the notation used in Equations (1-19) through (1-22), the mass equations for the two fluid model, become:

\[
\frac{\partial[(1-\alpha)\rho_l \vec{V}_l]}{\partial t} + \nabla \cdot [(1-\alpha)\rho_l \vec{V}_l] = -\Gamma \quad (1-23)
\]
Closure is obtained for these equations using normal thermodynamic relations and correlations for phase change, heat source and force terms. These equations do not directly require the quasi-steady assumption for the closure terms as long as the correct closure relations for the given transient exist. A real difficulty arises because, depending on how the closure relations were developed, a different set of closure relations may be required for each transient, and each set must comply with the assumptions associated with the definition of the time- and volume-averaging used in the field equations. If a steady- or quasi-steady-state database or a relationship derived from such a database is used to represent a closure relation, the code necessarily applies the quasi-steady assumption, as detailed in Appendix A. This latter case applies for the closure relations within TRACE.

The phase-change rate required by the equation set is evaluated from a simple thermal-energy-jump relation, often called a heat conduction limited model.

\[ \Gamma = \frac{-(q_{ig} + q_{il})}{(h_v' - h_l')} \]  

(1-25)

where the interfacial heat transfer per unit volume on the gas and liquid sides are

\[ q_{ig} = \frac{P}{P} h_{ig} a_i (T_{sv} - T_v) \]  

(1-26)

and

\[ q_{il} = h_{il} a_i (T_{sv} - T_l) . \]  

(1-27)

Here \( a_i \) is the interfacial area per unit volume, \( h_{ig} \) and \( h_{il} \) are HTCs at the liquid/gas interface, and \( T_{sv} \) is the saturation temperature corresponding to the partial steam pressure (\( P_v \)). Chapter 5 discusses the closure relationships used to define \( a_i, h_{ig}, \) and \( h_{il} \). The quantities \( h_v' \) and \( h_l' \) are the appropriate enthalpies of the vapor and liquid, respectively. These enthalpies are the bulk fluid enthalpy for the phase moving to the interface and the saturation enthalpy for the product of the phase change. This choice of enthalpies was inherited from both the RELAP and TRAC code series. Use of bulk enthalpy for the phase moving to the interface was necessary to prevent unphysical thermal runaways.

One example of such runaway behavior can occur when subcooled liquid is driving the condensation of a superheated vapor and the interfacial heat transfer on the gas side is very low. In this situation the bulk gas temperature increases if steam is removed at the interface at the saturation temperature, but no significant interfacial heat transfer (diffusion) from bulk gas to
interface is present to provide a balancing cooling effect for the bulk gas. Removal of steam at a temperature less than the bulk temperature, leaves the remaining gas hotter. The root of this problem is in the use of the heat conduction limited model. It is meant for a diffusion dominated process and the heat transfer coefficients selected to represent the boundary conditions at the interface assume diffusion dominates the energy transfer. In fact when the full advection/diffusion problem is considered the diffusive heat flux at the boundary is strongly enhanced as the advection becomes important (see, for example, the temperature profiles in the advection/diffusion example presented by Roach (Ref. 1-8)). In this limit of negligible interfacial heat transfer on the gas side, use of the bulk gas temperature to evaluate the steam enthalpy in Eqs. (1-22) and (1-25) is rigorously correct. In any case, except for very unusual circumstances, temperatures are close enough to saturation that use of a bulk enthalpy rather than a saturation enthalpy in Eqs. (1-22) and (1-25) will make much less difference in results than the inherent range of uncertainty associated with interfacial heat transfer equations.

Using Newton’s law of cooling extended to a thermal nonequilibrium situation, the wall heat-transfer terms assume the form

\[ q_{wg} = h_{wg} a_w (T_w - T_g) = q'_{wg} a_w \]  

(1-28)

and

\[ q_{wl} = h_{wl} a_w (T_w - T_l) = q'_{wl} a_w \]  

(1-29)

where \( a_w \) is the heated surface area per volume of fluid (only meaningful in a volume averaged or finite volume context). The heat transfer coefficients \( h_{wg} \) and \( h_{wl} \) include the information regarding the portion of the wall having gas and liquid contact. Chapter 6 discusses the closure relationships used to define \( h_{wg} \) and \( h_{wl} \).

Force terms \( f_i \), \( f_{wg} \), and \( f_{wl} \) are cast in the following forms, relying on correlations for friction coefficients \( C_i \), \( C_{wg} \), and \( C_{wl} \).

\[ f_i = C_i (\vec{V}_g - \vec{V}_i) \left| \vec{V}_g - \vec{V}_i \right| \]  

(1-30)

\[ f_{wg} = -C_{wg} \vec{V}_g \left| \vec{V}_g \right| \]  

(1-31)

\[ f_{wl} = -C_{wl} \vec{V}_l \left| \vec{V}_l \right| \]  

(1-32)

By representing interfacial force with Eq. (1-30), two contributions to interfacial force have been neglected. Terms proportional to acceleration (virtual mass terms) have been ignored because of no evidence of significance in reactor safety problems, combined with significant increase in
complexity of the solution procedure when they are present with semi-implicit or SETS solution procedures. Virtual mass terms will be reconsidered if higher order numerical methods are introduced into a future version of TRACE and a well-posed set of PDEs becomes important. Lift forces perpendicular to the flow direction have also been dropped. However, some representation of this term will be necessary in future TRACE versions containing the ability to do sub-channel analysis in a reactor core.

**Rearrangement of Equations for Numerical Solution**

TRACE does not solve the field equations in the form presented above. To cut complexity and computer time of the numerical solution, the fully conservative forms of the energy and momentum equations are rearranged to provide internal energy and motion equations. The steps to the next form of the field equations are rigorous mathematically, and involve no formal approximations. However, in finite volume form, the internal energy equations have problems with very large changes in pressure between two cells that are not present when the fully conservative forms of the energy equations are implemented directly into a finite volume approach. In such cases the prediction of temperature change between two volumes deteriorates significantly when the pressure change between the volumes is very large. This problem was inherited from RELAP and TRAC, and from a practical standpoint has only been apparent when the code has been used to model both the reactor primary and the containment during a LOCA. Fortunately, one portion of the TRACE development effort was a task to provide direct time step by time step linkage between parallel executions of TRACE and CONTAIN. CONTAIN was developed for the USNRC at Sandia National Laboratory to simulate a reactor containment’s transient behavior during a LOCA. In a coupled calculation TRACE only simulates the reactor coolant system (vessel, primary loops, and steam generator secondary system) while CONTAIN simulates the containment side of the problem. Development of the linkage between TRACE and CONTAIN included adjustments to the energy flux terms between the codes to preserve the correct temperature change in fluid as it moves from a high pressure volume in TRACE to a low pressure volume in CONTAIN.

Use of motion equations, rather than fully conservative momentum equations, generally works very well. However, exaggerated momentum transfer can occur in TRACE V5.0 (or earlier) when a steam/droplet mixture flows down towards the surface of a liquid pool (often in a downcomer during reflood). When practical, the solution to this problem is to engage the TRACE interface tracking model.

An internal energy conservation equation (gas or liquid) is obtained by taking the dot product of the corresponding momentum equation with its velocity and subtracting the results from the fully conservative energy equation. For gas the result is:

\[
\frac{\partial (\rho g e_g)}{\partial t} + \nabla \cdot (\rho g e_g \vec{V}_g) = -P \frac{\partial \alpha}{\partial t} - P \nabla \cdot (\alpha \vec{V}_g) + q_{wg} + q_{dg} + q_{ig} + \Gamma h_v, \tag{1-33}
\]
A similar operation is performed on the liquid energy equation, but rather than using it in that form, the result is added to the gas energy equation to produce a mixture energy conservation equation.

\[
\frac{\partial}{\partial t} \left[ (1-\alpha) \rho_l e_l + \alpha \rho_g e_g \right] + \nabla \cdot \left[ (1-\alpha) \rho_l V_l + \alpha \rho_g V_g \right] = 0
\]  

(1-34)

When included in the finite volume equation solution, the mixture energy equation makes it easier to deal with transitions from two-phase to single-phase flow during a step in the time integration. To fully achieve this advantage during a transition, a similar pair of gas and mixture mass equations must be used in the actual solution.

\[
\frac{\partial (\alpha \rho_g)}{\partial t} + \nabla \cdot [\alpha \rho_g V_g] = \Gamma
\]  

(1-35)

\[
\frac{\partial}{\partial t} \left[ (1-\alpha) \rho_l + \alpha \rho_g \right] + \nabla \cdot \left[ (1-\alpha) \rho_l V_l + \alpha \rho_g V_g \right] = 0
\]  

(1-36)

Motion equations are obtained by the standard means of multiplying the mass conservation equation for a phase (Eq. (1-23) or Eq. (1-24)) by that phase’s velocity, subtracting it from the corresponding momentum conservation equation (Eq. (1-19) or Eq. (1-20)), and dividing the result by the appropriate macroscopic density.

\[
\frac{\partial V_l}{\partial t} + V_l \cdot \nabla V_l = -\frac{1}{\rho_l} \nabla P + \frac{f_i - \Gamma (V_i - V_l) + f_wl}{(1-\alpha) \rho_l} + \dot{\gamma}
\]  

(1-37)

\[
\frac{\partial V_g}{\partial t} + V_g \cdot \nabla V_g = -\frac{1}{\rho_g} \nabla P + \frac{f_{wg} - f_i - \Gamma (V_g - V_i)}{\alpha \rho_g} + \dot{\gamma}
\]  

(1-38)

Eq. (1-37) and Eq. (1-38) are generally referred to as the nonconservative form of the momentum equations, because it is not possible to write a finite volume method that guarantees some numerical integral of momentum over a system does not change from one time step to the next in
the absence of force terms. Use of this form permits simpler numerical solution strategies particularly for a semi-implicit method, and can generally be justified because the presence of wall friction makes the fully conservative form of the momentum equation far less useful. When sharp flow-area changes exist, however, numerical solution of the nonconservative motion equations can produce significant errors. For these situations, the motion equations have been modified to force Bernoulli flow (see Conserving Convected Momentum later in this chapter).

Terms in the momentum equation associated with phase change at the interface can produce non-physical velocity runaways that are analogous to the thermal runaways discussed above. Consider the case of moving steam condensing onto a stratified relatively stagnant liquid. The interfacial drag term will not be significant, and the negative value of \( \Gamma \) combined with an interface velocity with any significant relation to the liquid velocity will result in a positive acceleration to the gas. To avoid such velocity runaways the interface velocity appearing in Equations (1-37) and (1-38) is set to \( V_l \) when \( \Gamma \) is positive (boiling) and to \( V_g \) when \( \Gamma \) is negative.

**Noncondensable Gas**

Normally only one noncondensable gas field is modeled with TRACE, but it supports multiple gas species if the user is willing to increase run time by using extra field equations. The noncondensable gas mixture is assumed to be in thermal equilibrium with any steam that is present and to move with the same velocity as the steam (mechanical equilibrium). Hence, only a single gas momentum (Eq. (1-38)) and a single gas energy equation (Eq. (1-33)) are needed. Mass conservation is provided with a total noncondensable mixture mass equation:

**Noncondensable Mixture Mass Equation**

\[
\frac{\partial (\alpha \rho_a)}{\partial t} + \nabla \cdot \left[ \alpha \rho_a V_g \right] = 0, \quad (1-39)
\]

and equations for each additional species in the mixture beyond the first.

**Additional Non-Condensable Mass Equations (k\(^{th}\) species)**

\[
\frac{\partial (\alpha X_k \rho_a)}{\partial t} + \nabla \cdot \left[ \alpha X_k \rho_a V_g \right] = 0 \quad (1-40)
\]

We could have skipped use of the mixture gas conservation Eq. (1-39) in favor of individual species equation (1-40) for all species present. However, in analogy to justification for use of a
full mixture mass equation (1-36), inclusion of the full mixture mass equation aids in enforcement of mass conservation when individual gas species disappear from a computational volume.

For pure non-condensable gases, air, and mixtures of these gases, an ideal gas equation of state is normally assumed. The only exception occurs when helium is the only noncondensable gas present in a flow simulation. In that case, you are permitted to select a non-ideal helium equation (see Chapter 11). In terms of the ideal gas model, the mixture density is obtained from:

\[ \rho_a = \frac{P}{R_{mix} T} \]  \hspace{1cm} (1-41)

With this field present, the total gas density and energy are sums of the vapor and the noncondensable components,

\[ \rho_g = \rho_v + \rho_a \]  \hspace{1cm} (1-42)

and

\[ e_g \rho_g = e_v \rho_v + e_a \rho_a \]  \hspace{1cm} (1-43)

where specific internal energy of the noncondensable mixture is the sum of mass weighted contributions from all noncondensable gas species.

\[ e_a = X_{NC,1} e_{NC,1} + X_{NC,2} e_{NC,2} + \ldots \]  \hspace{1cm} (1-44)

We assume Dalton’s law applies; therefore,

\[ P = P_v + P_a \]  \hspace{1cm} (1-45)

TRACE, by default, applies the thermodynamic properties for air to a single noncondensable gas. The code user may, however, select hydrogen, helium, nitrogen, argon, krypton, or xenon as the single gas, or use any of these in a mixture.

**Liquid Solute**

TRACE includes an optional mass-continuity equation for a solute (default is orthoboric acid) moving with the liquid field.
**Liquid-Solute Concentration Equation**

\[
\frac{\partial[(1-\alpha)m\rho_l]}{\partial t} + \nabla \cdot [(1-\alpha)m\rho_l \mathbf{V}_l] = S_m
\]  \hspace{1cm} (1-46)

where \(m\) is the solute concentration (mass of solute/unit mass of liquid water) in the liquid phase.

The solute does not affect the hydrodynamics directly. However, the amount of the dissolved and the plated-out orthoboric acid in a reactor core may affect the hydrodynamics indirectly through neutronic-reactivity feedback corresponding to user-specified input values obtained from a boron-mass reactivity-coefficient table (see Chapter 9, Reactivity Feedback). If the solute concentration exceeds the orthoboric-acid solubility at the liquid temperature in a specific hydrodynamic cell, TRACE assumes that the excess solute in that cell plates out. Plating on structures can occur if the cell liquid boils and thus increases the concentration beyond the solubility limit. TRACE also assumes that any plated-out solute instantaneously redissolves to the maximum allowable concentration if more liquid enters the cell. Because the solute does not affect the hydrodynamics directly, the solute variable may also be used as a tag to track the movement of liquid from a specific source through the system.

**Application Specific Usage of these Equations**

TRACE utilizes the time and volume averaged equations presented in the previous section in two contexts. The first is in a 1-D form in which fluid behavior in the other two dimensions is hidden by an average of the flow over the cross-section of the flow channel. As will be seen below, this procedure permits modeling of flow channels with variable cross-sectional area, but loses the ability to capture the effects of flow structures (e.g. recirculation zones) associated with changes in cross-sectional area. The second context is 3-D modeling, where a porous media approach is followed in the actual implementation. When the field equations are averaged over a 3-D region, provisions are made for metal structures filling portions of the geometric volumes and bounding flow areas, reducing the actual space available for flow. Changes of available flow area within this context, combined with sizes of the averaging volumes will also mask details of flow patterns. In both cases empirical modeling is required to capture the average effects of flows not resolved. The primary contribution to this modeling seen by the user is the need to specify empirical loss coefficients for the momentum equations.

**1-D Equations**

The use of the term "one-dimensional" in association with the equations used by TRACE to model piping in reactors or experiments can be an immediate source of confusion. The tendency is to think in terms of three-dimensional Cartesian geometry, and a pipe running straight in a single direction. However, piping runs in these systems have a number of bends, and a true one-
dimensional equation has only one "momentum" equation. What is done in TRACE, and was done in its predecessors TRAC and RELAP, is to think in terms of a coordinate system in which the one dimension follows the centerline of the entire piping run. Within this view, the flows in all piping segments shown in Figure 1-1 are all one-dimensional, and the vectors at the entrance and exit of each example are in the same coordinate direction.

Figure. 1-1. Sample 1-D Piping Segments

The first pipe segment in Figure 1-1 represents the standard view of 1-D flow and a single coordinate momentum equation will work well as long as the flow is turbulent, giving a flat velocity profile over most of the flow cross-section. For the second pipe segment, the dimension along the pipe could be the theta direction in a cylindrical coordinate system. Although this change in coordinate system simplifies the construction of an area averaged momentum equation, the turn can’t always be ignored. For single phase flow centrifugal force terms alter velocity profiles and can have a small impact of the wall friction term. For two phase flow, the centrifugal force term in the un-modeled radial momentum equation can have a significant effect on flow regime, and through that, the relative velocity between the phases and the wall heat transfer (e.g. helical heat exchanger tube). In sharper bends separation should be expected for flow coming past the inside of the bend, and irrecoverable pressure losses will occur up to the limit predicted by a simple two-dimensional right angle turn analysis. All of these details are lost in averaging over the flow cross-section, and if important must be captured with special sub-grid models.

Similar loss of information occurs for flow through a straight run of variable area pipe (see Figure 1-2). Recirculation zones downstream of an expansion, vena contracta downstream of a contraction, and pressure distributions associated with these phenomena will not be captured. That is a job for CFD. The approach in TRACE and its predecessors has been to structure the discrete implementation to introduce the minimum irrecoverable loss at an abrupt area change and to rely on user input of loss coefficients to model physical processes lost in the coarse nodalization. For the flow illustrated in Figure 1-2 the goal is to have a discrete form of the momentum equation that, absent wall friction terms, produces a pressure change between inlet and outlet that is as consistent as possible with Bernoulli flow. Irrecoverable pressure losses associated with unresolved details of the flow are again covered by user input loss coefficients.
Pseudo 2-D Flow

One-dimensional modeling is complicated by the fact that pipes modeled by one dimensional cross-section averaged equations can have connections through their walls from other pipes. Within reactor systems these connections are necessary to model Emergency Core Cooling Systems (ECCS) and jet pumps. Topologically, connections can range from a right angle "T", through angled connections to the wall, to injection pipes that are interior and parallel to a larger pipe at the point of injection (see Figure 1-3).

Figure. 1-2. Abrupt Expansion and Contraction

Figure. 1-3. Tee connections

Derivations of the finite volume equations in the next section include provisions for such side junctions to a 1-D flow path. However, there are certain limitations within the current TRACE
implementation that should be noted now. For reactor system transients the injection flow patterns illustrated in Figure 1-3 are the situations where the momentum transport terms are the most significant. In particular it is very important to transfer momentum correctly within a jet pump model, and in situations where ECCS liquid is being injected into a steam flow through a reactor coolant pipe. A rigorous formulation for momentum transfer terms has not been developed for the case were flow is out through the side connection. When this happens in normal reactor scenarios, the split in mass flows between the main and side legs of the connection is driven by pressure rather than momentum terms. In addition TRACE currently expects the main channel to have a constant cross-sectional area over the volume with the side flow connection. Abrupt area changes across a volume containing a side junction can lead to distortions in momentum transfer terms. If the impact of momentum transfer in such a location is not clearly understood to be minimal, user guidelines on nodalization at a side junction should be followed.

One aspect of outflow from a side junction has been given special treatment. When the main channel has stratified two-phase flow and a large enough pressure drop occurs through the side connection, the volume fraction of fluid pulled through the side junction is not equal to the mean volume fraction in the main flow channel. TRACE uses a special offtake model, documented in Chapter 10, to determine the void fraction of the fluid convected out of the side junction.

3-D Equations

The 3-D implementation of the field equations suffer from two primary limitations. The first has already been mentioned. There is no model for turbulent diffusion and shear between fluid cells, making TRACE unsuitable for modeling circulation patterns in large open regions. The second is related to the large computational volumes used in models of reactor vessels. Flow turns from the cold leg into the downcomer and normally from the downcomer to the lower plenum within a single volume. This yields an irrecoverable pressure loss within the calculation that is the same as can be obtained from a simple back of the envelop calculation for a sharp right angle turn. In fact the streamlines curve, and the pressure distribution is such that the actual pressure loss will be less than the right angle limit.

Basic Finite-Volume Approximations to the Flow Equations

To avoid confusion a few words are necessary about notation used in this section. We use a fairly standard notation to represent a volume integral. For example mass in a volume would be written as

$mass = \int_V \rho dV \quad (1-47)$
Unfortunately, an upper case "V" is also used when writing velocities. However, there will be no integration over velocities in this documentation, so that the combination of a "$V$" below an integral sign and a "$dV$" should always be interpreted as a volume integral. To avoid confusion when integrals are not present in notation, we define

\[ Vol = \int_V dV \]  

(1-48)

Integrals are further abbreviated through use of overbar averaging notation. For example the mean density in a volume is expressed as

\[ \bar{\rho} = \frac{\left( \int_V \rho dV \right)}{Vol} \]  

(1-49)

The field equations introduced in the previous section have gone through a volume averaging process to generate the wall terms in the energy and momentum equations, and fit well with a finite volume solution approach. Consider the region in a flow channel illustrated in Figure 1-4. In this example the surface bounding the volume of fluid is divided into the channel wall area, and three areas ($A_1$, $A_2$, $A_3$) through which flow can occur. The integral form of the gas mass conservation equation for this volume is:

\[ \frac{\partial}{\partial t} \int_V \alpha \rho g dV + \int_V \nabla \cdot (\alpha \rho g \vec{V}_g) \, dV = \int_V \Gamma \, dV \]  

(1-50)

or applying Gauss’ Theorem:

\[ \frac{\partial}{\partial t} \int_V \alpha \rho g dV + \oint_S \alpha \rho g \vec{V}_g \cdot d\vec{S} = \int_V \Gamma \, dV. \]  

(1-51)

Hence the time derivative of the total gas mass in the region can be written as:

\[ \frac{\partial (\alpha \rho g)}{\partial t} \mid_{Vol} + \left( \alpha \rho g \vec{V}_g \right)_1 \cdot \vec{A}_1 + \left( \alpha \rho g \vec{V}_g \right)_2 \cdot \vec{A}_2 + \left( \alpha \rho g \vec{V}_g \right)_3 \cdot \vec{A}_3 = \vec{\Gamma} \cdot Vol \]  

(1-52)

where the positive sense of an area vector is directed out from the volume.
Four approximations must be made to convert Eq. (1-52) to a useful discrete approximation to the gas mass conservation equation. First the volume average of vapor macroscopic density must be related to the volume centered values. In TRACE, the simple first order assumption is made that state quantities are constant throughout a volume, so the volume average is taken to be equal to the volume center value. The next approximation converts the partial derivative with respect to time to a simple algebraic expression, given as

$$\frac{\partial (\bar{\alpha} \rho_g)}{\partial t} = \frac{\bar{\alpha} \rho_g^{n+1} - \bar{\alpha} \rho_g^n}{\Delta t},$$  \hspace{1cm} (1-53)

where:

1) a superscript "n" denotes known values at the current level in time;

2) a superscript "n + 1" denotes a value at the next level in time that must be determined from solution of the equations; and

3) $\Delta t$ is the increment in time between levels $n$ and $n + 1$.

The third approximation is that for all expressions, the average of a product is equal to the product of individual average state variables. In this case, Eq. (1-52) becomes

$$\frac{\partial \bar{\alpha} \rho_g}{\partial t} V_{ol} + \left(\bar{\alpha} \rho_g \bar{V}_g\right)_1 \cdot \vec{A}_1 + \left(\bar{\alpha} \rho_g \bar{V}_g\right)_2 \cdot \vec{A}_2 + \left(\bar{\alpha} \rho_g \bar{V}_g\right)_3 \cdot \vec{A}_3 = \bar{\Gamma} \cdot V_{ol}.$$ \hspace{1cm} (1-54)

The fourth approximation relates values of state variables at volume edge flow faces to volume centered quantities. In the case of Eq. (1-54), when void fraction and gas density are needed to
calculate a mass flux at a flow surface \((A_1, A_2, \text{ or } A_3)\), the values are obtained from the nearest volume center upstream (as determined by gas velocity) from the flow surface. This is a first order upwind method. Momentum equations are evaluated at the edges of the volumes used for mass and energy conservation, so no upwind approximation is needed to obtain the velocity used in mass flux terms. One important piece of information missing from Eq. (1-54) is the time level of state variables in the mass flux terms. Options for this choice within TRACE are discussed later in this chapter.

Similar derivations can be followed to obtain discrete forms for other mass and energy conservation equations. For liquid mass or energy equations, the upwind cell center is determined from the liquid velocity.

Generation of a discrete approximation to the momentum equation is more complex due to the fact that velocities and associated momentum equations are not evaluated at the same locations as thermodynamic state variables. Momentum equations and the primary associated velocities are evaluated at the surfaces separating the volumes used for conservation of mass and energy. Figure 1-5 illustrates the edge (labeled \(j + 1/2\)) between two adjacent mass/energy conservation volumes (\(j\) and \(j + 1\)). It illustrates the fact that a given computational volume can have a non-uniform cross-sectional area, and that discontinuous changes in flow area can be modeled at the junction between volumes. The center of a mass conservation volume is taken to be halfway between the bounding flow surfaces along the center of the flow channel. Dotted lines through these center points represent surfaces that will bound a volume to be used in the derivation of the finite volume form of the momentum equation. Since the fundamental evaluation of velocities is not at these dotted surfaces through points \(j\) and \(j + 1\), a special averaging procedure is needed to obtain velocities at these surfaces for use in momentum transport terms. This needs to be consistent with the upwind procedure discussed for the mass conservation equation. However,
because rapid area changes are permitted from volume to volume, the upwind approach is applied to volumetric flow rather than velocity and for the flow direction chosen in Figure 1-5 we get

\[ V_{j+1} = \frac{A_{j+1/2} V_{j+1/2}}{A_{j+1}} \]

and

\[ V_j = \frac{A_{j-1/2} V_{j-1/2}}{A_j} \]

A detailed derivation of the discrete momentum equation and an alternative derivation based upon kinetic energy are provided in Appendix B. However, key steps in the process are provided here. Figure 1-6 focuses on the momentum volume consisting of the right half of mass volume \( j \) and left half of mass volume \( j+1 \). To cut the length of subscript notation, the surfaces at locations \( j \) and \( j+1 \) in Figure 1-5 are now designated by subscripts 1 and 2 respectively and assigned areas \( A_1 \) and \( A_2 \). The central surface between the two mass volumes is given a subscript \( c \), and to cover side junctions in the derivation, side flow through an area \( A_3 \) is permitted. Users need to know that more than one such side junction may exist. Because of the upstream approximations used for spatial averages, only those side junctions upstream from the center of the momentum cell can contribute to momentum fluxes. In the final implementation of the finite volume momentum equation, this upstream requirement can result in a shift in association of a side junction from one momentum volume to its immediate neighbor as flow velocities switch sign.

![Figure 1-6. Momentum Volume](image)

Basic approximations used in generation of the final discrete equations are modified slightly. Thermodynamic state variables such as density, pressure, and volume fraction are still constant.
over mass conservation volumes, so within the momentum volume, density (for example) has one uniform value upstream of the central flow area \((A_c)\), and a second uniform value downstream of the central area. However, it is the product of velocity and channel flow area (volumetric flow) that is treated as constant on either side of the central flow area.

As a simple example of generation of a discrete momentum equation, integrate the gas momentum equation over the momentum volume associated with flow surface \(A_c\) located between two mass/energy conservation volumes.

\[
\int \frac{\partial}{\partial t} (\alpha \rho_g \mathbf{V}_g) dV + \int \left( \alpha \rho_g \mathbf{V}_g \mathbf{V}_g \right) \cdot d\mathbf{S} + \int \alpha \nabla P dV = \int (\Gamma \mathbf{V}_i + \mathbf{f}_i + \mathbf{f}_w + \alpha \rho_g \mathbf{V}_g) dV
\]  
(1-55)

or

\[
\int \frac{\partial}{\partial t} (\alpha \rho_g \mathbf{V}_g) dV + \sum_{k=1,3} \left( \alpha \rho_g \mathbf{V}_g \mathbf{V}_g \right)_k \cdot \mathbf{A}_k + \int \alpha \nabla P dV = \int (\Gamma \mathbf{V}_i + \mathbf{f}_i + \mathbf{f}_w + \alpha \rho_g \mathbf{V}_g) dV. \quad (1-56)
\]

Next integrate the mass conservation equations over the portions of the volume to the left and right of \(A_c\). Area vectors for areas 1 through 3 are chosen to have a positive sense out of the momentum volume. The area vector associated with an area splitting the momentum volume in the middle has a sign convention that is positive towards end area 2.

\[
\int \frac{\partial}{\partial t} (\alpha \rho_g) dV - \left( \alpha \rho_g \mathbf{V}_g \right)_c \cdot \mathbf{A}_c + \left( \alpha \rho_g \mathbf{V}_g \right)_2 \cdot \mathbf{A}_2 = \int \Gamma dV
\]  
(1-57)

and

\[
\int \frac{\partial}{\partial t} (\alpha \rho_g) dV + \left( \alpha \rho_g \mathbf{V}_g \right)_1 \cdot \mathbf{A}_1 + \left( \alpha \rho_g \mathbf{V}_g \right)_c \cdot \mathbf{A}_c + \left( \alpha \rho_g \mathbf{V}_g \right)_3 \cdot \mathbf{A}_3 = \int \Gamma dV
\]  
(1-58)

Changing notation to use of the volume and area averages seen in the derivation of the finite volume mass equation, the integrated momentum equation can be written as:
The mass equations for the left (subscript $l$) and right (subscript $r$) halves of the momentum volume are:

\[
\frac{\partial}{\partial t} (\alpha \rho_g \mathbf{V}_g) Vol_{j+1/2} + \sum_{k=1,3} (\alpha \rho_g \mathbf{V}_g)_k \cdot \mathbf{A}_k
\]

\[+ \alpha \nabla \rho_{Vol} Vol_{j+1/2} = \left( \Gamma \mathbf{V}_i + \hat{\mathbf{j}}_l + \hat{\mathbf{j}}_w + \alpha \rho_g \hat{\mathbf{j}} \right) Vol_{j+1/2} \]  

(1-59)

Next rearrange these mass equations to get end fluxes along the primary direction of flow.

\[
\frac{\partial}{\partial t} (\alpha \rho_g) Vol_{l} + (\alpha \rho_g \mathbf{V}_g)_l \cdot \mathbf{A}_1 + (\alpha \rho_g \mathbf{V}_g)_c \cdot \mathbf{A}_c + (\alpha \rho_g \mathbf{V}_g)_3 \cdot \mathbf{A}_3 = \Gamma_l Vol_l
\]

(1-60)

and

\[
\frac{\partial}{\partial t} (\alpha \rho_g) Vol_{r} - (\alpha \rho_g \mathbf{V}_g)_c \cdot \mathbf{A}_c - (\alpha \rho_g \mathbf{V}_g)_2 \cdot \mathbf{A}_2 = \Gamma_r Vol_r
\]

(1-61)

Next rearrange these mass equations to get end fluxes along the primary direction of flow.

\[
\frac{\partial}{\partial t} (\alpha \rho_g) Vol_{l} - (\alpha \rho_g \mathbf{V}_g)_c \cdot \mathbf{A}_c - (\alpha \rho_g \mathbf{V}_g)_3 \cdot \mathbf{A}_3 = \Gamma_l Vol_l
\]

(1-62)

and

\[
\frac{\partial}{\partial t} (\alpha \rho_g) Vol_{r} + (\alpha \rho_g \mathbf{V}_g)_c \cdot \mathbf{A}_c
\]

(1-63)

At this point we use the assumption that the volume average of the products is equal to the product of the volume averages. By this point all velocities are time averaged, and turbulence effects have been included in wall and interfacial force terms, so no further loss of turbulence effects is implied. As mentioned in the previous section, this assumption works well in most cases, but some cases exist where this will introduce difficulties. To simplify notation beyond this point we will drop the bar over flow variables. Eq. (1-59) becomes:

\[
\frac{\partial}{\partial t} (\alpha \rho_g \mathbf{V}_g) Vol_{j+1/2} + \sum_{k=1,3} (\alpha \rho_g \mathbf{V}_g)_k \cdot \mathbf{A}_k
\]

\[+ (\alpha \nabla \rho) Vol_{j+1/2} = \left( \Gamma \mathbf{V}_i + \hat{\mathbf{j}}_l + \hat{\mathbf{j}}_w + \alpha \rho_g \hat{\mathbf{j}} \right) Vol_{j+1/2} \]

(1-64)
Flux terms in Eq. (1-64) are expanded by multiplying Eq. (1-62) by $V_{g,1}$ and Eq. (1-63) by $V_{g,2}$, giving us

\[ (\alpha \rho_g \vec{V}_g \vec{V}_g)_1 \cdot \vec{A}_1 = \Gamma_l V_{g,1} Vol_l - V_{g,1} \frac{\partial}{\partial t} (\alpha \rho_g) Vol_l \]

\[ - V_{g,1} (\alpha \rho_g \vec{V}_g)_c \cdot \vec{A}_c - V_{g,1} (\alpha \rho_g \vec{V}_g)_3 \cdot \vec{A}_3 \]

\[ (\alpha \rho_g \vec{V}_g \vec{V}_g)_2 \cdot \vec{A}_2 = \Gamma_r V_{g,2} Vol_r - V_{g,2} \frac{\partial}{\partial t} (\alpha \rho_g)_r Vol_r + V_{g,2} (\alpha \rho_g \vec{V}_g)_c \cdot \vec{A}_c . \]  

(1-66)

Eq. (1-65) and Eq. (1-66) provide expressions for the first two terms in the momentum flux summation from Eq. (1-64), giving:

\[ \sum_{k=1,3} (\alpha \rho_g \vec{V}_g \vec{V}_g)_k \cdot \vec{A}_k = \vec{V}_{g,2} (\alpha \rho_g \vec{V}_g)_c \cdot \vec{A}_c - \vec{V}_{g,1} (\alpha \rho_g \vec{V}_g)_c \cdot \vec{A}_c \]

\[ + (\vec{V}_{g,3} - \vec{V}_{g,1}) (\alpha \rho_g \vec{V}_g)_3 \cdot \vec{A}_3 + \Gamma_r \vec{V}_{g,2} Vol_r + \Gamma_l \vec{V}_{g,1} Vol_l \]

\[ - \vec{V}_{g,2} \frac{\partial}{\partial t} (\alpha \rho_g)_r Vol_r - \vec{V}_{g,1} \frac{\partial}{\partial t} (\alpha \rho_g)_l Vol_l \]

or

\[ \sum_{k=1,3} (\alpha \rho_g \vec{V}_g \vec{V}_g)_k \cdot \vec{A}_k = (\alpha \rho_g \vec{V}_g)_c \cdot \vec{A}_c (\vec{V}_{g,2} - \vec{V}_{g,1}) \]

\[ + (\vec{V}_{g,3} - \vec{V}_{g,1}) (\alpha \rho_g \vec{V}_g)_3 \cdot \vec{A}_3 + \Gamma_r \vec{V}_{g,2} Vol_r + \Gamma_l \vec{V}_{g,1} Vol_l \]

\[ - \vec{V}_{g,2} \frac{\partial}{\partial t} (\alpha \rho_g)_r Vol_r - \vec{V}_{g,1} \frac{\partial}{\partial t} (\alpha \rho_g)_l Vol_l \]

(1-68)

Given that the only permitted location for area discontinuity is at the center of the momentum volume, and that the final numerical method is restricted to first order accuracy, we can write:
Eqs. (1-69) and (1-70) can be substituted into Eq. (1-68), and the result substituted into Eq. (1-64), to give a simpler form of the finite volume momentum equation.

\[
\frac{\partial}{\partial t}(\alpha \rho_g \vec{V}_g)Vol_{j+1/2} - \vec{V}_{g,2} \frac{\partial}{\partial t}(\alpha \rho_g)Vol_r
\]

and

\[
\Gamma \vec{V}_i Vol_{j+1/2} - \Gamma_r \vec{V}_{g,2} Vol_r - \Gamma_l \vec{V}_{g,1} Vol_l = \Gamma(\vec{V}_i - \vec{V}_g)Vol_{j+1/2}
\]

At this point, to obtain results useful for a computer solution, we need to employ the previously mentioned assumptions about the spatial dependence of state variables within the volumes of interest. Here void fraction, densities, and pressure are taken as constant within the left portion of the momentum volume and a separate set of constant values over the right portion of the momentum volume. The basis functions for velocities are slightly modified to deal with the possibility of discontinuous change in area at the center of the momentum volume. Rather than taking the velocity to be constant, the product of area averaged velocity and area is taken as constant.

Expressions for volume averages need to be reexamined under the first order assumptions to provide useful forms for these terms. One additional quantity that will be useful in this context will be the distance "dx" along the primary flow path between bounding areas \( A_1 \) and \( A_2 \). Three of the averages in Eq. (1-71) are:
Evaluation of the total contribution of pressure forces is greatly simplified by the first order assumption that state variables are constant over sub-regions of the integration volume. For this particular case with pressure and void constant to the left and right of \( A_c \), we divide the integral of the pressure force term into integration over three sub-volumes. One is centered on \( A_c \) with an infinitesimal thickness perpendicular to \( A_c \). The other two sub-volumes cover the remainder of the momentum volume to the left and right of \( A_c \). The integral over these two large volumes will be zero because the pressure gradient is zero throughout both. However, the integral over the central volume is non-zero due to the discontinuity in pressure. The result is obtained through use of Heaviside step functions to represent the functional forms of pressure and void fraction.

\[
\int V \alpha \nabla P dV = A_c \int V \nabla P dx = A_c \left( \frac{\alpha_l + \alpha_r}{2} \right) (P_r - P_l) \tag{1-75}
\]
For those accustomed to the derivation of loss coefficients for an abrupt expansion, this approximation will look wrong. In the classic abrupt expansion case, the pressure $P_1$ is assumed to also be appropriate in the right sub-volume over the wall area aligned with the center surface of the momentum volume. Unfortunately, the finite volume calculation must be able to deal with a wide variety of channel shapes. Rather than doing subgrid calculations to obtain better values of surface pressure distributions, we have elected to account for the discrepancy by using loss coefficients. The approach taken in Eq. (1-75) produces the lowest irrecoverable pressure loss of all possible assumptions about wall pressure distribution. It is up to the user to provide loss coefficients in the model’s input specification that result in the correct irrecoverable pressure loss.

The force terms for interfacial and wall shear have proportionality to velocity, so the volume multiplying those terms ($Vol_{j+1/2}$) can be converted to the product $A_c \cdot dx$. Substituting all of the approximations to the volume integrals into the last form of the momentum equation and dividing everything by $\alpha \rho_g A_c dx$ gives

$$
\frac{\partial}{\partial t} \left( \vec{V}_g \right) + \frac{(\alpha \rho_g \vec{V}_g)_c}{\alpha \rho_g A_c dx} \cdot A_c \left( \vec{V}_{g,2} - \vec{V}_{g,1} \right) + \frac{(\alpha \rho_g \vec{V}_g)_3}{\alpha \rho_g A_c dx} \cdot A_3 \\
+ \frac{\vec{\alpha}(p_r - p_l)}{\alpha \rho_g dx} \cdot \hat{i} = \frac{1}{\alpha \rho_g} \left[ \Gamma (\vec{V}_{i,c} - \vec{V}_{g,c}) + f_{i,c} + f_{w,c} + \alpha \rho_g g \cdot Vol_{j+1/2} \right] 
$$

(1-76)

The actual momentum equations in TRACE were derived from a finite difference approach, and ratios with the product of volume fraction and density in numerator and denominator are set to one.

$$
\frac{\partial}{\partial t} \left( \vec{V}_g \right) + \frac{(\vec{V}_g)_c}{A_c dx} \cdot A_c \left( \vec{V}_{g,2} - \vec{V}_{g,1} \right) + \frac{(\vec{V}_g)_3}{\alpha \rho_g A_c dx} \cdot A_3 \\
+ \frac{\vec{\alpha}(p_r - p_l)}{\alpha \rho_g dx} \cdot \hat{i} = \frac{1}{\alpha \rho_g} \left[ \Gamma (\vec{V}_{i,c} - \vec{V}_{g,c}) + f_{i,c} + f_{w,c} \right] + \vec{g} 
$$

(1-77)

To this point the time and volume averaged momentum equation is still 3-D. Three steps are necessary to make it useful for a 1-D model. First the equation is recast into a coordinate system in which one dimension follows the flow channel. From the standpoint of this coordinate system, there are no bends in the piping. The piping’s centerline can be treated as the axis of the primary dimension. Second, take the dot product of Eq. (1-77) with a unit vector along the primary dimension to isolate the component of the velocity along the piping. Finally introduce a term to account for irrecoverable losses lost in the volume averaging and collapse to one dimension. This
accounts for wall pressure distributions and effects of recirculation zones not resolved due the scale of volume averaging.

\[
\frac{\partial V_g}{\partial t} + \frac{(V_g)_c}{dx} \left( V_{g,2} - V_{g,1} \right) + \frac{V_{g,3} \cos \phi - V_{g,1}}{\alpha \rho_g A_c dx} (\alpha \rho_g V_g)_3 A_3 \\
+ \frac{\alpha(p_r - p_l)}{\alpha \rho_g dx} = \frac{1}{\alpha \rho_g} \left[ \Gamma \left( V_{i,c} - V_{g,c} \right) + f_{i,c} + f_{w,c} \right] + \tilde{g} \cos \theta
\]  

(1-78)

In the above equation \( \phi \) is the angle between the pipe centerline and the primary flow direction through face \( A_3 \), and \( \theta \) is the angle between a vector along the centerline in a positive direction and a vector pointing vertically upward (against gravity).

During the evolution of the TRACE momentum equation implementation several deviations have occurred from the formal definition of terms in this derivation.

- The mean volume fraction of gas used in the pressure gradient term is currently a cell length weighted rather than simple average.
- The value of \( \alpha \rho_g \) in the denominator of the flux term for side connection momentum is currently donor cell averaged rather than cell length weighted.
- The final coefficient for the gravitational source term must be consistent with static gravitational pressure head in a two phase column of liquid
- \( V_1 \) and \( V_2 \) are obtained from area scaling of upwind edge velocities, and in the momentum flux term \( V_{g,c} \) is a simple area weighted average of \( V_1 \) and \( V_2 \), chosen this way to give Bernoulli equation results in the limit of steady state and constant density.

**Time Level Selection**

TRACE contains the option to select one of two related numerical methods for solution of the two-phase-flow equations. The default Stability Enhancing Two-Step (SETS) method has the advantage of avoiding Courant stability limits on time-step size but the disadvantage of relatively high numerical diffusion. A namelist input option permits selection of a semi-implicit method that can have substantially less numerical diffusion but has time-step sizes restricted by a material Courant limit. This should be the method of choice for BWR stability analysis. Currently, a single method must be used for the entire system. It is not possible, for example to use a semi-implicit vessel and SETS for the 1-D loops.

Both basic finite-volume models are descendents of the Implicit Continuous Eulerian technique (ICE) (Ref. 1-9). The key improvement introduced by Liles and Reed (Ref. 1-10) in their semi-implicit method was a tighter coupling of the energy equation to the mass and momentum equations than that used in ICE. This coupling is crucial to stable modeling of two-phase flows.
with substantial boiling or condensation. The SETS method (Refs. 1-11 and 1-12) includes the semi-implicit method at its core and increases stability with an additional evaluation of each field equation during each time step.

In the following subsections, the semi-implicit and SETS methods will be described at three levels of detail. The basic aspects of each method are illustrated for simple 1D single-phase-flow equations as follows:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho V) = 0, \quad (1-79)
\]

\[
\frac{\partial (\rho e)}{\partial t} + \frac{\partial}{\partial x} (\rho eV) = -P \frac{\partial V}{\partial x} + h_{vol} \frac{A_w}{A_w} (T_w - T), \quad (1-80)
\]

and

\[
\frac{\partial V}{\partial t} + V \frac{\partial V}{\partial x} = -\frac{1}{\rho} \frac{\partial P}{\partial x} - KV |V|, \quad (1-81)
\]

where \( K \) is a wall friction coefficient that may be a function of velocity and fluid properties and \( T_w \) is a pipe wall temperature. More detail is then provided through explanation of special adaptations to improve robust simulation of single- and/or two-phase flow. Finally, the full two-phase-flow equations are presented.

Fairly standard notation is used in presenting the finite-volume equations. A superscript “\( n \)” indicates known values at the beginning of a step in the time integration (old-time value). A superscript “\( n + 1 \)” labels a variable value at the end of the current time step (new-time value), which must be obtained as part of the solution of the equations. Subscripts provide information on spatial location as illustrated in Figure 1-5. Integer subscripts such as “\( j \)” or “\( j + 1 \)” label volume center information (e.g., \( P_j^{n+1} \) is the new-time pressure in volume “\( j \)”). A half-integer subscript indicates a value obtained at the surface separating two volumes (e.g., \( V_{j+1/2}^n \) is the old-time velocity at the surface separating volume “\( j \)” from volume “\( j + 1 \)”).

When values of cell-centered variables are needed at cell edges, an average of some form is required. The methods discussed here use values only from the volumes immediately adjacent to the given edge, so the averages are always in the following form:

\[
\langle Y \rangle_{j+1/2} = w_{j+1/2} Y_j + (1 - w_{j+1/2}) Y_{j+1}. \quad (1-82)
\]
For simple 1D flow, terms expressing mass and energy flow for the \( j^{th} \) finite volume then have the following form:

\[
\frac{\partial}{\partial x} (YV) = \frac{\langle Y \rangle_{j+1/2} V_{j+1/2} - \langle Y \rangle_{j-1/2} V_{j-1/2}}{\Delta x} = \frac{\left[ w_{j+1/2} Y_{j} + \left( 1 - w_{j+1/2} \right) Y_{j+1} \right] V_{j+1/2} - \left[ w_{j-1/2} Y_{j-1} + \left( 1 - w_{j-1/2} \right) Y_{j} \right] V_{j-1/2}}{\Delta x} \quad (1-83)
\]

The form is more complex for 1D flow with a spatially varying cross-sectional flow area. In this case the mass flux term is abbreviated as

\[
\nabla j \cdot (YV) = \frac{\left[ w_{j+1/2} Y_{j} + \left( 1 - w_{j+1/2} \right) Y_{j+1} \right] A_{j+1/2} V_{j+1/2} - \left[ w_{j-1/2} Y_{j-1} + \left( 1 - w_{j-1/2} \right) Y_{j} \right] A_{j-1/2} V_{j-1/2}}{v_{olj}} \quad , \quad (1-84)
\]

where \( A_{j+1/2} \) is the flow area between cells \( j \) and \( j+1 \) and \( v_{olj} \) is the volume of the \( j^{th} \) cell.

The related derivative used in the finite-difference momentum flux involves the use of a more complicated averaging method. This is driven by a need to model Bernoulli flows when appropriate and to conserve momentum properly when a side-junction flow is present. Details of this methodology are presented in \textbf{Conserving Convected Momentum}. To aid in understanding the basic numerical methods, it is worth noting that with no area changes or side junctions, the numerical form of the velocity gradient is

\[
\frac{\partial V}{\partial x} \bigg|_{j+1/2} = \frac{(1 - w_{j+1/2}) V_{j+3/2} + (2w_{j+1/2} - 1) V_{j+1/2} - w_{j+1/2} V_{j-1/2}}{\Delta x} \quad . \quad (1-85)
\]

For flows in 1D channels with variable cross-sectional area, the momentum-transfer term is abbreviated as \( V_{j+1/2} \nabla j+1/2 \).

Although the basics of the finite volume spatial discretization have already been covered, further details are provided in later sections of this document. \textbf{3D Finite-Difference Methods} presents a generalization of the methods to 3D geometry. Special treatment of transition to single-phase flow and conditions beyond the critical point is described in \textbf{Modifications to the Basic Equation Set}. The section \textbf{Conserving Convected Momentum} describes details of special treatment used for momentum-flux terms. The actual solution of these equations is described in \textbf{Chapter 2}. 
**Basics of the Semi-Implicit Method**

When fluid flow is modeled with a fully explicit method, time-step sizes are restricted by the Courant limit as

\[
\Delta t \leq k \cdot \frac{\Delta x}{|V| + c},
\]

where \(\Delta x\) is a characteristic mesh length, \(V\) is the flow velocity, \(c\) is the speed of sound, and parameter \(k\) varies in value depending on the details of the method, but here can be taken to be 1.0. This simple class of methods is appropriate when it is important to track the details of pressure wave propagation (e.g., shock waves). However, in most reactor transients, this level of detail is not important. At most, continuity waves (moving liquid levels or froth fronts) must be followed. Frequently the transient is simply an evolution between quasi-steady states.

Both the ICE and semi-implicit methods relax the explicit restrictions on time-step size by evaluating terms involved in pressure wave propagation at the new \((n+1)\) time level. For a simple form of the momentum equation, this requires new-time values in the pressure gradient term as given by

\[
\frac{\left( V_{j+1/2}^{n+1} - V_{j+1/2}^n \right)}{\Delta t} + \left. V_{j+1/2}^n \frac{\partial V^n}{\partial x} \right|_{j+1/2} + \frac{1}{\langle \rho \rangle_{j+1/2}^n} \frac{(P_{j+1}^{n+1} - P_j^{n+1})}{\Delta x} + K^n_{j+1/2} V_{j+1/2}^{n+1} \left| V_{j+1/2}^n \right| = 0
\]

Similarly, relaxation of the restrictions on time-step size also requires that velocities involved in flux of mass and energy be evaluated at the new-time level. The equations then become

\[
\frac{(\rho_{j+1}^{n+1} - \rho_j^n)}{\Delta t} + \frac{\partial}{\partial x_j}(\rho^n V^{n+1}) = 0
\]

and

\[
\frac{(\rho_{j+1}^{n+1} e_{j+1}^{n+1} - \rho_j^n e_j^n)}{\Delta t} + \frac{\partial}{\partial x_j}(\rho^n e^n V^{n+1}) + P_{j+1}^{n+1} \left( \frac{V_{j+1/2}^{n+1} - V_{j-1/2}^{n+1}}{\Delta x} \right) = \text{heat sources (W/m}^3)\]

=heat sources (W/m^3)
By using the above equation structure, information on a pressure disturbance in any cell is available to any other cell during the same time step. This eliminates the sound speed from the Courant stability limit, leaving what is commonly referred to as the “material Courant” stability limit \((\Delta t < (\Delta x)/|V|)\). The absolute value of flow velocity remains in the denominator of the expression because information relevant to continuity waves is still propagated only one cell per time step by the semi-implicit method. It is worth noting here that the numerical diffusion associated with a semi-implicit method is at a minimum when the time step is equal to the material Courant stability limit (see Reference 1-7). Numerical diffusion increases as the time step decreases approaching that of a fully implicit or SETS method in the limit of very small time steps.

Completion of the problem definition requires a choice of two independent variables from the four thermodynamic variables: pressure, temperature, density, and specific internal energy. Density is not a good choice because of the need to model liquid solid regions. Given the low compressibility of liquid, a small error in a solution for density can translate to a significant error in pressure. When pressure is designated as an independent variable, a small error in the solution for pressure results in an even smaller fractional error in density. The choice of the second independent variable is driven by considerations beyond the simple equations presented above. Multi-phase and multi-component systems tend toward an equilibrium in which the phases and/or components are all at the same temperature. This behavior is reflected in constitutive relations for interphase (or wall-to-fluid) heat transfer that depend on differences of temperatures and that must be evaluated implicitly with respect to these temperature differences in the numerical equations. When the gas phase contains a mixture of species, all species are assumed to be at the same temperature. Selecting temperature as an independent variable in these situations can significantly simplify final solution of the equations.

Equations of state provide density and internal energy as functions of pressure and temperature. The relationships are generally nonlinear; therefore, the combination of discretized flow equations and state equations yields a coupled set of nonlinear equations. A key feature of TRACE is the use of an iterative method (see Chapter 2) to obtain a solution to the nonlinear equations. The nonlinear equations are not simply replaced by a linearized approximation, as is done in RELAP5 (Ref. 1-16).

A stability analysis of these semi-implicit equations introduces limitations on weighting factors used for cell-edge averages. The equations are unconditionally unstable unless

\[
\begin{align*}
&w_{j+1/2} \geq \left(1/2\right) \left(1 + \frac{\Delta t |V_{j+1/2}|}{\Delta x_{j+1/2}}\right) \quad \text{for} \quad V_{j+1/2} \geq 0 \quad \text{and} \\
&w_{j+1/2} \leq \left(1/2\right) \left(1 - \frac{\Delta t |V_{j+1/2}|}{\Delta x_{j+1/2}}\right) \quad \text{for} \quad V_{j+1/2} < 0.
\end{align*}
\]
When the inequalities are replaced with equalities in the above expression, a difference scheme with the minimal permitted numerical diffusion results. However, experience with a range of two-phase-flow problems has resulted in the final adoption of the following more robust choice of weighting factors:

$$
w_{j+1/2} = \begin{cases} 
1 & \text{for } V_{j+1/2} \geq 0 \\
0 & \text{for } V_{j+1/2} < 0 
\end{cases}.
$$

(1-91)

This is the standard donor-cell or first order upwind difference method.

**Enhancements to the Semi-Implicit Method**

The finite-volume equations given above reflect the semi-implicit method as implemented in early versions of TRAC-PF1 (Ref. 1-16). However, the discovery of instabilities in bubbly flow (Ref. 1-13) resulted in improvements to the wall friction term in Eq. (1-87) and, more importantly, to the interfacial friction term in the two-phase momentum equations. Optimal stability would be obtained by evaluating the friction terms fully implicitly. Unfortunately, this would result in serious complications for the solution procedure outlined in Chapter 2. The existing solution procedure relies on the finite-difference motion equations containing no more than the first power of the new-time velocity. This permits a direct solution for \( V^{n+1} \) as a linear function of adjacent new-time pressures.

More stable force terms can be obtained from linearization of a fully implicit force term. First, assume that the new-time velocity is not very different from the old-time velocity, or

$$
V^{n+1}_{j+1/2} = V^n_{j+1/2} + \delta V_{j+1/2}.
$$

(1-92)

Now, substitute this expression into the fully implicit wall friction term as follows:

$$
K^n_{j+1/2} V^{n+1}_{j+1/2} \left| V^n_{j+1/2} + \delta V_{j+1/2} \right| = K^n_{j+1/2} \left| V^n_{j+1/2} + \delta V_{j+1/2} \right| V^n_{j+1/2} + \delta V_{j+1/2}.
$$

(1-93)

$$
= 2 K^n_{j+1/2} \left| V^n_{j+1/2} \right| \delta V_{j+1/2} + K^n_{j+1/2} V^n_{j+1/2} \left| V^n_{j+1/2} \right| + O(\delta V^2)
$$

Finally, drop terms containing \( \delta V^2 \) and replace \( \delta V \) with the difference between the new- and old-time velocity to give
\[
K^n_{j+1/2} V^{n+1}_{j+1/2} \left| V^{n+1}_{j+1/2} \right| \approx 2 K^n_{j+1/2} V^n_{j+1/2} \left| V^n_{j+1/2} \right| \left[ K^n_{j+1/2} V^n_{j+1/2} - K^n_{j+1/2} V^n_{j+1/2} \right]. \quad (1-94)
\]

In the two-phase-flow equations, the same linearized implicit approximation is applied to the interfacial drag term.

The history of use of the semi-implicit equations within TRACE has resulted in a related approximation in the momentum flux terms for the semi-implicit method. When using the semi-implicit equations as part of the SETS method, it was found that a linearization of the implicit momentum-flux term can improve the stability of the motion equation. Details of this linearization are presented in the next subsection. Within the context of a pure semi-implicit equation the consistent development has been that the momentum flux term originally written in Eq. (1-87) is changed to:

\[
V^{n+1}_{j+1/2} \frac{\partial V^n_{j+1/2}}{\partial x}_{j+1/2} \quad (1-95)
\]

when the velocity derivative is positive. When the velocity derivative is negative, the form in Eq. (1-87) must be maintained to avoid an instability. The momentum flux term can be written in a single expression as:

\[
V_{j+1/2} \frac{\partial V^n_{j+1/2}}{\partial x}_{j+1/2} = \left[ \beta V^{n+1}_{j+1/2} + (1 - \beta) V^n_{j+1/2} \right] \frac{\partial V^n_{j+1/2}}{\partial x}_{j+1/2}, \quad (1-96)
\]

where

\[
\beta = \begin{bmatrix}
1 & \text{for } \frac{\partial V^n_{j+1/2}}{\partial x} \geq 0 \\
0 & \text{for } \frac{\partial V^n_{j+1/2}}{\partial x} < 0
\end{bmatrix}. \quad (1-97)
\]

With the special modifications to momentum flux and friction terms, the finite-difference form of the motion equation becomes
Semi-Implicit Method Adapted to Two-Phase Flow

Extension of the numerical method to the two-phase, two-fluid model is relatively straightforward. Special modifications to the method are necessary to treat changes from two-phase to single-phase flow and are described below. Source terms are present to model phase change and heat transfer. These are generally implicit in any driving temperature difference and explicit in any coefficient. The importance of gravitationally driven liquid flow requires an accurate model of gravitational force along the direction of motion. This uses an input angle (\( \theta \)) between a vector from the center of cell \( j \) to the center of cell \( j+1 \) and a vector directed against gravity. In the application of the code, \( \theta \) is more generally the inverse cosine (\( \cos^{-1} \)) of the change in elevation between cell centers divided by the flow length between cell centers.

To shorten notation in the following difference equations, some subscripts associated with location have been eliminated. For velocities not contained in spatial differences, the subscript denoting spatial location is assumed to be \( j+1/2 \). For cell-centered variables, the assumed subscript is \( j \). The phrase “combined gas” refers to the mixture of noncondensable gas and steam, which is assumed to move with no interspecies diffusion.

Semi-Implicit Equations of Motion

Combined Gas

\[
\frac{(V_g^{n+1} - V_g^n)}{\Delta t} + [\beta V_g^{n+1} + (1 - \beta) V_g^n] \nabla_{j+1/2} V_g^n \\
+ \frac{C_i^n | V_g^n - V_l^n |}{(\alpha \rho_g^n)_{j+1/2}} [2(V_g^{n+1} - V_l^{n+1}) - (V_g^n - V_l^n)] = 0
\]
\[ + \frac{1}{\rho^*_g} (P^*_j + 1 - P^*_j) \frac{\Delta x}{j + 1/2} + \frac{\Gamma^*_j}{\rho^*_g} (V^*_i + 1 - V^*_l) \]

\[ + \frac{\Gamma^*_j}{\rho^*_g} (V^*_g - V^*_l) \mid V^*_g \mid + g \cos \theta = 0. \quad (1-99) \]

Liquid

\[ \frac{V^*_l + 1 - V^*_l}{\Delta t} + \frac{\beta^*_l V^*_l + 1 + (1 - \beta^*_l) V^*_l}{\Delta x} \nabla \frac{V^*_l}{j + 1/2} \]

\[ + \frac{C_i}{\rho^*_l} \frac{\beta^*_l V^*_l - c^*_l}{\rho^*_l} \cdot \left[ 2(V^*_l + 1 - V^*_g) - (V^*_l - V^*_g) \right] \]

\[ + \frac{1}{\rho^*_l} (P^*_j + 1 - P^*_j) \frac{\Delta x}{j + 1/2} - \frac{\Gamma^*_j}{\rho^*_g} (V^*_l + 1 - V^*_g) \]

\[ + \frac{C_{w/l}}{(1 - \rho^*_g)} (2V^*_l + 1 - V^*_l) \mid V^*_l \mid + g \cos \theta = 0. \quad (1-100) \]

**Semi-Implicit Mass Equations**

Combined Gas

\[ \frac{\alpha^*_j + 1 - \alpha^*_j}{\Delta t} + \nabla \cdot \left[ \alpha^*_j \rho^*_g V^*_g \right] = \Gamma^*_l + 1. \quad (1-101) \]

Noncondensable Gas

\[ \frac{\alpha^*_j + 1 - \alpha^*_j}{\Delta t} + \nabla \cdot \left[ \alpha^*_j \rho^*_a V^*_g \right] = 0. \quad (1-102) \]

Additional Noncondensable Mass Equations (kth species)

\[ \frac{\alpha^*_j + 1 - \alpha^*_j}{\Delta t} + \nabla \cdot \left[ \alpha^*_j V^*_g \right] = 0 \]

(1-103)
Liquid

\[
\frac{[(1-\alpha_j^{n+1})\rho_{lj}^{n+1} - (1 - \alpha_j^n)\rho_{lj}^n]}{\Delta t} + \nabla_j \cdot [(1-\alpha^n)\rho_l^n V_l^{n+1}] = -\Gamma^{n+1} .
\]  

(1-104)

**Semi-Implicit Energy Equations**

Combined Gas

\[
\frac{[\alpha_j^{n+1} \rho_{gj}^{n+1} e_{gj}^{n+1} - \alpha_j^n \rho_{gj}^n e_{gj}^n]}{\Delta t} + \nabla_j \cdot [\alpha^n \rho_g^n e_g^n V_g^{n+1}]
\]

\[= q_{wg}^{n+1} + q_{dg}^n + q_{ig}^{n+1} + \Gamma^{n+1} h_{sg}^{n+1} .
\]  

(1-105)

Total Fluid (gas and liquid)

\[
\frac{[\alpha_j^{n+1} \rho_{gj}^{n+1} e_{gj}^{n+1} + (1-\alpha_j^{n+1})\rho_{lj}^{n+1} e_{lj}^{n+1}]}{\Delta t} - \alpha_j^n \rho_{gj}^n e_{gj}^n + (1-\alpha_j^n)(\rho_{lj}^n e_{lj}^n)
\]

\[+ \nabla_j \cdot [\alpha^n \rho_g^n e_g^n V_g^{n+1} + (1-\alpha^n)\rho_l^n e_l^n V_l^{n+1}]
\]

\[+ P^{n+1} \nabla_j \cdot [(1-\alpha^n)V_l^{n+1} + \alpha^n V_g^{n+1}]
\]

\[= q_{wg}^{n+1} + q_{wl}^{n+1} + q_{dl}^n + q_{dg}^n .
\]  

(1-106)

The wall heat transfer to the gas and liquid, \( q_{wg} \) and \( q_{wl} \), and the interfacial mass-transfer rate, \( \Gamma \), also require further definition. Note the mixture of old- and new-time values in these terms. The choice of old-time heat-transfer coefficients was driven by the desire to simplify the implementation of the method, but can result in bounded instabilities during calculations. These terms are given by

\[q_{wl}^{n+1} = h_w a_w (T_w^{n+1} - T_l^{n+1}) ,
\]  

(1-107)

and

\[q_{wg}^{n+1} = h_w a_w (T_w^{n+1} - T_g^{n+1}) ,
\]  

(1-108)
\( \Gamma^{n+1} = \frac{-q_{ig}^{n+1} + q_{il}^{n+1}}{(h_i')^{n+1} - (h_i')^{n+1}} \)  

(1-109)

where

\( q_{ig}^{n+1} = h_{ig}^{n} a_i^{n} (T_{sat}^{n+1} - T_{g}^{n+1}) \)  

(1-110)

and

\( q_{il}^{n+1} = h_{il}^{n} a_i^{n} (T_{sat}^{n+1} - T_{l}^{n+1}) \)  

(1-111)

The interfacial heat transfer coefficients \( (h_{il}, h_{ig}) \), wall heat transfer coefficients \( (h_{wl}, h_{wg}) \), interfacial drag coefficient \( (C_i) \) and wall friction coefficients \( (C_{wg}, C_{wl}) \) all are the result of nonlinear functions associated obtained from correlations. Old time (explicit) evaluation of these coefficients can result in bounded instabilities.

Further definition is also needed for a special set of density averages used in the momentum equations. Cell-edge densities used in the denominator of Eq. (1-99) and Eq. (1-100) are defined to produce a good prediction of hydrostatic pressure heads. For example, the edge-average gas macroscopic density is defined as

\[
\langle \alpha \rho \rangle_{j+1/2}^{n} = \frac{\Delta x_{j} \langle \alpha \rho \rangle_{j}^{n} + \Delta x_{j+1} \langle \alpha \rho \rangle_{j+1}^{n}}{\Delta x_{j} + \Delta x_{j+1}}.
\]

(1-112)

A similar definition holds for the cell-edge liquid macroscopic density. The edge-average microscopic densities are somewhat more complex. For example,

\[
\langle \rho_{g} \rangle_{j+1/2}^{n} = \langle \alpha \rho_{g} \rangle_{j+1/2}^{n} \left[ \frac{\Delta x_{j} \alpha_{j}^{n} + \Delta x_{j+1} \alpha_{j+1}^{n}}{\Delta x_{j} + \Delta x_{j+1}} \right]^{-1}.
\]

(1-113)

This particular average is necessary for consistency within the SETS equations (see The SETS Method Adapted to Two-Phase Flow), where macroscopic densities have a more fundamental importance within the solution.

The above finite-volume-flow equations hold only when a two-phase mixture is present at both the old- and new-time levels. Modifications are necessary when the old- or new-time-level fluid state is single phase; these are described in Modifications to the Basic Equation Set
Liquid Solute

Treatment of the liquid solute field (defaults to boric acid) requires a bit more discussion than the basic equations above. The primary variable used for following the solute is its mass fraction \( m \). Because the rate of transition between the dissolved and plated components of the solute field is taken to be instantaneous when the solubility limit is reached, the time evolution of solute mass fraction (concentration) is modeled in a two step process. First the change in solute mass fraction over a time step is predicted based upon a standard mass conservation equation accounting for fluid flow alone.

\[
\frac{1}{\Delta t} \left[ (1-\alpha)^{n+1} m^{n+1} \rho_l^{n+1} - (1-\alpha)^n \rho_l^n \right] + \nabla_j \cdot \left[ ((1-\alpha)^n m^n \rho_l^n V_l^{n+1} \right] = 0, \quad (1-114)
\]

Next a correlation is checked for the maximum mass fraction \( m_{max} \) of solute that can be dissolved in the liquid at the current temperature. This is either a correlation for boric acid or a replacement provided by a TRACE user as optional input. The highest possible dissolved mass fraction at the end of a time step is the sum of the result from Eq. (1-114) and available mass of plated solute per mass of liquid in the volume. The final end of time step mass fraction must be the smaller of this limit and \( m_{max} \).

\[
m^{n+1} = \min \left[ \frac{S_c^n}{(1-\alpha)^{n+1} \rho_l^{n+1}} \cdot m_{max}, m_{max} \right], \quad (1-115)
\]

In the above equation \( S_c \) is the plated solute mass divided by the volume of the computational cell in which it is plated. Whatever plated solute was not taken into solution by Eq. (1-115) remains in the inventory of plated solute at the end of the step. This can be expressed mathematically as:

\[
S_c^{n+1} = (\tilde{m}^{n+1} - m_{\max}^n)(1-\alpha)^n \rho_l^{n+1} + S_c^n. \quad (1-116)
\]

Basics of the SETS Method

The goal of the SETS method was to eliminate the material Courant stability limit with minimal alterations to the existing semi-implicit method. Given the success of the semi-implicit method in propagating information about sound waves, a correction step was devised to perform a similar propagation of information on continuity waves. As a very simple example, consider the single-phase mass equation. For each time step, the semi-implicit method is used to establish the new-time velocity field. Next, the following correction (or “stabilizer”) step is used to obtain a final value of the new-time density:
On the surface, this appears to be a fully implicit finite-difference equation. It is not, however, because the new-time velocities \( V^{n+1} \) are all known numbers, obtained from the semi-implicit step. New-time densities are the only unknowns in this system of equations. Information about a density change in any given computational cell is propagated to all other cells within the same time step. Formal stability analysis and direct testing confirm expectations based on information propagation. The material Courant stability limit actually is eliminated. This does not imply unconditional stability for the method. The only modifications to the semi-implicit method involve flux terms. The continued practice of evaluating heat-transfer and friction coefficients at the old time results in other poorly defined problems with bounded instabilities.

One unusual aspect of SETS as implemented in the code is that the pattern of evaluation of semi-implicit and stabilizer equations is not the same for the motion equations as it is for the mass and energy equations. All mass and energy equations follow the above pattern of a semi-implicit step followed by a stabilizer step. However, the analogous momentum-stabilizer equation is evaluated before the evaluation of the semi-implicit equations. This pattern was established during the original development of SETS through tests of the various combinations of equation ordering. In these tests, two-phase-flow problems ran smoothly at significantly higher time steps with the current equation ordering than with others. The physical explanation for this behavior is the importance of the pressure gradient term in problems of interest. A solution is better behaved when the velocity used for transport of mass and energy is a direct result of a pressure-balanced solution.

For our special example of 1D single-phase flow, the SETS difference equations are

\[
\frac{(\rho_j^{n+1} - \rho_j^n)}{\Delta t} + \partial_{x_j}(\rho_j^{n+1} V_j^{n+1}) = 0. \tag{1-117}
\]

\[
\rho_j^{n+1} + \partial_{x_j}(\rho_j^{n+1} V_j^{n+1}) = V_j^{n+1} + \frac{\rho_{j+1/2}^{n+1} - \rho_j^{n+1}}{\Delta x} + \frac{P_{j+1}^n - P_j^n}{\Delta x} + K_{j+1/2}^{n} \left( V_{j+1}^{n+1} - V_j^{n+1} \right) V_j^{n+1} = 0. \tag{1-118}
\]
**Semi-Implicit Equation Step**

\[
\left( \frac{V_{j+1/2}^{n+1} - V_{j+1/2}^n}{\Delta t} \right) + \left. \frac{\partial \tilde{V}}{\partial x} \right|_{j+1/2}^{n+1} + \frac{1}{\langle \rho \rangle_{j+1/2}^n} \left( \tilde{P}_{j+1}^n - \tilde{P}_{j}^n \right) \Delta x + K_{j+1/2}^n \left( 2 \left| \frac{V_{j+1/2}^{n+1} - V_{j+1/2}^n}{\Delta t} \right| \right) V_{j+1/2}^n = 0 , \tag{1-119}
\]

\[
\frac{\tilde{\rho}_j^{n+1} - \tilde{\rho}_j^n}{\Delta t} + \frac{\partial}{\partial x_j} \tilde{\rho}_j^n V_{j+1}^{n+1} = 0 , \text{ and} \tag{1-120}
\]

\[
\frac{\tilde{\rho}_j e_j^{n+1} - (\rho e)_j^n}{\Delta t} + \frac{\partial}{\partial x_j} \tilde{\rho}_j^n e_j^n V_{j+1}^{n+1} + \tilde{P}_{j+1}^n - V_{j+1/2}^{n+1} \frac{V_{j+1/2}^{n+1} - V_{j+1/2}^n}{\Delta x} = 0 . \tag{1-121}
\]

**Stabilizer Mass and Energy Equations**

\[
\frac{\tilde{\rho}_j^{n+1} - \tilde{\rho}_j^n}{\Delta t} + \frac{\partial}{\partial x_j} (\tilde{\rho}_j^{n+1} V_{j+1}^{n+1}) = 0 , \text{ and} \tag{1-122}
\]

\[
\frac{(\rho e)_j^{n+1} - (\rho e)_j^n}{\Delta t} + \frac{\partial}{\partial x_j} \left[ (\rho e)_j^{n+1} V_{j+1}^{n+1} \right] + \tilde{P}_{j+1}^n - V_{j+1/2}^{n+1} \frac{V_{j+1/2}^{n+1} - V_{j+1/2}^n}{\Delta x} = 0 . \tag{1-123}
\]

A tilde above a variable indicates that it is a first estimate of the new-time value. Actual new-time variables have a superscript “n + 1” and no tilde. Note that the only result of the above semi-implicit step appears to be just a new-time velocity field. In practice the situation is more complex. To save computational time, temperatures and pressures that are fully consistent with the densities and energies obtained from solving the stabilizer mass and energy equations are never calculated. If the correlation used to obtain an old-time wall friction coefficient requires temperature or pressure, the values used would be those obtained during the solution of the semi-implicit equation step.

As will be clear in the discussion of the solution of the SETS equations, each of the above equations is solved once per time step. During development of the method, attempts were made to make repeated evaluations of a form of the SETS equations during each time step to produce an iterative solution to the fully implicit method. This approach was found to converge poorly or not at all, particularly at time steps in excess of the material Courant limit.
Enhancements to the SETS Method

As with the semi-implicit method, linearized implicit terms are introduced in the motion equation to improve the behavior of friction and momentum transfer. The improved friction terms are identical to those derived in Enhancements to the Semi-Implicit Method. The momentum-transfer terms are somewhat more complex. First, the new-time velocity and velocity gradient are linearized in the following forms:

\[
\tilde{V}_{j+1/2}^{n+1} = V_{j+1/2}^n + \delta V_{j+1/2}^n \quad \text{and} \quad (1-124)
\]

\[
\nabla \tilde{V}_{j+1/2}^{n+1} = \nabla \tilde{V}_{j+1/2}^n + \delta(\nabla V_{j+1/2}^n). \quad (1-125)
\]

Substitution of these relationships into the implicit form of the momentum-transfer term gives

\[
V_{j+1/2}^{n+1} \nabla \tilde{V}_{j+1/2}^{n+1} = \left( V_{j+1/2}^n + \delta V_{j+1/2}^n \right) \left( \nabla \tilde{V}_{j+1/2}^n + \delta(\nabla V_{j+1/2}^n) \right) \quad (1-126)
\]

\[
= V_{j+1/2}^n \nabla \tilde{V}_{j+1/2}^n + \delta V_{j+1/2}^n \nabla \tilde{V}_{j+1/2}^n + V_{j+1/2}^n \delta(\nabla V_{j+1/2}^n) + \delta V_{j+1/2}^n \delta(\nabla V_{j+1/2}^n)
\]

Keeping only terms with no more than the first power of a variation and back-substituting the variations in terms of differences between old- and new-time variables gives

\[
\tilde{V}_{j+1/2}^{n+1} \nabla \tilde{V}_{j+1/2}^{n+1} \approx V_{j+1/2}^n \nabla \tilde{V}_{j+1/2}^{n+1} + \left( \tilde{V}_{j+1/2}^{n+1} - V_{j+1/2}^n \right) \nabla \tilde{V}_{j+1/2}^n. \quad (1-127)
\]

The difference in base points for the linearizations of Eqs. (1-124) and (1-125) is not an error in the equations. It is the result of numerical experimentation with the three possible alternatives. The situation is further complicated by instabilities resulting from negative values of the gradient or sign discrepancies between final and intermediate (tilde) velocities. Numerical experimentation resulted in the following robust form of the linearized implicit momentum-transfer term:

\[
\tilde{V}_{j+1/2}^{n+1} \nabla \tilde{V}_{j+1/2}^{n+1} \approx V_{j+1/2}^n \nabla \tilde{V}_{j+1/2}^{n+1} + \beta \left( \tilde{V}_{j+1/2}^{n+1} - V_{j+1/2}^n \right) \nabla \tilde{V}_{j+1/2}^n \quad (1-128)
\]

where
With these modifications, the final form of the stabilizer motion equation is

\[
\left( \frac{\tilde{V}_{j+1/2}^{n+1} - V_{j+1/2}^n}{\Delta t} \right) + V_{j+1/2}^n \nabla \tilde{V}_{j+1/2}^{n+1} + \beta \left( \tilde{V}_{j+1/2}^{n+1} - V_{j+1/2}^n \right) \nabla \tilde{V}_{j+1/2}^{n+1} \\
+ \frac{1}{\langle \rho \rangle_{j+1/2}^n} \left( P_{j+1/2}^{n+1} - P_{j+1/2}^n \right) + K_{j+1/2}^n \left( 2 \tilde{V}_{j+1/2}^{n+1} - V_{j+1/2}^n \right) \left| V_{j+1/2}^n \right| = 0.
\]

(1-130)

The following revised form of the motion equation in the semi-implicit step contains the revised flux term to increase the robustness of the method:

\[
\left( \frac{V_{j+1/2}^{n+1} - V_{j+1/2}^n}{\Delta t} \right) + V_{j+1/2}^n \nabla \tilde{V}_{j+1/2}^{n+1} + \beta \left( V_{j+1/2}^{n+1} - V_{j+1/2}^n \right) \nabla \tilde{V}_{j+1/2}^{n+1} \\
+ \frac{1}{\langle \rho \rangle_{j+1/2}^n} \left( P_{j+1/2}^{n+1} - P_{j+1/2}^n \right) + K_{j+1/2}^n \left( 2 \tilde{V}_{j+1/2}^{n+1} - V_{j+1/2}^n \right) \left| V_{j+1/2}^n \right| = 0.
\]

(1-131)

One significant modification is introduced in the stabilizer mass and energy equations. To save computational effort and overhead associated with the communication of more variables, the stabilizer equations listed in the previous section are not directly solved. Instead, the actual equations solved are the result of subtracting the semi-implicit equations from the corresponding stabilizer equations.

**Stabilizer Mass and Energy Equations as Solved**

\[
\left( \frac{\rho_j^{n+1} - \rho_j^n}{\Delta t} \right) + \frac{\partial}{\partial x_j} \left( \rho_j^{n+1} V_j^{n+1} \right) = \frac{\partial}{\partial x_j} \left( \rho^n V^n \right),
\]

(1-132)
Note that these appear to be conservation equations, but on close examination what appears to be a time derivative is in fact a difference between two time derivatives. The advantage of this approach is more apparent in the application of the method to the full two-phase-flow equations. In that case, all source terms (mass and energy transfer) are canceled out of the equations to be solved. The disadvantage of this approach is that the rigorous mass conservation of Eq. (1-122) is lost. Mass conservation associated with Eq. (1-132) depends on the level of convergence of the iterative solution for the semi-implicit equations.

The SETS Method Adapted to Two-Phase Flow

The two-phase forms of the SETS equations contain some significant modifications. The first, which improves code robustness, is an initial evaluation of the equations of motion that is used solely to provide an improved prediction of the interfacial force terms needed in the standard stabilizer motion equations.

Equations for Prediction of Interfacial Drag Force

Combined Gas

\[
\frac{(\rho e)^{n+1}_j - \rho_j^{n+1}}{\Delta t} + \frac{\partial}{\partial x_j} ((\rho e)^{n+1}_j V^{n+1}_j) = \frac{\partial}{\partial x_j} ((\rho e)^{n}_j V^{n}_j). \tag{1-133}
\]

\[
\frac{V^{n+1}_g - V^n_g}{\Delta t} + V^n_g \nabla_{j+1/2} V^n_g + \beta (V^{n+1}_g - V^n_g) \nabla_{j+1/2} V^n_g + C_i \frac{\rho^n_g - \rho^n_i}{\langle \alpha \rho \rangle^n_{j+1/2}} \left[ 2(V^{n+1}_g - \hat{V}^{n+1}_g) - (V^n_g - \hat{V}^n_i) \right] \\
+ \frac{1}{\langle \rho^n_g \rangle_{j+1/2}} \frac{(P^{n+1}_{j+1} - P^n_{j+1})}{\Delta x_{j+1/2}} + \frac{\Gamma^n_{j+1/2}}{\langle \alpha \rho^n_g \rangle_{j+1/2}} (V^{n+1}_g - \hat{V}^{n+1}_i) \\
+ \frac{C_{wq}}{\langle \alpha \rho^n_g \rangle_{j+1/2}} (2 \hat{V}^{n+1}_g - V^n_g) V^n_g + g \cos \theta = 0, \tag{1-134}
\]

where
\[ \beta = \begin{bmatrix} 0 & \text{if } \nabla_{j+1/2} V^n < 0 \text{ and } V^n \tilde{V}^n < 0 \\\n & \text{if } \nabla_{j+1/2} V^n \geq 0 \text{ and } V^n \tilde{V}^n \geq 0 \end{bmatrix} \]  

(1-135)

Liquid

\[
\frac{(\hat{V}^{n+1}_l - V^n_l)}{\Delta t} + V^n_l \nabla \hat{V}^n_l + \beta (\hat{V}^{n+1}_l - V^n_l) \nabla \hat{V}^n_l + \frac{C_w}{\rho} [2(\hat{V}^{n+1}_l - \hat{V}^{n+1}_g) - (V^n_l - V^n_g)]
\]

\[
+ \frac{1}{\rho_j^{n+1/2}} \left( \frac{\Gamma^n_j}{\Delta x} \right) + \frac{\rho^n_j}{\rho_j^{n+1/2}} (\hat{V}^{n+1}_l - \hat{V}^{n+1}_g)
\]

\[
+ \frac{C_{wl}}{\rho_j^{n+1/2}} (2 \hat{V}^{n+1}_l - V^n_l) V^n_l + g \cos \theta = 0. \quad \text{(1-136)}
\]

Edge-average densities follow the definitions provided in the discussion of the semi-implicit method [Eqs. (1-112) and (1-113)].

The velocities obtained from the above equations are used to decouple the vapor and liquid stabilizer motion equations. The prediction of the interfacial force term is good enough that the interfacial force term in the following stabilizer equations does not need to depend on the new-time stabilizer velocities. As a result, the liquid stabilizer motion equation contains only liquid stabilizer (tilde) velocities as unknowns. The liquid and gas equations are two completely independent systems of equations, which are solved separately.

**Stabilizer Equations of Motion**

Combined Gas

\[
\frac{(\hat{V}^{n+1}_g - V^n_g)}{\Delta t} + V^n_g \nabla \hat{V}^{n+1}_g + \beta (\hat{V}^{n+1}_g - V^n_g) \nabla \hat{V}^n_g
\]
Field Equations

\[ C_i^n \left[ \frac{V^n - V^n_l}{\langle \alpha \rho_g \rangle_{j+1/2}^n} \right] [2(\hat{V}^{n+1} - \hat{V}_l^{n+1}) - (V^n - V_l^n)] \]

\[ + \frac{1}{\langle \rho_g \rangle_{j+1/2}^n} \frac{(P^n_j - P^n_j)}{\Delta x_{j+1/2}} + \frac{\Gamma_{j+1/2}^n}{\langle \alpha \rho_g \rangle_{j+1/2}^n}(\hat{V}^{n+1} - \hat{V}_l^{n+1}) \]

\[ + \frac{C_{wg}^n}{\langle \alpha \rho_g \rangle_{j+1/2}^n} (2 \hat{V}_g^{n+1} - V_g^n) \left| V_g^n \right| + g \cos \theta = 0. \] (1-137)

Liquid

\[ \frac{\hat{V}_l^{n+1} - V_l^n}{\Delta t} + V_l^n \nabla \hat{V}_l^{n+1} + \beta (\hat{V}_l^{n+1} - V_l^n) \nabla \hat{V}_l^{n+1} \]

\[ + \frac{C_{wg}^n}{\langle (1-\alpha) \rho \rangle_{j+1/2}^n} [2(\hat{V}_l^{n+1} - \hat{V}_g^{n+1}) - (V_l^n - V_g^n)] \]

\[ + \frac{1}{\langle \rho \rangle_{j+1/2}^n} \frac{(P^n_j - P^n_j)}{\Delta x_{j+1/2}} - \frac{\Gamma_{j+1/2}^n}{\langle (1-\alpha) \rho \rangle_{j+1/2}^n}(\hat{V}_l^{n+1} - \hat{V}_g^{n+1}) \]

\[ + \frac{C_{wl}^n}{\langle (1-\alpha) \rho \rangle_{j+1/2}^n} (2 \hat{V}_l^{n+1} - V_l^n) \left| V_l^n \right| + g \cos \theta = 0. \] (1-138)

**Equations of Motion for the SETS Semi-Implicit Step**

The equations solved during the semi-implicit step are almost identical to those presented in **Semi-Implicit Method Adapted to Two-Phase Flow** but are reproduced here in their entirety to avoid ambiguity in details of the implementation. The primary difference between the motion equation in a pure semi-implicit method and its corresponding form in the semi-implicit step of SETS is the use of stabilizer velocities for momentum transport.

Combined Gas

\[ \frac{(V_g^{n+1} - V_g^n)}{\Delta t} + V_g^n \nabla \hat{V}_g^{n+1} + \beta (V_g^{n+1} - V_g^n) \nabla \hat{V}_g^{n+1} \]

50
Field Equations

\[ C^n_i \left[ V^n_g - V^n_l \right] \frac{\rho^n}{\alpha \rho^n_{j+1/2}} [2(V^{n+1}_g - V^{n+1}_l) - (V^n_g - V^n_l)] \]

\[ + \frac{1}{\rho^n_{j+1/2}} \frac{(\tilde{P}^{n+1}_j - \tilde{P}^{n+1}_g)}{\Delta x_{j+1/2}} + \frac{\Gamma_{j+1/2}^{n+1}}{(\alpha \rho^n_{j+1/2})} (V^{n+1}_g - V^{n+1}_l) \]

\[ + \frac{C^n_{wg}}{(\alpha \rho^n_{j+1/2})} (2V^{n+1}_g - V^n_g) |V^n_g| + g\cos \theta = 0. \]  

(1-139)

Liquid

\[ \frac{(V^{n+1}_l - V^n_l)}{\Delta t} + V^n_l \nabla \tilde{V}^{n+1}_l + \beta (V^{n+1}_l - V^n_l) \nabla_{j+1/2} \tilde{V}^n_l \]

\[ + \frac{C^n_i}{((1 - \alpha) \rho^n_{j+1/2})} \left[ 2(V^{n+1}_l - V^n_l) - (V^n_l - V^n_l) \right] \]

\[ + \frac{1}{\rho^n_{j+1/2}} \frac{(\tilde{P}^{n+1}_j - \tilde{P}^{n+1}_g)}{\Delta x_{j+1/2}} - \frac{\Gamma_{j+1/2}^{n}}{(1 - \alpha) \rho^n_{j+1/2}} (V^{n+1}_l - V^n_l) \]

\[ + \frac{C^n_{wl}}{(1 - \alpha) \rho^n_{j+1/2}} (2V^{n+1}_l - V^n_l) |V^n_l| + g\cos \theta = 0. \]  

(1-140)

**Basic Semi-Implicit Mass Equations**

These equations differ from those in a pure semi-implicit method; the resulting void fraction and new-time thermodynamic variables are intermediate results. Final new-time values for these variables are formally set by the stabilizer mass and energy equations. Individual thermodynamic variables also are carefully distinguished from products that comprise macroscopic densities and energies. These macroscopic quantities [e.g., \((\alpha \rho_g)\)] are a direct result of the solution of the stabilizer mass and energy equations at the end of the previous time step. Another key difference is found in the modified form of the divergence operator, which can involve an unusual mixture of new- and old-time values [see Eq. (1-147)].

Combined Gas
Field Equations

\[ \frac{[\alpha_j^\rho_{g j} - (\alpha_j^\rho_{g j})^n]}{\Delta t} + \nabla_j \cdot \left[ (\alpha_j^\rho_{g j})^n V_{g j}^{n+1} \right] = \tilde{\Gamma}_g^{n+1}. \quad (1-141) \]

Noncondensable Mixture

\[ \frac{[\tilde{\alpha}^\rho_{a j} - \tilde{\alpha}^\rho_{a j}]}{\Delta t} + \nabla_j \cdot \left[ (\alpha_j^\rho_{a j})^n \tilde{V}_{g j}^{n+1} \right] = 0 \quad (1-142) \]

Additional Noncondensable Mass Equations (kth species)

\[ \frac{[\tilde{\alpha} X_k \rho_{a j} - \tilde{\alpha} X_k \rho_{a j}]}{\Delta t} + \nabla_j \cdot \left[ ((\alpha X_k \rho_{a j})^n \tilde{V}_{g j}^{n+1} \right] = 0 \quad (1-143) \]

Liquid

\[ \frac{\left(1 - \tilde{\alpha}_j^{n+1}\right) \tilde{\alpha}_j^{n+1} - \left(1 - \alpha \right) \rho_j^n}{\Delta t} + \nabla_j \cdot \left[ (1 - \alpha) \rho_j^n \tilde{V}_l^{n+1} \right] = -\tilde{\Gamma}_l^{n+1}. \quad (1-144) \]

**Basic Energy Equations**

Combined Gas

\[ \frac{[\tilde{\alpha}_j^{\rho_{g j} e_{g j} - (\alpha_j^\rho_{g j} e_{g j})^n]}{\Delta t} + \nabla_j \cdot \left[ (\alpha_j^\rho_{g j} e_{g j})^n V_{g j}^{n+1} \right] \\
+ \tilde{P}_{g j}^{n+1} \left[ \frac{\tilde{\alpha}_j^{n+1} - \alpha^n}{\Delta t} + \nabla_j \cdot (\alpha_j^n V_{g j}^{n+1}) \right] \\
= q_{wg}^n + q_{dg}^n + q_{ig}^n + \tilde{\Gamma}_g^{n+1} \tilde{\rho}_{g j}^{n+1}. \quad (1-145) \]

Total Fluid (gas and liquid)

\[ \frac{[\tilde{\alpha}_j^{\rho_{g j} e_{g j} - (1 - \alpha_j^\rho_{g j} e_{g j})^n} + (1 - \alpha_j^\rho_{g j} e_{g j})^n]}{\Delta t} + \nabla_j \cdot \left[ (\alpha_j^\rho_{g j} e_{g j})^n V_{g j}^{n+1} + (1 - \alpha) \rho_j^n V_l^{n+1} \right] \]
The divergence operator is revised during the semi-implicit step to improve modeling accuracy of situations in which flux can be predominately attributed to phase change in the cell for which the continuity equation is being evaluated. The idea is to use new-time information for that portion of the flux associated with the same cell as the equation (cell $j$). This makes the local solution more sensitive to variation in phase-change rates. In terms of the notation used for the basic definition of the divergence operator, the revised form is

$$
\nabla_j \cdot [q_{\text{wg}}^{n+1} + q_{\text{wl}}^{n+1} + q_{\text{dl}}^{n+1} + q_{\text{dg}}^{n+1}]
= \rho_{V}^{n+1} \cdot \left[ (1 - \alpha) \frac{Y_j^n}{Y_j^{n+1}} V_{l}^{n+1} + \alpha \frac{Y_j^n}{Y_j^{n+1}} V_{g}^{n+1} \right]
\tag{1-146}
$$

The special feature of this operator is that all occurrences of $Y_j^n$ in the normal finite volume divergence operator are replaced by a mixed time average defined as

$$
Y_j' = \gamma Y_j^{n+1} + (1 - \gamma) Y_j^n.
\tag{1-148}
$$

The weighting factor $\gamma$ is determined by several considerations. For flow that is single phase over the entire time step, $\gamma$ is set to zero. When the net predicted flow out of a cell of either phase exceeds the current mass in that cell, the weight is set to one (new-time cell-centered quantities are fluxed). For less dramatic situations, three ratios are computed. The first ratio has as a numerator the sum of the change in cell vapor mass for the time step due to all mass fluxes plus twice the change due to boiling. The ratio’s denominator is the cell’s mass decrease due only to outwardly directed vapor mass flows (positive number). The second ratio is the analog of the first as applied to the liquid phase. For the third ratio, the numerator adds half the old-time cell liquid mass to the predicted change in cell liquid mass for the time step. The denominator is half of the mass change due to outwardly directed flows at the cell’s edges (negative number). When other considerations are not in control, the maximum of the three ratios is limited to the range of zero through one and is used for $\gamma$.

The ratios used to compute the weighting factor were obtained after a long period of experimentation with two-phase-flow problems. The first two ratios force the use of a cell-centered implicit value when outflow of a phase is almost exclusively the result of phase-change terms. The factor will also force this implicit evaluation when phase change is not significant and inflow significantly exceeds the outflow. The third ratio becomes important when some liquid outflow is present and a prediction is made that over half of the existing liquid mass will flow or boil away during the time step.
The mixture of old- and new-time values of the quantity being fluxed results in a difference scheme for this step that is not rigorously conservative. However, the standard finite-volume divergence operator is applied in the stabilizer mass and energy equations, restoring conservation to the final fluxes of mass and energy.

To understand the stabilizer mass and energy equations, it is important to remember what is unknown and what quantities have fixed values. In this respect, the superscript “$n + 1$” can be deceptive. New-time velocity values are fixed by the semi-implicit step, as are all new-time terms marked with a tilde. In the stabilizer combined-gas mass equation, the only unknown new-time variables are the macroscopic gas densities $(\alpha \rho_g)^{n + 1}$. For the noncondensable mass equation, the only unknowns are the terms $(\alpha \rho_a)^{n + 1}$, and for the liquid mass equation, the only unknowns are the terms $[(1 - \alpha) \rho_l]^{n + 1}$. In the stabilizer combined-gas energy equation, the only unknown new-time variables are the macroscopic gas energy densities $(\alpha \rho_g e_g)^{n + 1}$. For the liquid energy equation, the only unknowns are the terms $[(1 - \alpha) \rho_l e_l]^{n + 1}$.

**Stabilizer Mass Equations**

**Combined Gas**

$$
\frac{[(\alpha \rho_g)^{n + 1}_j - (\alpha \rho_g)^n_j]}{\Delta t} + \nabla_j \cdot [(\alpha \rho_g)^{n + 1} V_g^{n + 1}] = \tilde{\Gamma}^{n + 1}_j .
$$

(1-149)

**Noncondensable Gas**

$$
\frac{[(\alpha \rho_a)^{n + 1}_j - (\alpha \rho_a)^n_j]}{\Delta t} + \nabla_j \cdot [(\alpha \rho_a)^{n + 1} V_g^{n + 1}] = 0 .
$$

(1-150)

**Additional Noncondensable Mass Equations (kth species)**

$$
\frac{[\alpha X_k \rho_a]^{n + 1}_j - [\alpha X_k \rho_a]^n_j}{\Delta t} + \nabla_j \cdot [(\alpha X_k \rho_a)^{n + 1} V_g^{n + 1}] = 0
$$

(1-151)

**Liquid**

$$
\frac{[(1 - \alpha) \rho_l]^{n + 1}_j - [(1 - \alpha) \rho_l]^n_j}{\Delta t} + \nabla_j \cdot \{(1 - \alpha) \rho_l)^{n + 1} V_l^{n + 1} \} = - \tilde{\Gamma}^{n + 1}_j .
$$

(1-152)

Liquid Solute (see the semi-implicit section for a description)
\[
\frac{[(1 - \alpha)^{n+1} m^{n+1}_j \rho_{lj} - (1 - \alpha)^n m^n_j \rho^n_{lj}]}{\Delta t} + \nabla_j \cdot \left( (1 - \alpha)^{n+1} m^{n+1}_l \rho^n_i V^{n+1}_l \right) = 0 \quad (1-153)
\]

\[
m^{n+1}_j = \min \left[ m^{n+1}_j + \frac{S^n_{cj}}{(1 - \alpha)^{n+1} \rho^n_{lj}}, m_{\text{max}} \right], \quad \text{(1-154)}
\]

and

\[
S^{n+1}_{cj} = (m^{n+1}_j - m^n_j)(1 - \alpha)^{n+1} \rho^n_{lj} + S^n_{cj}. \quad \text{(1-155)}
\]

**Stabilizer Energy Equations**

Combined Gas

\[
\frac{[(\alpha \rho_g e_g)^{n+1}_j - (\alpha \rho_g e_g)^n_j]}{\Delta t} + \nabla_j \cdot \left( (\alpha \rho_g e_g)^{n+1} V^{n+1}_g \right)
\]

\[
+ \tilde{P}^{n+1}_j \left[ \left( \frac{\tilde{\alpha}^{n+1}_j - \alpha^n_j}{\Delta t} \right) + \nabla_j \cdot \left( \alpha^n V^{n+1}_g \right) \right]
\]

\[
= q^{n+1}_{wg} + q^n_{dg} + q^{n+1}_{ig} + \tilde{\Gamma}^{n+1}_j \hat{h}_{sg} \quad \text{(1-156)}
\]

Liquid

\[
\frac{[(1 - \alpha) \rho_i e_i)^{n+1}_j - [(1 - \alpha) \rho_i e_i]_j^n}{\Delta t} + \nabla_j \cdot \left\{ [(1 - \alpha) \rho_i e_i]^{n+1} V^{n+1}_i \right\}
\]

\[
+ \tilde{P}^{n+1}_j \left\{ \left( \frac{\alpha^n_j - \tilde{\alpha}^{n+1}_j}{\Delta t} \right) + \nabla_j \cdot \left( (1 - \alpha)^n V^{n+1}_i \right) \right\}
\]

\[
= q^{n+1}_{wl} + q^n_{dl} - q^{n+1}_{ig} - \tilde{\Gamma}^{n+1}_j \hat{h}_{sg} \quad \text{(1-157)}
\]

As indicated in **Enhancements to the SETS Method**, the code does not directly solve all of the above stabilizer equations. The actual equations solved are differences between these equations and their corresponding equations from the semi-implicit step. For the case of solute transport, no corresponding equation exists in the semi-implicit step. As a result, the stabilizer solute-transport equation, Eq. (1-154), is solved exactly as listed above. The final forms of the other equations as set in TRACE follow:
Stabilizer Mass Equations

Combined Gas

\[
\frac{[(\alpha \rho_g)_{j}^{n+1} - \tilde{\alpha}^{n+1} \rho_{gj}^{n+1}]}{\Delta t} + \nabla_j \cdot [(\alpha \rho_g)^{n+1} V_g^{n+1}] = \nabla_j \cdot [(\alpha \rho_g)^n V_g^n].
\]

(1-158)

Noncondensable Gas

\[
\frac{[(\alpha \rho_a)_{j}^{n+1} - \tilde{\alpha}^{n+1} \rho_{aj}^{n+1}]}{\Delta t} + \nabla_j \cdot [(\alpha \rho_a)^{n+1} V_g^{n+1}] = \nabla_j \cdot [(\alpha \rho_a)^n V_g^n].
\]

(1-159)

Additional Noncondensable Mass Equations (kth species)

\[
\frac{[\alpha X_k \rho_a]_{j}^{n+1} - [\tilde{\alpha} X_k \rho_a]_{j}^{n+1}}{\Delta t} + \nabla_j \cdot [(\alpha X_k \rho_a)^{n+1} V_g^{n+1}] = \nabla_j \cdot [(\alpha X_k \rho_a)^n V_g^n].
\]

(1-160)

Liquid

\[
\frac{[(1 - \alpha) \rho_l]_{j}^{n+1} - (1 - \tilde{\alpha}^{n+1}) \rho_{lj}^{n+1}}{\Delta t} + \nabla_j \cdot \{(1 - \alpha) \rho_l\}^{n+1} V_l^{n+1} = \nabla_j \cdot \{(1 - \alpha) \rho_l\}^n V_l^n.
\]

(1-161)

Stabilizer Energy Equations

Combined Gas

\[
\frac{[(\alpha \rho_g e_g)_{j}^{n+1} - \tilde{\alpha}^{n+1} \rho_{gj}^{n+1} e_{gj}^{n+1}]}{\Delta t} + \nabla_j \cdot [(\alpha \rho_g e_g)^{n+1} V_g^{n+1}] = \nabla_j \cdot [(\alpha \rho_g e_g)^n V_g^n].
\]

(1-162)

Liquid

\[
\frac{\left\{(1 - \alpha) \rho_l e_l\right\}_{j}^{n+1} - (1 - \tilde{\alpha}^{n+1}) \rho_{lj}^{n+1} e_{lj}^{n+1}}{\Delta t} + \nabla_j \cdot \{(1 - \alpha) \rho_l e_l\}^{n+1} V_l^{n+1} = \nabla_j \cdot \{(1 - \alpha) \rho_l e_l\}^n V_l^n.
\]
\[ \nabla \cdot \left\{ [(1 - \alpha) \rho_l e_l] v^{n+1}_l \right\} = 0. \]  

(1-163)

Source terms in the SETS equations follow the definitions provided during the discussion of the semi-implicit methods. They are redefined below to clarify the use of intermediate variables.

\[ \tilde{q}_{wl}^{n+1} = h_{wl}^n a_w (T_w^n - \tilde{T}_l^{n+1}) \],

(1-164)

\[ \tilde{q}_{wg}^{n+1} = h_{wg}^n a_w (T_w^n - \tilde{T}_g^{n+1}) \],

(1-165)

and

\[ \tilde{\Gamma}^{n+1} = \frac{\left( \tilde{q}_{ig}^{n+1} + \tilde{q}_{il}^{n+1} \right)}{(h_i')^{n+1} - (h_i')^{n+1}} \],

(1-166)

where

\[ \tilde{q}_{ig}^{n+1} = h_{ig}^n a_i (\tilde{T}_{sat} - \tilde{T}_g^{n+1}) \]

(1-167)

and

\[ \tilde{q}_{il}^{n+1} = h_{il}^n a_i (\tilde{T}_{sat} - \tilde{T}_l^{n+1}) \].

(1-168)

As mentioned in **Enhancements to the SETS Method**, an important subtlety in the SETS application is the use of thermodynamic variables in the evaluation of specific terms. The current form of the SETS solution provides only final new-time values for void fraction \((\alpha)\), macroscopic densities \([\alpha \rho_g, \alpha \rho_a, (1 - \alpha) \rho_l]\), and macroscopic energies \([\alpha \rho_g e_g, (1 - \alpha) \rho_l e_l]\). A final call to the thermodynamics equation-of-state does not occur after the solution of the stabilizer mass and energy equations. As a result, when basic thermodynamic variables are needed for evaluation of properties such as viscosity or heat-transfer coefficients, values obtained from the previous semi-implicit step are used.

Eq. (1-134) and Eq. (1-136) do not involve any implicit coupling between cells and can be solved directly for the gas and liquid (caret) velocities at each mesh-cell interface. Eq. (1-137) and Eq. (1-138) are not coupled to each other. Each of these systems is implicitly coupled in space through the momentum-convection term, and each requires the solution of a tridiagonal linear system. Equations (1-139) through (1-146), combined with the necessary thermodynamic and constitutive equations, form a coupled system of nonlinear equations. Eq. (1-139) and Eq. (1-140) are solved directly to obtain \(V_{g}^{n+1}\) and \(V_{l}^{n+1}\) as linear functions of \(\tilde{P}^{n+1}\). After substituting these equations for velocity into Eqs. (1-141) through (1-146), the resulting system is solved with
a standard Newton iteration for the independent variables $\tilde{P}^{n+1}$, $\tilde{T}_a^{n+1}$, $\tilde{T}_g^{n+1}$, $\tilde{T}_l^{n+1}$, $\tilde{\alpha}^{n+1}$ and any $\tilde{X}_k^{n+1}$ with $k > 1$, including all coupling between cells. In practice, the linearized equations solved during this Newton iteration are reduced easily to a system is tridiagonal or dominately tridiagonal involving only total pressures. The final stabilizer mass and energy equations [Eq. (1-149) through Eq. (1-157)] also are simple tridiagonal linear systems because $V_g^{n+1}$ and $V_l^{n+1}$ are known after solving Eq. (1-139) through Eq. (1-146).

**3D Finite-Difference Methods**

All basic equations and stabilizer equations for the 3D VESSEL component are solved in the same form as the 1D components. The vector form of the motion equation separates into three orthogonal-coordinate velocity-component motion equations. We present only the combined-gas equations with the understanding that the liquid equations are treated analogously. The 3D VESSEL component can be modeled by the TRACE user in either cylindrical or Cartesian geometry. The following equations in cylindrical geometry convert to Cartesian geometry by replacing the $r$ divisor by unity and deleting the $V^2/r$ term in the divergence operator that models momentum convection. The $r$ and $\theta$ dependence is replaced by $x$- and $y$-dependence. For an orthogonal, right-handed, cylindrical coordinate system, the three velocity-component forms of the combined-gas motion differential equation are as follows:

**Axial Velocity ($z$) Component**

$$\frac{\partial V_g}{\partial t} + \left( V_{gr} \frac{\partial V_g}{\partial r} + \frac{V_{g\theta}}{r} \frac{\partial V_g}{\partial \theta} + V_{gz} \frac{\partial V_g}{\partial z} \right) = -\frac{1}{\rho_g \frac{\partial \bar{P}}{\partial z}} - \frac{\Gamma^+}{\alpha \rho_g} (V_g - V_l)$$

$$- \frac{C_{iz}}{\alpha \rho_g} (V_g - V_l) \bar{V}_g - \frac{C_{wgz}}{\alpha \rho_g} V_g \bar{V}_g - g_g$$

(1-169)

**Radial Velocity ($r$) Component**

$$\frac{\partial V_{gr}}{\partial t} + \left( V_{gr} \frac{\partial V_{gr}}{\partial r} + \frac{V_{gr}}{r} \frac{\partial V_{gr}}{\partial \theta} + \frac{V_{gr}^2}{r} + V_{gz} \frac{\partial V_{gr}}{\partial z} \right) = -\frac{1}{\rho_g \frac{\partial \bar{P}}{\partial r}} - \frac{\Gamma^+}{\alpha \rho_g} (V_{gr} - V_{lr})$$

$$- \frac{C_{ir}}{\alpha \rho_g} (V_{gr} - V_{lr}) \bar{V}_g - \frac{C_{wgr}}{\alpha \rho_g} V_{gr} \bar{V}_g - g_{gr}$$

(1-170)

**Azimuthal Velocity ($\theta$) Component**
In the last term of each equation, \( g \) is the gravitational acceleration constant and \( g_z, g_r, \) and \( g_\theta \) are the directional components of the gravity vector based on the orientation of the 3D VESSEL component. By default, TRACE internally defines \( g_z = 1, g_r = 0, \) and \( g_\theta = 0, \) where the \( z \)-axis is oriented vertically upward for all VESSEL components in the system model. The user may, however, redefine through input the orientation of each VESSEL component to something more general.

TRACE uses a staggered-mesh scheme (Ref. 1-14) similar to that used for the 1D components in which the velocities \( (V) \) are defined at the mesh-cell interfaces and the pressure \( (P) \), gas volume fraction \( (\alpha) \), temperature \( (T) \), internal energy \( (e) \), and density \( (\rho) \) are defined at the mesh-cell centers. The scalar field equations (mass and energy) apply to a mesh cell, whereas the velocity-component motion equations apply to an interface between mesh cells in the three velocity-component directions. The wall heat transfer and the interfacial mass transfer required by the field equations are defined with a form similar to Eqs. (1-164) through (1-168).

The difference scheme for each motion equation is lengthy because of the cross-derivative terms. Therefore, to illustrate the procedure, we will describe only the combined-gas velocity-component, \( z \)-direction, finite-difference basic equation of motion for a typical mesh cell interface, together with the gas basic mass and energy equations, for a typical mesh cell. The gas velocity-component basic equations of motion in the \( \theta \) and \( r \) directions along with all of the liquid basic equations are similar in form. The stabilizer motion, mass, and energy equations will not be illustrated; the reader is referred to the 1D component equations - Eq. (1-134) to Eq. (1-146) and Eq. (1-149) to Eq. (1-163) - where time-level parameters with \( \dot{\cdot}, \ddot{\cdot}, \cdot \), and \( \cdot + 1 \) superscripts are changed in going from the basic equations to the stabilizer equations. The superscript \( n \) indicates a current-time quantity; the superscript \( n + 1 \) indicates a new-time quantity. The functional dependence \( (r, \theta, z) \) points to the cell center. By incrementing \( r \) or \( \theta \) or \( z \) by \( \pm 1 \), one moves to the adjacent cell in the direction based on which coordinate is incremented and on the sign of the increment. The functional dependencies \( (r - 1/2, \theta, z) \) and \( (r + 1/2, \theta, z) \) point to the inside and outside radial faces of the cell, respectively; \( (r, \theta - 1/2, z) \) and \( (r, \theta + 1/2, z) \), the right and left azimuthal faces of the cell (based on a perspective of looking radially out of the cell), respectively; and \( (r, \theta, z - 1/2) \) and

\[
\frac{\partial V_{\theta}}{\partial t} + \left( V_{gr} \frac{\partial V_{\theta}}{\partial r} + \frac{V_{g\theta}}{r} \frac{\partial V_{\theta}}{\partial \theta} + \frac{V_{gz}}{r} \frac{\partial V_{\theta}}{\partial z} + V_{g\theta} \frac{\partial V_{\theta}}{\partial z} \right) = - \frac{1}{r \rho_g \partial \theta} \frac{\partial P}{\partial \theta} - \frac{\Gamma^+}{\alpha \rho_g} (V_{g\theta} - V_{l\theta})
\]

\[
- \frac{C_{\theta}}{\alpha \rho_g} (V_{g\theta} - V_{l\theta}) \left( \hat{V}_y - \hat{V}_z \right) - \frac{C_w \rho \alpha}{\alpha \rho_g} V_{g\theta} \left( \hat{V}_y - g g_{\theta} \right)
\]

(1-171)
(r, θ, z + 1/2), the bottom and top axial faces of the cell, respectively. The subscript \( g \) (for gas) is dropped unless it is needed for clarity.

The finite-difference combined-gas basic equation of motion in the \( z \)-direction has the following form:

**Combined-Gas Basic Equation of Motion in the \( z \)-Direction**

\[
V_z^{n+1}(r, \theta, z + 1/2) = V_z^n(r, \theta, z + 1/2) - \Delta t \left[ \frac{(V_z \Delta_r V_z^{n+1})}{\Delta r} + \frac{V_\theta \Delta_\theta V_z^{n+1}}{r \Delta \theta} + \frac{1}{2} \left( \frac{A_{z+1/2}}{A_{z+1}} + \frac{A_{z+1/2}}{A_z} \right) \right] \frac{V_z^{n+1}(r, \theta, z + 1/2)}{\Delta z}
\]

\[
\frac{A_{z+1/2}}{A_{z+1}} V_z^{n+1}(r, \theta, Z + 1/2) - \frac{A_{Z-1/2}}{A_Z} V_z^{n+1}(r, \theta, Z - 1/2)
\]

\[
- \frac{[P(r, \theta, z + 1) - P(r, \theta, z)]^{n+1}}{\rho^n(r, \theta, z + 1/2) \Delta z} - \frac{C_{iz}^{n}(r, \theta, z + 1/2)}{(\alpha, \rho)^n(r, \theta, z + 1/2)}
\]

\[
\times \left\{ \left[ \nabla_g - \nabla_l \right]^n + \frac{((V_g - V_{lz})^n(r, \theta, z + 1/2))^2}{\nabla_g - \nabla_l^n} \right\} (V_g - V_{lz})^{n+1}(r, \theta, z + 1/2)
\]

\[
- \frac{((V_g - V_{lz})^n(r, \theta, z + 1/2))^3}{\nabla_g - \nabla_l^n}
\]

\[
- \frac{\Gamma^+(r, \theta, z + 1/2)(V_g - V_{lz})^{n+1}(r, \theta, z + 1/2)}{(\alpha, \rho)^n(r, \theta, z + 1/2)} - gg_x
\]

\[
C_{wz}^{n}(r, \theta, z + 1/2) \left\{ \left[ \nabla_g^n + \frac{(V_g^n(r, \theta, z + 1/2))^2}{\nabla_g^n} \right] V_z^{n+1}(r, \theta, z + 1/2) - \frac{(V_g^n(r, \theta, z + 1/2))^3}{\nabla_g^n} \right\}
\]

\[
(\alpha, \rho)^n(r, \theta, z + 1/2)
\]
where $Z = z$ if $V^m_z(r, \theta, z + 1/2) \geq 0$ and $Z = z+1$ if $V^m_z(r, \theta, z + 1/2) < 0$

Any finite-difference scheme requires certain quantities at locations where they are not defined formally; therefore, additional relations are needed. TRACE obtains the volume-averaged properties $\alpha \rho$ and $\rho$ at the cell axial interface from a cell-length weighted average,

\[
(\alpha \rho)(r, \theta, z + 1/2) = \frac{\Delta z(z) \alpha(r, \theta, z) \rho(r, \theta, z) + \Delta z(z+1) \alpha(r, \theta, z+1) \rho(r, \theta, z+1)}{\Delta z(z) + \Delta z(z+1)}
\]

and

\[
\rho(r, \theta, z + 1/2) = \frac{(\alpha \rho)(r, \theta, z + 1/2)}{\alpha(r, \theta, z + 1/2)} = \frac{\Delta z(z) \alpha(r, \theta, z) \rho(r, \theta, z) + \Delta z(z+1) \alpha(r, \theta, z+1) \rho(r, \theta, z+1)}{\Delta z(z) \alpha(r, \theta, z) + \Delta z(z+1) \alpha(r, \theta, z+1)}
\]

This averaging is necessary to compute pressure heads accurately. The code obtains $\Gamma$ at the cell interface from its phasic velocity donor cell as follows:

The cross-derivative term $V_r \Delta_r V^m_z + 1$ reflects a donor-cell average:

\[
V_r \Delta_r V^m_z + 1 = \tilde{V}_r(r + 1/2, \theta, z + 1/2)[\tilde{V}_z(r + 1, \theta, z + 1/2) - \tilde{V}_z(r, \theta, z + 1/2)] + \tilde{V}_r(r - 1/2, \theta, z + 1/2)[\tilde{V}_z(r, \theta, z + 1/2) - \tilde{V}_z(r - 1, \theta, z + 1/2)],
\]

where

\[
\tilde{V}_r(r + 1/2, \theta, z + 1/2) = \min \left[ \frac{SC_r(r + 1/2, \theta, z + 1) \tilde{V}_r(r + 1/2, \theta, z + 1) \Delta z(z) + SC_r(r + 1/2, \theta, z) \tilde{V}_r(r + 1/2, \theta, z) \Delta z(z+1)}{\Delta z(z) + \Delta z(z+1)}, 0 \right].
\]

and

\[
\tilde{V}_r(r - 1/2, \theta, z + 1/2) = \min \left[ \frac{SC_r(r - 1/2, \theta, z + 1) \tilde{V}_r(r - 1/2, \theta, z + 1) \Delta z(z) + SC_r(r - 1/2, \theta, z) \tilde{V}_r(r - 1/2, \theta, z) \Delta z(z+1)}{\Delta z(z) + \Delta z(z+1)}, 0 \right].
\]
In the above equations, “min” and “max” are the mathematical functions of minimum and maximum values of the terms inside the brackets. \( SC_r(r+1/2, \theta, z) \) is the product of an orifice factor that is 0 (when an orifice plate is present at the \( r+1/2 \) interface) or 1 and the ratio of the flow area through the \( r+1/2 \) interface to the \( r \) cell flow area in the radial direction, \( \text{vol}(r, \theta, z)/\Delta r_{cell} \). The orifice factor is simply a statement that transverse momentum is not transported across an orifice. This assumption is particularly valid at the upper and lower core support plates. The area ratio contained in \( SC \) is consistent with the discussion later in this chapter of use of area ratios in momentum flux terms. An analogous expression holds for the \( V_\theta \Delta \theta V_z^{n+1} \) term.

Note that the \( V_z \) differences in the \( r \) and \( \theta \) directions do not contain the \( z \)-direction flow-area weighting form. The \( SC_r \) and \( SC_\theta \) factors make this correction for \( z \)-direction momentum convection in the \( r \) and \( \theta \) directions, respectively.

In the interfacial drag terms, the magnitude of the relative velocity is defined as follows:

\[
\left| \hat{V}_g - \hat{V}_l \right| = \left\{ \left[ V_{zg}(r, \theta, z + 1/2) - V_{zl}(r, \theta, z + 1/2) \right]^2 
+ 0.25 \left[ (V_{rg}(r+1/2, \theta, z) + V_{rg}(r-1/2, \theta, z) 
- V_{rl}(r+1/2, \theta, z) - V_{rl}(r-1/2, \theta, z) \right]^2 
+ 0.25 \left[ V_{\theta g}(r, \theta + 1/2, z) + V_{\theta g}(r, \theta - 1/2, z) 
- V_{\theta l}(r, \theta + 1/2, z) - V_{\theta l}(r, \theta - 1/2, z) \right]^2 \right\}^{1/2}.
\]

(1-178)

The convective terms in the finite volume relations for the scalar field equations are in conservative form. The finite-difference form of the combined-gas basic mass equation is
**Combined-Gas Basic Mass Equation**

\[
(\tilde{\rho})^{n+1} = (\alpha \rho)^n - \left[\frac{\Delta t}{vol}\right] \left\{ A_{z+1/2} \langle (\alpha \rho)^n V_{z}^{n+1} \rangle_{z+1/2} - A_{z-1/2} \langle (\alpha \rho)^n V_{z}^{n+1} \rangle_{z-1/2} \right. \\
+ A_{r+1/2} \langle (\alpha \rho)^n V_{r}^{n+1} \rangle_{r+1/2} - A_{r-1/2} \langle (\alpha \rho)^n V_{r}^{n+1} \rangle_{r-1/2} \\
+ A_{\theta+1/2} \langle (\alpha \rho)^n V_{\theta}^{n+1} \rangle_{\theta+1/2} - A_{\theta-1/2} \langle (\alpha \rho)^n V_{\theta}^{n+1} \rangle_{\theta-1/2} \right\} + \Delta t \tilde{\Gamma}^{n+1} 
\]  
(1-179)

The combined-gas basic energy equation is

**Combined-Gas Basic Energy Equation**

\[
(\tilde{\rho}e)^{n+1} = (\alpha \rho e)^n - \left[\frac{\Delta t}{vol}\right] \left\{ A_{z+1/2} \langle (\alpha \rho e)^n V_{z}^{n+1} \rangle_{z+1/2} - A_{z-1/2} \langle (\alpha \rho e)^n V_{z}^{n+1} \rangle_{z-1/2} \right. \\
+ A_{r+1/2} \langle (\alpha \rho e)^n V_{r}^{n+1} \rangle_{r+1/2} - A_{r-1/2} \langle (\alpha \rho e)^n V_{r}^{n+1} \rangle_{r-1/2} \\
+ A_{\theta+1/2} \langle (\alpha \rho e)^n V_{\theta}^{n+1} \rangle_{\theta+1/2} - A_{\theta-1/2} \langle (\alpha \rho e)^n V_{\theta}^{n+1} \rangle_{\theta-1/2} \right\} \\
- \tilde{P}^{n+1} (\tilde{\alpha}^{n+1} - \alpha^n) \\
- \left[\frac{\tilde{P}^{n+1}}{vol} \Delta t\right] \left\{ A \alpha^n V_{z}^{n+1} \rangle_{z+1/2} - \langle A \alpha^n V_{z}^{n+1} \rangle_{z-1/2} \right. \\
+ \langle A \alpha^n V_{r}^{n+1} \rangle_{r+1/2} - \langle A \alpha^n V_{r}^{n+1} \rangle_{r-1/2} \\
+ \langle A \alpha^n V_{\theta}^{n+1} \rangle_{\theta+1/2} + \langle A \alpha^n V_{\theta}^{n+1} \rangle_{\theta-1/2} \right\} + \Delta t (\tilde{q}_{wg}^{n+1} + \tilde{q}_{dg}^{n+1} + \tilde{q}_{ig}^{n+1} + \tilde{\Gamma}^{n+1} \tilde{h}_{sg}^{n+1}) 
\]  
(1-180)

The discrete forms for the other scalar equations (the total mass and energy equations, the noncondensable-gas mass equation, and the liquid-solute mass equation) are similar. The time level of the convected mass \(\alpha \rho\) and convected energy \(\alpha \rho e\) is \(n + 1\) in the stabilizer equations. If the stabilizer mass and energy equations are not evaluated (pure semi-implicit method), the tilde parameters in Eq. (1-179) and Eq. (1-180) are defined without tildes.
All the field equations in the 3D VESSEL component can have additional source terms to allow one or more 1D component junctions to be connected to a mesh-cell interface anywhere in the 3D VESSEL component. The source terms in the mass and energy equations follow below. The subscripts 1D and 3D indicate that quantities are obtained from the 1D component-junction interface or junction cell and the 3D VESSEL-component mesh cell, respectively. The $\langle \rangle$ indicates the convected quantity has either the subscript 1D or 3D of the upstream donor cell based on the direction of the phase velocity at the source-connection 1D component-junction interface, illustrated by Eqs. (1-82) and (1-91). Each of these source terms is added to the downstream mesh cell’s mass or energy equation and an equivalent sink term is subtracted from the upstream mesh cell’s equation.

**Total Basic Mass-Equation Source Term**

$$\left[ \frac{\Delta t}{\text{vol}} \right] \{ \langle (\alpha \rho_g) V_{g}^{n+1} \rangle_{1D} + \langle (1 - \alpha) \rho_l V_{l}^{n+1} \rangle_{1D} \} .$$

(1-181)

**Combined-Gas Basic Mass-Equation Source Term**

$$\left[ \frac{\Delta t}{\text{vol}} \right] \langle (\alpha \rho_g) V_{g}^{n+1} \rangle_{1D} .$$

(1-182)

**Total Basic Energy Equation Source Term**

$$\left[ \frac{\Delta t}{\text{vol}} \right] \{ \langle [(1 - \alpha) \rho_l e_l] V_{l}^{n+1} \rangle_{1D} A_{1D} + \langle [\alpha \rho_g e_g] V_{g}^{n+1} \rangle_{1D} A_{1D} \} + P_{3D} \{ \langle \alpha V_{g}^{n+1} \rangle_{1D} A_{1D} + \langle (1 - \alpha) V_{l}^{n+1} \rangle_{1D} A_{1D} \} \} .$$

(1-183)

**Combined-Gas Basic Energy Equation Source Term**

$$\left[ \frac{\Delta t}{\text{vol}} \right] \{ \langle (\alpha \rho_g e_g) V_{g}^{n+1} \rangle_{1D} A_{1D} + P_{3D} \langle \alpha V_{g}^{n+1} \rangle_{1D} A_{1D} \} .$$

(1-184)

**Mixture Noncondensable-Gas Basic Mass-Equation Source Term**

$$\left[ \frac{\Delta t}{\text{vol}} \right] \langle (\alpha \rho_g) V_{g}^{n+1} \rangle_{1D} A_{1D} .$$

(1-185)
Additional Noncondensable Mass Equation Source Terms \((kth\ species)\)

\[
\left[ \frac{\Delta t}{vol} \right] \langle (\alpha X_k \rho_a)^n V_g^{n+1} \rangle_{1D} A_{1D}
\]  

\(1-186\)

Liquid-Solute Basic Mass-Equation Source Term

\[
\left[ \frac{\Delta t}{vol} \right] \langle [(1-\alpha) X_k m \rho_l]^n V_l^{n+1} \rangle_{1D} A_{1D}
\]  

\(1-187\)

The momentum source term is complicated by the staggered differencing and by the fact that the actual 1D component may enter at an arbitrary angle. For TRACE, we assume that the 1D component attaches normal (perpendicular) to the vessel mesh-cell interface. The interface flow area \(A_{3D}\) and velocity \(V_{3D}\) are defined on the opposite side of the 3D mesh cell from the interface where the 1D component-junction source convection is made. It is that opposite mesh-cell interface from the source-convection interface that has in its motion equation the following momentum-convection source term for the combined-gas or liquid basic equation of motion when \(V_{3D} \pm 1/2\) flows away from the 1D component source-convection interface into the \(3D + 1\) mesh cell. An \(S\) factor is applied to the 1D component so that its positive flow direction becomes the positive flow direction of the vessel.

Basic Equation-of-Motion Source Term

\[
\frac{\Delta t}{2} \left( \frac{A_{3D}}{vol_{3D} / \Delta x_{3D}} + \frac{A_{3D}}{vol_{3D} / \Delta x_{3D}} \right) V_{3D}^{n+1} \left[ \frac{A_{1D} S \bar{V}_{1D}^{n+1}}{vol_{1D} / \Delta x_{1D}} \right]
\]  

\(1-188\)

As with the 1-D semi-implicit equations, independent variables \(\tilde{P}^{n+1}, \tilde{P}_a^{n+1}, \tilde{T}_g^{n+1}, \tilde{T}_l^{n+1}, \tilde{\alpha}^{n+1}\) and any \(\tilde{X}_k^{n+1}\) with \(k > 1\) are used during the iterative solution of the non-linear set of flow equations. Motion equations are solved for new time liquid and gas velocities as linear functions of new time pressures, making these velocities dependent variables in the solution process. Densities and internal energies are also treated as dependent variables by using the thermal equations of state,

\[
\rho_l = \rho_l(P,T), \quad \rho_v = \rho_v(P_a,T_g), \quad \text{and} \quad \rho_a = \rho_a(P_a,T_g);
\]  

\(1-189\)

the caloric equations of state,

\[
e_l = e_l(P,T), \quad e_v = e_v(P_a,T_g), \quad \text{and} \quad e_a = e_a(P_a,T_g);
\]  

\(1-190\)
and the definitions for \( \rho_g \), \( e_g \), and \( P \) (Eqs. 1-42 through 1-45).

If one or more hardware structures exist in the 3D mesh cells, the interface flow area \( A \) for fluid flow and the mesh-cell fluid volume \( vol \) are reduced from their geometric mesh-cell values by the user through inputting fractions of their geometric area and volume. These fractions can be input with values greater than unity, but it is recommended that the user not do so for the model to be physically valid. Thus, \( A \) should be less than or equal to the geometric mesh-cell side area and “\( vol \)” should be less than or equal to the geometric mesh-cell volume. Mesh-cell fluid volumes are constrained to be \( \geq 1 \times 10^{-12} \text{ m}^3 \) by TRACE. When the flow area is defined to be zero, fluid flow across the mesh-cell interface is zero. This procedure allows large obstacles, such as the downcomer walls and flow channels, to be modeled within the VESSEL component.

**Modifications to the Basic Equation Set**

Because of the choice of independent variables in the solution of the 1D or 3D basic equations (total pressure, air partial pressure, void fraction, combined-gas and liquid temperatures, and mass fractions of any noncondensable species beyond the first), the basic equation set becomes singular at void fractions of zero and one. To avoid this solution difficulty the combined gas mass equation (1-141) is replaced with a simple equation setting \( \alpha = 0 \) or \( \alpha = 1 \). The combined-gas energy equation is replaced with an equation setting the temperature of the missing phase to the saturation temperature based on the total pressure.

When the transition from single-phase gas or liquid to a two-phase fluid first occurs, the combined-gas and liquid mass equations are evaluated but the replacement equation for the gas energy equation is used for one more time step. This forces the second phase to initially appear at saturation conditions, which is generally a very good approximation. It drastically reduces sporadic numerical problems associated with the use of two energy equations in which the first appearance of a phase can be associated with an exceptionally bad predicted value of its temperature. Special considerations are also made during the linearization for the Newton solution of the semi-implicit equations. When an explicit mass test suggests the first appearance of a second phase, flux of the second phase is used to estimate the new-time void fraction. If air is just appearing in a cell, an initial estimate is also made of the air partial pressure. Both of these estimates are used to specify the base state for the linearization associated with the current Newton iteration.

When the pressure exceeds the critical-point pressure, the basic equations can become singular. However, care has been taken to place a minimum value on the difference between liquid and vapor density wherever it appears in a constitutive equation. This results in a two-phase equation set that drives itself rapidly to single phase when pressure is above the critical point.
**Conserving Convedted Momentum**

The backward difference approach given in Eq. (1-85) to determine the $V \cdot \nabla V$ term in a momentum equation is known to be stable numerically. For smooth area changes, however, this backward or upwind difference scheme is not accurate and does not conserve momentum. For abrupt area changes, it can be shown that the upwind difference scheme combining Eq. (1-85) and Eq. (1-91) for $V \cdot \nabla V$ will result in pressure changes that include both reversible and irreversible effects. Upwind differencing is accurate for abrupt expansions and overestimates the pressure change for an abrupt contraction. (see Chapter 7, *Form Loss Models* for details.)

It has been shown that the accuracy of a central difference representation of $V \cdot \nabla V$ is quite good for smooth area changes and for the reversible portion of an abrupt area change. It can be shown, however, through linear stability analysis, that central differencing is, in general, unconditionally unstable. An approach was developed (originally for TRAC-PF1/MOD2 and carried over into TRACE) to improve momentum conservation by determining factors based on geometry that change the upwind differencing of the $V \cdot \nabla V$ so that its accuracy is consistent with central differencing. The assumption used in developing these factors is constant volumetric flow from the cell center to the cell edge.

A central difference $V \cdot \nabla V$ for 1D flow yields

$$V \cdot \nabla V = \frac{V dV}{dx} \equiv \frac{0.5 d(V^2)}{dx} \equiv \frac{0.5(V_{j+1}^2 - V_j^2)}{\Delta x_{j+1/2}}. \quad (1-191)$$

Equation (1-191) can be rewritten as

$$V \cdot \nabla V = \frac{0.5(V_{j+1}^2 + V_j^2)(V_{j+1} - V_j)}{\Delta x_{j+1/2}} \quad (1-192)$$

In TRACE, velocities are calculated at cell edges, therefore cell-center velocities must be estimated from cell-edge velocities. Equation (1-192) can be written in terms of the cell-edge velocities by applying the following equations based on constant volumetric flow from cell center to the cell edge:

$$A_{j+1} V_{j+1} = A_{j+1/2} V_{j+1/2}, \quad (1-193)$$

$$A_j V_j = A_{j+1/2} V_{j+1/2}, \quad (1-194)$$
and

\[ A_j V_j = A_{j-1/2} V_{j-1/2}. \]  

(1-195)

If Eqs. (1-193) and (1-194) are substituted into the summed portion of Eq. (1-192), and Eqs. (1-193) and (1-195) are substituted into the difference portion of Eq. (1-192), an upwind difference form that is as accurate as central differencing is obtained for \( V \cdot \nabla V \).

\[
V \cdot \nabla V_{j+1/2} = \frac{0.5 \left( \frac{A_{j+1/2}}{A_{j+1}} + \frac{A_{j+1}}{A_j} \right) V_{j+1/2} \left( \frac{A_{j+1/2}}{A_{j+1}} \frac{V_{j+1/2}}{A_{j+1}} - \frac{A_{j-1/2}}{A_j} \frac{V_{j-1/2}}{A_j} \right)}{\Delta x_{j+1/2}} 
\]

(1-196)

These equations assume that \( V_{j+1/2} \geq 0 \) but similar sets of equations can be derived for \( V_{j+1/2} < 0 \). In TRACE, Eq. (1-196) is the approximation used in both the 1D and 3D momentum-convection terms to improve the conservation of momentum.

In general, TRACE, even with the corrected \( V \cdot \nabla V \) term, is still solving a nonconserving momentum equation. What follows is a simplified version of the derivation leading to Eq. (1-78). A conserving form of the momentum equation for single-phase flow with no momentum sources or sinks can be written as

\[
\frac{d(\rho V)}{dt} = \frac{d(\rho VA V)}{A dx} = 0 
\]

(1-197)

Expanding the derivatives of Eq. (1-197) yields

\[
V \left[ \frac{d(\rho)}{dt} + \frac{d(\rho VA)}{A dx} \right] + \rho \left[ \frac{d(V)}{dt} + V \frac{d(V)}{dx} \right] = 0. 
\]

(1-198)

The continuity equation for single-phase flow with no sources or sinks can be written as

\[
\frac{d(\rho)}{dt} + \frac{d(\rho VA)}{A dx} = 0 
\]

(1-199)

Therefore, Eq. (1-198) can be written as
\[
\frac{d(V)}{dt} + V \frac{d(V)}{dx} = 0.
\]

Equation (1-200) represents the type of nonconserving form of the momentum equation solved by the TRACE code. This derivation indicates that TRACE will conserve momentum with the nonconserving form of the momentum equation if mass is conserved on a point-by-point basis. TRACE conserves mass within each hydraulic cell and assumes that within that cell, the density and void fractions are constant. This assumption may lead to errors in conserving momentum, since the nonconserving momentum equation is solved from cell center to cell center and the geometry area ratio factors developed for Eq. (1-196) assume constant density and void fraction from cell center to cell edge.

If we assume constant volumetric flow from cell edge \( j-1/2 \) to cell edge \( j+1/2 \), Eq. (1-196) in the form of the Bernoulli equation is equivalent to

\[
P_{j+1} - P_j + \frac{\rho}{2} \left( \left( \frac{A_{j+1/2}}{A_{j+1}} V_{j+1/2} \right)^2 - \left( \frac{A_{j-1/2}}{A_{j}} V_{j-1/2} \right)^2 \right) + \rho g \Delta x_{j+1/2} \cos \theta = 0.
\]

Substitute the constant volumetric-flow relations \( A_{j+1/2} V_{j+1/2} = A_{j+1} V_{j+1} \) and \( A_{j-1/2} V_{j-1/2} = A_{j} V_{j} \) into the momentum-convection term of Eq. (1-201) to obtain the Bernoulli equation

\[
P_{j+1} - P_j + \frac{1}{2} \rho \left[ V_{j+1}^2 - V_j^2 \right] + \rho g \Delta x_{j+1/2} \cos \theta = 0.
\]

We see from the above derivation of the momentum-convection term and the assumptions made that the equation of motion for single-phase liquid (a near-incompressible fluid) to a very good approximation satisfies the Bernoulli equation. Convected momentum flux between momentum cells should be nearly conserved. Reversible form losses caused by flow-area and elevation changes should be evaluated correctly. This has been demonstrated (Ref. 1-15) for single-phase liquid with a variable flow-area and elevation flow-channel test problem having a total of seven 1D PIPE and VESSEL components connected in series with a FILL-component velocity and BREAK-component pressure boundary condition at each end of the flow channel, respectively. Each 1D VESSEL component was evaluated in each of three Cartesian-coordinate directions in separate calculations. Wall losses in the flow channel with flow area varying from 0.1 to 0.6 \( m^2 \) were minimized by increasing the flow-channel hydraulic diameter by a factor of 100.

A plot of the Bernoulli expression \( P_j/\rho_j + V_j^2/2 + gh_j \) (as calculated using TRAC-PF1/MOD2) versus flow-channel cell number \( j \) for four different PIPE- and VESSEL-component models is
shown in Figure 1-7, with and without flow-area ratios applied in the momentum-convection term of the liquid equation of motion. Each of the four models comprised a different combination of PIPE and/or 1D VESSEL components, yet each gave the same results. The momentum equation currently used in TRACE provided an accurate evaluation of the Bernoulli equation as demonstrated by the constant value of the Bernoulli expression when flow-area ratios are applied in the momentum-convection term. Similar calculations were performed for single-phase vapor wherein TRAC-PF1/MOD2 was temporarily modified to evaluate a constant vapor microscopic density (making vapor an incompressible fluid). The results determined were similar to those of liquid, which served as a check that the combined-gas equation of motion as well as the liquid equation of motion are programmed correctly for both 1D and 3D components.

![Graph showing Bernoulli expression](image)

**Figure. 1-7.** The Bernoulli expression \( P_j/\rho_j + V_j^2/2 + gh_j \) vs. flow-channel cell number \( j \) from a 1D flow-channel test problem having variable flow area and elevation. This calculation was performed with TRAC-PF1/MOD2.

For a compressible single-phase vapor, the change in its microscopic density because of fluid pressure and temperature variation over a mesh-cell distance generally is small. Approximating constant density within a fluid cell should cause only a small error in conserving convected vapor momentum flux between momentum cells. However, a significant spatial variation in the fluid void fraction across a mesh cell can result in a momentum-flux conservation error, in part because of the constant volumetric-flow assumption. However, for rapidly changing void fractions the larger problem in momentum conservation can be traced to the assumption equating two different averages of macroscopic density, leading to the difference between Eq. (1-76) and Eq. (1-77).
Reversible and Irreversible Form Losses.

With flow-area ratios in the momentum-convection term, TRACE approximately conserves convected momentum and evaluates only the reversible form losses of the Bernoulli equation. The TRACE user is therefore responsible for supplying input that specifies all irreversible form losses due to abrupt or semi-abrupt flow-area expansions and contractions, thin-plate-orifice-type flow restrictions, and flow redirection (turning) at an elbow or tee, as discussed in Chapter 7, Form Loss Models.

TRACE users who are adapting old TRAC-PF1/MOD1 input files need to be aware of a conflict in the way form losses are applied between TRACE and that older code. The TRAC-PF1/MOD1 momentum-convection term does not include the flow-area ratios illustrated in Eq. (1-196). That results in a numerically produced irreversible form loss that is about right for an abrupt expansion and approximately twice the irreversible form loss of an abrupt contraction. Code users who have prepared TRAC-PF1/MOD1 input-data plant models have compensated for this numerically generated irreversible form-loss error by not including other irreversible form losses at flow restrictions or at elbows and tees in order to evaluate the correct overall pressure drop through a portion or all of a flow loop. TRACE users who inherit and convert such TRAC-PF1/MOD1 input-data files into TRACE input-data files need to be aware that their plant model may have built-in compensating-error features for TRAC-PF1/MOD1 that, when evaluated by TRACE, give pressure losses along flow paths that are significantly low. The user’s response to this situation should be to never use converted TRAC-PF1/MOD1 input-data files blindly. All mesh-cell interface flow areas and mesh-cell volumes and lengths (whose ratio defines mesh-cell flow area) need to be checked against plant specifications, and all input-specified FRICs or K-factors (and those that have not been specified) need to be defined to account for their actual irreversible form losses at abrupt or semi-abrupt flow-area changes, flow restrictions, and flow turns (redirections).

TRACE assists code users by not requiring them to determine values loss coefficients at abrupt expansion or contraction 1D component mesh-cell interfaces for input specification. At all such interfaces, TRACE internally evaluates the standard K-factor formulas in Chapter 7, Form Loss Models, for abrupt-expansion \[ K = (1-A_{\text{min}}/A_{\text{max}})^2 \] and abrupt-contraction \[ K = 0.5 - 0.7(A_{\text{min}}/A_{\text{max}}) + 0.2 (A_{\text{min}}/A_{\text{max}})^2 \] form losses based on mesh-cell flow areas and adds them to the any input-specified loss coefficients. This feature is extended in TRACE to 3D VESSEL components as well.

Special Cases

The definition of flow-area ratios and irreversible form losses when evaluating momentum convection in BREAK, PLENUM, TEE (and, more generally, side junctions), and VESSEL components needs further consideration.
**BREAK Component**

TRACE models a BREAK component as a volume in which state conditions are prescribed by the user rather than generated through the solution of flow equations. The user specifies the volume of the cell and a characteristic length perpendicular to it’s connection area. A momentum equation is evaluated at the BREAK junction area, and when an area is required from the BREAK side for use in the momentum transfer terms, it is obtained by dividing the BREAK volume by the BREAK characteristic length. TRACE user’s need to think carefully about the physical configuration within which the BREAK is being used as a boundary condition to isolate a subsystem. If in the real system piping continues beyond BREAK junction, the pipe geometry must be considered in setting the BREAK geometry. If piping ends at the BREAK junction and flow enters a very large volume (e.g. containment), the ratio of volume to length in the break should give an area much larger than the flow area at the BREAK junction. The characteristic length input for the BREAK should not, however, be a characteristic length for the large physical volume. It is used in the pressure gradient term in the junction momentum equation, and should be small to reflect the fact that pressure changes rapidly as it enters the large volume. The standard guideline for TRACE is to set the length for the BREAK equal to the length of the computational volume immediately adjacent to the BREAK.

As with other points of abrupt area change, when the flow area changes between the BREAK mesh cell and the adjacent-component mesh cell, we recommend user specification of an appropriate irrecoverable loss coefficient. This can be done either as a specific coefficient, or a request that TRACE calculate an appropriate coefficient. It is important to provide a dissipative term in the equation of motion to determine the correct and numerically stable solution. A BREAK component is a pressure boundary condition that locally removes a degree of freedom from the hydrodynamic solution. The equation set becomes locally stiffer and more sensitive to error growth when there is not a dissipative term.

**PLENUM Component**

In general, we no longer recommend use of the PLENUM component when developing new TRACE input models. We document it here for completeness in case you find yourself maintaining or using a legacy model that includes such a component type.

The PLENUM component is a single mesh cell with a user selected number of junction interfaces connected to 1D components. Momentum can be transferred into a plenum but not across a plenum from one connecting face to another. The input for a plenum requests a characteristic length associated with each connection. This can be considered as twice the distance from the connecting face to the center of the plenum. When a plenum area is needed as part of the momentum transfer term, it is calculated as the ratio of plenum volume divided by the characteristic length associated with the junction at which the momentum equation is evaluated. When a velocity is needed from the plenum side for use in the momentum transfer term it is taken to be zero. For example if face j+1/2 in Eq. (1-196) is a plenum junction, and volume j is the plenum, the equation becomes:
where $A_j$ is the previously mentioned ratio of plenum volume to characteristic length.

1D Side Junctions (including the TEE Component)

The TEE component has been maintained in TRACE for legacy TRAC input models, and its functionality has been captured with the side junction capability in other 1-D components. The key aspect of a TEE component or the more modern side junction is the introduction of source terms to the 1-D motion equations to properly capture the influence of momentum from the side leg flow on the momentum in the primary 1-D flow path. Less complicated capabilities are also provided to transfer momentum from the primary to secondary flow path via the boundary conditions at the side junction.

The momentum source model used for any TRACE side junction (including the TEE and other TEE-based components like the JETP or SEPD) was directly inherited from TRAC-PF1/MOD2. The basic momentum source term can be seen in Eq. (1-78) as:

$$ V_g, 3 \cos \phi - V_g, 1 \left( \frac{\alpha \rho g}{\alpha \rho g A_c} \right) (\alpha \rho g V_g)_3 A_3 $$

Within the final difference equation form we evaluate this source term in a linearized implicit manner analogous to the treatment of the other momentum flux terms. In the standard SETS notation, the source term is:

$$ A_3 \rho_n \frac{A_3 \rho_n}{\alpha \rho_g A_c} \left[ \tilde{V}_{g, 3}^{n+1} \left( 2 \tilde{V}_{g, 3}^{n} \cos \theta + \tilde{V}_{g, 1}^{n} \right) \right. $$

$$ + \left. \tilde{V}_{g, 3}^{n} \tilde{V}_{g, 1}^{n+1} - \tilde{V}_{g, 3}^{n} \left( \tilde{V}_{g, 3}^{n} \cos \theta + \tilde{V}_{g, 1}^{n} \right) \right] $$

A similar term appears in the liquid momentum equation.

One limitation of the current implementation is that it was inherited directly from TRAC-PF1/MOD2 where a straight pipe assumption was enforced in proximity to the side connection. Best results are obtained if there are no flow area changes at any edges of the volume to which the side leg connects. In addition the cell averaged flow area in the first volume of the 1-D flow
component connected to the side junction should be the same as the side junction’s area. These restrictions will be lifted with TRACE v6.0.

Differences in implementation of the momentum transport terms also affect irrecoverable loss coefficients. The option for automatic internal calculation of these coefficients is disabled at the edges of a volume containing a side junction. If area changes are present the code user needs to carefully check that pressure drops through the primary flow path are acceptable. If more pressure loss is needed, then specific values of loss coefficients should be supplied via the input. If too much pressure loss is obtained adjacent to a junction volume, then renodalization may be required.

A discussion of the side junction (TEE) model inherited from TRAC-PF1/MOD2 is given in Reference 1-17.

**VESSEL Component.**

Using flow-area ratios to correctly donor-cell the approximate momentum flux at a mesh-cell center (based on its interface-defined velocity a half mesh-cell distance away) is done only for momentum that is convected by its own component-direction velocity. This is not done in the cross-derivative terms of the divergence operator for momentum convection as shown in Eqs. (1-176) and (1-177).

Flow-area ratios are evaluated using the mesh-cell average flow area, \( vol_{i,j,k} / \Delta_d \), where \( d = i, j, \) or \( k \) defines the component direction of the equation of motion. When the structure volume fraction within a 3D mesh cell is nonuniform in the \( d \) direction, the average flow area for the mesh cell can be incorrectly defined by \( vol_{i,j,k} / \Delta_d \). Nonphysical mesh-cell flow areas affect the pressure solution through the Bernoulli equation by not approximating the donor-cell-approximated velocity components at the mesh-cell centers correctly. Locating 3D mesh-cell interfaces on planes of structure volume-fraction discontinuity can minimize this modeling difficulty. A modeling example that is difficult to handle correctly is representing the internal structure curved surface of a pressure vessel that bisects mesh cells in the vessel lower plenum.

A source connection to a 3D VESSEL component by a 1D component uses the \( vol_{i,j,k} / \Delta_d \) geometry parameters of the \( (i,j,k) \) mesh cell (where \( d \) refers to the edge direction to which the 1-D flow is connected), to define the 3D mesh-cell flow area for evaluating the source-connection junction momentum-convection term flow-area ratios. The actual \( d \)-direction flow area in the VESSEL component that the 1D component flow is expanding or contracting into may be significantly different from \( vol_{i,j,k} / \Delta_d \). The sides of the mesh-cell volume \( vol_{i,j,k} \) that the source-connection flow expands or contracts into may not be physical-structure surfaces that limit the flow area as in a 1D component pipe. Again the user needs to be aware of this when defining
mesh-cell interface planes and source connections to 3D mesh cells. The effect that the resulting
incorrect flow-area ratios has on evaluating a Bernoulli-equation solution needs to be recognized.
These area ratios also affect the irreversible flow loss coefficients that can by user request be
evaluated by TRACE at the 1D to 3D junction.

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This chapter describes the solution methods employed by TRACE for evaluating the fluid equations. First, the overall solution strategy and general solution steps are outlined for the two numerical methods approximating the flow equations (semi-implicit and SETS). Next, we describe the basic solution strategy, as illustrated by a simple 1D problem, and extensions to the solution strategy required for 3D flows, respectively. A summary is provided of the Newton iteration used to solve the system of non-linear equations required by both numerical methods, as well as the solution of the sparse system of linear equations produced during each iteration of the nonlinear solution and all stabilizer steps of the SETS method. One section, in particular, is devoted to a description of the special capacitance matrix solution applied to any 3D blocks of a system matrix. Finally, we describe the treatment of a special numerical situation called water packing.

Nomenclature

Before presenting the solution methods, we need to define certain terminology. In our nomenclature, the term "gas" implies a general mixture of water vapor and the noncondensable gas. The subscript $g$ will denote a property or parameter applying to the gas mixture; the subscript $v$ indicates a quantity applying specifically to water vapor (referred to as simply "vapor"); and the subscript $a$ (for "air") signifies a noncondensable-gas quantity. The term "liquid" implies pure liquid water, and the subscript $l$ denotes a quantity applying specifically to liquid water. For convenience, we define the following terms that will be used in the subsequent equations and list them alphabetically, with the Greek symbols and subscripts to follow. The reader may note in various places that dummy variables are used. Although the dummy variables are not listed in the following nomenclature, their significance becomes obvious to the reader by reading the text. A caret (\^{\prime}) above a variable denotes an explicit predictor value. A tilde (\tilde{\cdot}) above a variable denotes an intermediate result. A double line underneath a symbol refers to a matrix, whereas a single line underneath means a vector (1D array).

\begin{align*}
a, b, c &= \text{non-zero matrix/vector elements} \\
{\underline{A}} &= \text{a known matrix}
\end{align*}
\text{Solution Methods}

\[ B = \text{banded portion of matrix } A \text{ in capacitance matrix method} \]
\[ b = \text{a known vector} \]
\[ e = \text{internal energy} \]
\[ E = \text{element of matrix product in capacitance matrix method} \]
\[ I = \text{intermediate result in capacitance matrix method} \]
\[ K = \text{form-loss coefficient or wall friction coefficient} \]
\[ M = \text{number of rows in matrix } A \text{ having non-zero elements outside the tridiagonal bandwidth} \]
\[ N = \text{total number of rows and columns in matrix } A \]
\[ P = \text{fluid pressure or total pressure} \]
\[ R = \text{element of matrix product in capacitance matrix method} \]
\[ r, s, t, x = \text{non-zero elements of the } A \text{ matrix in capacitance matrix method} \]
\[ t = \text{time} \]
\[ T = \text{temperature} \]
\[ V = \text{magnitude of the velocity} \]
\[ x = \text{distance} \]
\[ z = \text{unknown vector to be solved (density, velocity, energy, pressure) in capacitance matrix method} \]

\text{Greek}

\[ \alpha = \text{gas volume fraction} \]
\[ \beta = \text{momentum-convection temporal expansion flags} \]
\[ \rho = \text{density} \]
\[ \Delta P = \text{pressure difference} \]
\[ \Delta t = \text{time-step size} \]
\[ \Delta V = \text{velocity change} \]
\[ \Delta x = \text{cell length for 1D components} \]
\[ \delta P = \text{linear Taylor series expansion term for pressure} \]
\[ \delta T = \text{linear Taylor series expansion term for temperature} \]
\[ \delta \alpha = \text{linear Taylor series expansion term for void fraction} \]

\text{Subscripts}

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\[ a = \text{noncondensable gas} \]
\[ g = \text{gas mixture} \]
\[ j + 1 = \text{downstream cell-center index} \]
\[ j + 1/2 = \text{downstream cell-edge index} \]
\[ j - 1 = \text{upstream cell-center index} \]
\[ j - 1/2 = \text{upstream cell-edge index} \]
\[ l = \text{liquid} \]
\[ r = \text{radial} \]

**Superscripts**

\[ i, i + 1 = \text{denotes an iteration level} \]
\[ n = \text{current-time quantity} \]
\[ n + 1 = \text{new-time quantity} \]
\[ ' = \text{last estimate} \]

**Overall Solution Strategy**

Solving the equations should be viewed from two perspectives. In the broadest view, we are solving an approximation to the partial differential equations modeling two-phase flow. In this context, time and spatial location are independent variables, and physical properties (pressure, temperature, etc.) are dependent variables of the system. Initial and boundary conditions are available, and the solution is integrated forward in time over the spatial domain of the problem. The size of the next step forward in time is selected based on a complex time step selection algorithm.

The second perspective on the solution ignores the original partial differential equations. Within a given time step, one or more systems of algebraic equations must be solved to obtain the state of the system at the end of the time step. In this context, time and spatial location are not independent variables. They are just contributions to constants within the algebraic equations. The independent variables for the algebraic equations are end-of-time-step state variables (e.g., velocity, temperature, pressure, and void fraction). This chapter has been written from this perspective, dealing with the solution of the algebraic equations defined in Chapter 1, *Basic Finite-Volume Approximations to the Flow Equations*.

Details of the solution within a given step in time are broken into three stages - a pre-pass, outer iteration (also sometimes called the semi-implicit step), and post-pass. The complexity of each stage is a function of the specific solution methodology being employed (i.e. semi-implicit or
SETS). When using the semi-implicit approximation to the flow equations, each stage represents a rather straightforward set of steps in the solution of the difference equations. First, all quantities dependent only on the state at the beginning of the time step are evaluated. This includes heat-transfer and friction coefficients and physical properties such as viscosity and conductivity. Next, the algebraic difference equations are solved. Finally, the end-of-step values are generated for various other variables needed for edits or to start the next time step.

For the SETS method, the situation is somewhat more complicated. The outer iteration step involves equations basically identical to those of the semi-implicit method and is accomplished by the same coding. However, this semi-implicit step is preceded by a solution of motion equations for “stabilizer” velocities (calculated during the pre-pass). In addition, stabilizer mass and energy equations are solved after the semi-implicit step, during the post-pass. As a result, SETS involves the solution of flow equations at all three stages of a time step.

Each equation solution follows a similar flow within the program. First, a loop is made over all system components to evaluate terms in the equation and store these terms in a system-wide database. Next, the full system of equations is solved. Finally, another loop over all components copies the values of the independent variables from the system-wide database into the component data structure and, when necessary, evaluates dependent variables.

**Basic Solution Methodology**

Almost all aspects of the equation solution procedure can be illustrated using the 1D single-phase-flow model introduced in Chapter 1, *Basic Finite-Volume Approximations to the Flow Equations*. For added clarity, examples will be presented based on some specific flow-path configurations. The solution of equations in the pure semi-implicit method is identical to the solution of the semi-implicit (or “basic”) step in SETS. As a result, no specific discussion is provided for solution when the semi-implicit method is selected (namelist variable NOSETS=1).

To illustrate the 1D portion of the solution, we will describe a specific example for flow in a closed loop, as shown in Figure 2-1. Cells and cell faces in Figure 2-1 have been given absolute numbers to facilitate discussion of full system-equation coupling. In terms of component numbering, cells 1–4 in this figure are considered to be cells 1–4 of PIPE 1, and cells 5–8 in the figure are considered to be cells 1–4 of PIPE 2.

**Solution of the 1D Stabilizer Motion Equations**

The stabilizer motion equations are purely linear in the unknown stabilizer velocities. If the tilde and superscript are dropped for simplicity, the general form for this linear system for the flow loop in Figure 2-1 is
One standard linear algebra trick to solve this problem is to break it into blocks that can be more easily solved. One obvious approach would be to isolate the last row and column of the matrix as follows:
This can then be written more clearly as the following problem:

\[
\begin{pmatrix}
  a_{1,1} & a_{1,2} & 0 & 0 & 0 & 0 & 0 & a_{1,8} \\
  a_{2,1} & a_{2,2} & a_{2,3} & 0 & 0 & 0 & 0 \\
  0 & a_{3,2} & a_{3,3} & a_{3,4} & 0 & 0 & 0 \\
  0 & 0 & a_{4,3} & a_{4,4} & a_{4,5} & 0 & 0 \\
  0 & 0 & 0 & a_{5,4} & a_{5,5} & a_{5,6} & 0 \\
  0 & 0 & 0 & 0 & a_{6,5} & a_{6,6} & a_{6,7} \\
  0 & 0 & 0 & 0 & 0 & a_{7,6} & a_{7,7} \end{pmatrix}
\begin{pmatrix}
  V_1 \\
  V_2 \\
  V_3 \\
  V_4 \\
  V_5 \\
  V_6 \\
  V_7 \
\end{pmatrix}
= \begin{pmatrix}
  b_1 \\
  b_2 \\
  b_3 \\
  b_4 \\
  b_5 \\
  b_6 \\
  b_7 \\
\end{pmatrix} \quad (2-2)
\]

and

\[
a_{8,1} V_1 + a_{8,7} V_7 + a_{8,8} V_8 = b_8 \quad (2-3)
\]

Equation (2-3) is solved to obtain velocities \( V_1 \) through \( V_7 \) as linear functions of \( V_8 \). The existence of two constant vectors on the right-hand side of the equation means that two solutions of a \( 7 \times 7 \) system are required. However, use of an L-U (lower-upper) decomposition method substantially reduces the cost of the second solution. Once these solutions are available, the specific linear expressions for \( V_1 \) and \( V_7 \) as functions of \( V_8 \) are substituted into Eq. (2-4) and a value for \( V_8 \) is obtained. Back-substitution of this value into the equations for the other velocities completes the solution.
TRACE is not quite as selective as the previous example in isolating submatrices for solution. When the basic matrix structure is established, all rows are scanned for the presence of those coefficients not on the main (tridiagonal) band. These rows are designated as “network equations” and variables with the same index as “network variables.”

\[
\begin{pmatrix}
  a_{1,1} & a_{1,2} & 0 & 0 & 0 & 0 & 0 & a_{1,8} \\
  a_{2,1} & a_{2,2} & a_{2,3} & 0 & 0 & 0 & 0 & 0 \\
  0 & a_{3,2} & a_{3,3} & a_{3,4} & 0 & 0 & 0 & 0 \\
  0 & 0 & a_{4,3} & a_{4,4} & a_{4,5} & 0 & 0 & 0 \\
  0 & 0 & 0 & a_{5,4} & a_{5,5} & a_{5,6} & 0 & 0 \\
  0 & 0 & 0 & 0 & a_{6,5} & a_{6,6} & a_{6,7} & 0 \\
  0 & 0 & 0 & 0 & 0 & a_{7,6} & a_{7,7} & a_{7,8} \\
  a_{8,1} & 0 & 0 & 0 & 0 & 0 & a_{8,7} & a_{8,8}
\end{pmatrix}
\begin{pmatrix}
  V_1 \\
  V_2 \\
  V_3 \\
  V_4 \\
  V_5 \\
  V_6 \\
  V_7 \\
  V_8
\end{pmatrix}
= \begin{pmatrix}
  b_1 \\
  b_2 \\
  b_3 \\
  b_4 \\
  b_5 \\
  b_6 \\
  b_7 \\
  b_8
\end{pmatrix}.
\]  

(2-5)

Solving Eq. (2-5) is analogous to the steps outlined for Eq. (2-3). In this instance, the central tridiagonal matrix block is reduced to provide velocities \(V_2\) through \(V_7\) as linear functions of \(V_1\) and \(V_8\) (e.g., \(V_j = V_{0,j} + c_{j,1} V_1 + c_{j,8} V_8\)). The resulting equations are substituted into the two isolated rows of Eq. (2-5) to obtain the following pair of network equations involving only \(V_1\) and \(V_8\):

\[
(a_{1,1} + a_{1,2} c_{2,1}) V_1 + (a_{1,2} a_{2,8} + a_{1,8}) V_8 = b_1 - a_{1,2} V_{0,2},
\]  

(2-6)

and

\[
(a_{8,1} + a_{8,7} c_{7,1}) V_1 + (a_{8,7} a_{7,8} + a_{8,8}) V_8 = b_8 - a_{8,7} V_{0,7}.
\]  

(2-7)

This closed system is solved for \(V_1\) and \(V_8\). Back-substitution of these values into the equations for \(V_2\) through \(V_7\) completes the solution of the system.

**Solving the SETS Semi-Implicit Step**

After the stabilizer motion equations are solved, the version of SETS implemented in TRACE proceeds to solve the semi-implicit (or “basic”) equations for motion, mass, and energy. Apart
from the use of stabilizer velocities in the momentum-transport term (and the special flux operator for two-phase flow), these equations are equivalent to the standard semi-implicit method used in old versions of the TRAC series of codes before the SETS methodology was developed. Thus, solving the pure semi-implicit method and solving the semi-implicit step in SETS are identical.

The system solution begins by treating the new-time velocity as a dependent variable, reducing the motion equation at each cell edge to obtain the new-time velocity as a linear function of the pressure difference across that edge. In our single-phase example, Eq. (1-131) is rearranged to the form

\[
\frac{V^{n+1}_{j+1/2} - \Delta t}{V^n_{j+1/2} - \Delta t} \left( \nabla V^n_{j+1/2} - \beta V^n_{j+1/2} \nabla \bar{V}^n_{j+1/2} + \frac{P^n_{j+1} - \bar{P}^{n+1}_{j+1}}{\langle \rho \rangle^n_{j+1/2} \Delta x} \right)
\]

\[
= \frac{1 + \Delta t(2 K^n_{j+1/2} \left| V^n_{j+1/2} \right| + \beta \nabla \bar{V}^n_{j+1/2})}{\Delta x}
\]

\[(2-8)\]

For the two-phase equations, the equivalent step requires simultaneous solution of the liquid and gas momentum equations at each face (\(2 \times 2\) linear system). At the same time, the following key variable is defined and stored for later use in updating velocities as

\[
\left. \frac{dV}{dP} \right|_{j+1/2} = \frac{\Delta t}{\langle \rho \rangle^n_{j+1/2} \Delta x \left[ 1 + \Delta t(2 K^n_{j+1/2} \left| V^n_{j+1/2} \right| + \beta \nabla \bar{V}^n_{j+1/2}) \right]}
\]

\[(2-9)\]

The mass and energy equations are nonlinear in the independent variables and must be solved with an iterative technique. Here a standard Newton iteration is applied. If the \(i\)th approximation to the solution is given, the next level of approximation is written as

\[
\tilde{T}^{n+1, i+1}_{j} = \tilde{T}^{n+1, i}_{j} + \delta T_{j}
\]

\[(2-10)\]

and

\[
\tilde{P}^{n+1, i+1}_{j} = \tilde{P}^{n+1, i}_{j} + \delta P_{j}
\]

\[(2-11)\]

The pressure definition can be substituted into Eq. (2-8) and simplified with the definition in Eq. (2-9) to give the following expression for the latest approximation to velocity as a linear function of the latest pressure changes:
\[ V_{j+1/2}^{n+1,i+1} = V_{j+1/2}^{n+1,i} + \left. \frac{dV}{dP} \right|_{j+1/2} (\delta P_j - \delta P_{j+1}) \quad (2-12) \]

These expressions are applied to the semi-implicit mass and energy equations [see Chapter 1 Eqs. (1-120) and (1-121)] through the direct substitutions

\[ \tilde{P}_j^{n+1} \Rightarrow \tilde{P}_j^{n+1,i} + \delta P_j, \quad (2-13) \]

\[ \tilde{T}_j^{n+1} \Rightarrow \tilde{T}_j^{n+1,i} + \delta T_j, \quad \text{and} \]

\[ V_{j+1/2}^{n+1} \Rightarrow V_{j+1/2}^{n+1,i} + \left. \frac{dV}{dP} \right|_{j+1/2} (\delta P_j - \delta P_{j+1}) \quad (2-15) \]

Use of the state relationships \([\rho(P, T)]\) and \([e(P, T)]\) and a first-order Taylor series expansion produces the linearized mass equation

\[
\frac{\partial \rho}{\partial T_j} \delta T_j + \frac{\partial \rho}{\partial P_j} \delta P_j \left( \right) \Delta t
\]

\[
\Delta x
\]

\[ = -\frac{n+1,i}{\Delta t} \rho_j \left( \rho V^{n+1,i} \right) - \frac{\partial}{\partial x_j} \left( \rho V^{n+1,i} \right) \]

and the linearized energy equation

\[
\left( \frac{\partial \rho}{\partial T_j} \right)^{n+1,i} \delta T_j + \frac{\partial e}{\partial T_j} \left( \right) \Delta t
\]

\[
\Delta t
\]

\[
\left( \frac{\partial \rho}{\partial P_j} \right)^{n+1,i} \delta P_j + \frac{\partial e}{\partial P_j} \left( \right) \Delta t
\]
Solution Methods

\[ \frac{dV}{dP} \left( \frac{\delta P - \delta P_{j+1}}{\Delta x} \right) - \left( \rho e \right)_{n, j+1/2} \frac{dV}{dP} \left( \frac{\delta P_{j+1} - \delta P_{j}}{\Delta x} \right) + P_{j+1, i} \frac{dV}{dP} \left( \frac{\delta P_{j+1} - \delta P_{j}}{\Delta x} \right) \]

\[ = \left( \rho e \right)_{n, j+1/2} \frac{dV}{dP} \left( \frac{\delta P_{j+1} - \delta P_{j}}{\Delta x} \right) \]

For the particular block-reduction technique used to solve this system of linear equations, an auxiliary variable is defined as

\[ \Delta P_{j+1/2} = \delta P_{j+1} - \delta P_j. \]  

(2-18)

This results in a set of linear equations for each cell in the form

\[
\begin{bmatrix}
\frac{a_{j+1, 1}}{a_{j+1, 2}} \frac{a_{j, 1, 2}}{a_{j, 2, 1}}
\end{bmatrix}
\begin{bmatrix}
\delta P_j \\
\delta T_j
\end{bmatrix}
= \begin{bmatrix}
b_{j, 1} \\
b_{j, 2}
\end{bmatrix}
- \begin{bmatrix}
c_{1j, 1} \\
c_{1j, 2}
\end{bmatrix}
\Delta P_{j-1/2}
+ \begin{bmatrix}
c_{rj, 1} \\
c_{rj, 2}
\end{bmatrix}
\Delta P_{j+1/2}.
\]

(2-19)

The first row in the above linear system can be considered to be the linearized mass conservation equation and the second to be the linearized energy equation. At each cell, this system is solved for the pressure and temperature variations in the form

\[
\begin{bmatrix}
\delta P_j \\
\delta T_j
\end{bmatrix}
= \begin{bmatrix}
b'_{j, 1} \\
b'_{j, 2}
\end{bmatrix}
- \begin{bmatrix}
c'_{1j, 1} \\
c'_{1j, 2}
\end{bmatrix}
\Delta P_{j-1/2}
+ \begin{bmatrix}
c'_{rj, 1} \\
c'_{rj, 2}
\end{bmatrix}
\Delta P_{j+1/2}.
\]

(2-20)

At this point, the \(b'\) constants represent the linearized predictions of change in pressure and temperature assuming no further velocity changes at the cell faces. The \(c'\) coefficients account for contributions due to velocity changes (driven by changes in the pressure gradient).

The solution of the basic equations is completed in two steps. First, for each block represented by Eq. (2-20), the pressure equation is isolated and Eq. (2-18) is substituted to provide a set of 10 equations in the form
This results in a system with the same form as the stabilizer velocity equations,

\[
- c_{1j1} \delta P_{j-1} + (1 + c_{1j1} + c_{rj1}) \delta P_j - c_{rj1} \delta P_{j+1} = b_j .
\]  

(2-21)

which is solved with the same procedure outlined for Eq. (2-5). The resulting values of \( \delta P \)s are first substituted into Eq. (2-18) to obtain a set of \( \Delta P \) values, which are then substituted into the second row of Eq. (2-20) to provide values for temperature changes. The variations in pressure and temperature are substituted into Eq. (2-11) to provide an improved approximation to the new-time variables. The \( \Delta P \) values are also fed to Eq. (2-12) to obtain new-time velocities, which are consistent with the updated pressure field. If variations in pressure and temperature are small enough, the iteration is terminated. If not, the linearized equations are evaluated again to generate the next approximate solution.

The iteration usually is started by setting the initial guess at the solution to the beginning of time-step values (e.g., \( P_j^{n+1,0} = P_j^n \)). The only exceptions occur in the full two-phase equations. When the old-time void fraction is zero but a prediction-based flux and phase change indicates appearance of gas, an explicit evaluation of the gas mass equation is used to provide an initial estimate of the new-time void fraction. When the first appearance of noncondensable gas is predicted, information from an explicit noncondensable mass equation is added to provide an estimate of the new-time partial pressure of noncondensable gas.

Use of old-time quantities to start the iteration provides an easy cure to situations in which the initial guess is beyond the convergence radius of the method. The new-time values must approach the old-time values as the time-step size approaches zero. If an iteration fails to converge, the time-step size is reduced and the solution is retried at the new-time-step size. Preemptive action is also taken to minimize convergence problems. If more than five iterations...
are required to converge the solution on a given time step, the size of the next step is reduced by the ratio of five divided by the last iteration count.

**Solution of the SETS Stabilizer Mass and Energy Equations**

The final step in the SETS method is the solution of the stabilizer mass and energy equations. At this point, the new-time velocities have been determined and can be treated as constants in the solution of the equations. The equations vary from the mass and energy equations of the semi-implicit step only in that the densities and energies in flux terms are now evaluated at the new time.

The mass and energy equations are linear in $\rho^{n+1}$ and $(\rho e)^{n+1}$ respectively, with a structure that is basically tridiagonal. For the loop flow problem, the general form of the mass equation can be written as

$$
\begin{pmatrix}
  a_{1,1} & a_{1,2} & 0 & 0 & 0 & 0 & 0 & 0 \\
  a_{2,1} & a_{2,2} & a_{2,3} & 0 & 0 & 0 & 0 & 0 \\
  0 & a_{3,2} & a_{3,3} & a_{3,4} & 0 & 0 & 0 & 0 \\
  0 & 0 & a_{4,3} & a_{4,4} & a_{4,5} & 0 & 0 & 0 \\
  0 & 0 & 0 & a_{5,4} & a_{5,5} & a_{5,6} & 0 & 0 \\
  0 & 0 & 0 & 0 & a_{6,5} & a_{6,6} & a_{6,7} & 0 \\
  0 & 0 & 0 & 0 & 0 & a_{7,6} & a_{7,7} & a_{7,8} \\
  0 & 0 & 0 & 0 & 0 & 0 & a_{8,7} & a_{8,8}
\end{pmatrix}
\begin{pmatrix}
  \rho_1 \\
  \rho_2 \\
  \rho_3 \\
  \rho_4 \\
  \rho_5 \\
  \rho_6 \\
  \rho_7 \\
  \rho_8
\end{pmatrix}
=
\begin{pmatrix}
  b_1 \\
  b_2 \\
  b_3 \\
  b_4 \\
  b_5 \\
  b_6 \\
  b_7 \\
  b_8
\end{pmatrix},
$$

(2-23)

where superscripts representing new time $(n+1)$ have been dropped. This can be recognized as identical in form to Eq. (2-5) and is solved with the same procedure.

The linear system produced by the stabilizer energy equation has the same coefficient matrix as that of the mass equation. Time is saved by storing matrix factorization steps used in the mass equation solution and by applying the results during the solution of the energy equation.

**Final Solution for a New-Time Void Fraction**

Solving the stabilizer mass and energy equations provides new-time values only for macroscopic densities $[\alpha \rho_g, \alpha \rho_a, (1-\alpha)\rho_l]$ and macroscopic energy densities $[\alpha \rho_ge_g, (1-\alpha)\rho_le_l]$. 
Experience with the method has shown that when end-of-time-step values are needed in correlations for variables such as temperature or pressure, the values obtained during the solution of the semi-implicit step are adequate. However, the method is more robust if an attempt is made to obtain a better value of the new-time void fraction.

After the stabilizer solution is completed, an approximate solution is obtained in each computational volume to the following equations:

\[ \alpha_{j}^{n+1} \rho_{g,j}^{n+1} = (\alpha \rho_{g})_{j}^{n+1}, \]  \hspace{1cm} (2-24)

\[ \alpha_{j}^{n+1} \rho_{a,j}^{n+1} = (\alpha \rho_{a})_{j}^{n+1}, \]  \hspace{1cm} (2-25)

\[ (1-\alpha_{j}^{n+1}) \rho_{l,j}^{n+1} = [(1-\alpha) \rho_{l}]_{j}^{n+1}, \]  \hspace{1cm} (2-26)

\[ \alpha_{j}^{n+1} \rho_{g,j}^{n+1} e_{g,j}^{n+1} = (\alpha \rho_{g} e_{g})_{j}^{n+1}, \text{ and} \]  \hspace{1cm} (2-27)

\[ (1-\alpha_{j}^{n+1}) \rho_{l,j}^{n+1} e_{l,j}^{n+1} = [(1-\alpha) \rho_{l} e_{l}]_{j}^{n+1}. \]  \hspace{1cm} (2-28)

where the right-hand sides are the known results from the stabilizer equations. These equations are linearized with respect to the independent variables \( P_{g}^{n+1}, T_{g}^{n+1}, T_{l}^{n+1}, P_{a}^{n+1}, \) and \( \alpha^{n+1}. \) The starting point of the linearization is taken to be the values of the corresponding variables obtained after the last iteration of the solution to the semi-implicit step. Thus, the values of the independent variables become

\[ T_{g,j}^{n+1} = \tilde{T}_{g,j}^{n+1} + \delta T_{g,j}, \]  \hspace{1cm} (2-29)

\[ T_{l,j}^{n+1} = \tilde{T}_{l,j}^{n+1} + \delta T_{l,j}, \]  \hspace{1cm} (2-30)

\[ P_{j}^{n+1} = \tilde{P}_{j}^{n+1} + \delta P_{j}, \]  \hspace{1cm} (2-31)

\[ P_{a,j}^{n+1} = \tilde{P}_{a,j}^{n+1} + \delta P_{a,j}, \text{ and} \]  \hspace{1cm} (2-32)

\[ \alpha_{j}^{n+1} = \alpha_{j}^{n+1} + \delta \alpha_{j}. \]  \hspace{1cm} (2-33)
These are substituted into Eq. (2-26), and a first-order Taylor expansion is applied. As an example of the results, the linearized macroscopic gas energy density is

\[
\begin{align*}
&\left(\alpha_j + n + 1 \frac{\delta \rho_g}{\delta T} \right) n + 1 e_{g, j} + \alpha_j \rho_{g, j} \frac{\delta e_g}{\delta T} \right) \delta T_j \\
&+ \left(\alpha_j + n + 1 \frac{\delta \rho_g}{\delta P} \right) n + 1 e_{g, j} + \alpha_j \rho_{g, j} \frac{\delta e_g}{\delta P} \right) \delta P_j \\
&+ \rho_{g, j} e_{g, j} \delta \alpha_j = \left(\alpha \rho_g e_g\right) n + 1 - n - 1 - n + 1 \rho_{g, j} e_{g, j}
\end{align*}
\]

This equation, combined with the other four linearized equations, produces a $5 \times 5$ linear system that is solved by direct Gauss elimination. Although linearized approximations to all new-time variables are available after this solution, only the void fraction is kept for use in the next time step. The other variables are discarded as a result of numerical experiments comparing various approaches. The consistent pressure field resulting from the solution of the semi-implicit step provides the best initial guess for velocities at the next time step. The tendency of temperatures in two-phase problems to follow the saturation temperature makes selection of temperatures consistent with that pressure field a good strategy for the most robust code behavior.

**Considerations for 3D Solutions**

When VESSEL components are present, the above procedure is followed, with one key exception in each set of equations. When any VESSEL variable (velocity, $\delta P$, $\delta T$, or $\rho e$) occurs in a 1D equation, it is moved to the right-hand side with its coefficient and all 1D variables are solved as functions of the unknown VESSEL variables. These results are substituted as needed into the difference equations for the VESSEL to give a closed set of equations that can be solved for all vessel variables. Values for VESSEL variables are back-substituted into the 1D equations, and final values for all 1D unknowns are obtained.

Specific examples of this process are provided here for the system illustrated in Figure 2-2. As in Figure 2-1, cells are given “absolute” numbers rather than a combination of component number and component cell number. For this example, cells numbered 1–5 are in a pipe and cells 6–9 are in a 3D (collapsed to 2D here) VESSEL.

The full system of stabilizer momentum equations for the flow loop in Figure 2-2 is represented by Eq. (2-35). The last block in the coefficient matrix is associated with the radial velocities $V_0$ and $V_{10}$ and is completely isolated from equations for the axial velocities in the same “3D” region. This reflects the fundamental structure of the 3D stabilizer momentum equations. For example, the axial stabilizer momentum equations evaluate contributions from axial velocities only implicitly. Radial and azimuthal velocities appearing in momentum-transport terms are
evaluated explicitly. This results in no coupling coefficients between velocity variables in the axial momentum block and those in the radial (or azimuthal) blocks. In matrix notation, we have

\[
\begin{pmatrix}
  a_{1,1} & a_{1,2} & 0 & 0 & 0 & 0 & 0 & a_{1,8} & 0 & 0 \\
  a_{2,1} & a_{2,2} & a_{2,3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & a_{3,2} & a_{3,3} & a_{3,4} & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & a_{4,3} & a_{4,4} & a_{4,5} & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & 0 & a_{5,4} & a_{5,5} & a_{5,6} & 0 & 0 & 0 & 0 \\
  0 & 0 & 0 & a_{6,5} & a_{6,6} & a_{6,7} & 0 & 0 & 0 & 0 \\
  a_{7,1} & 0 & 0 & 0 & 0 & a_{7,6} & a_{7,7} & a_{7,8} & 0 & 0 \\
  0 & 0 & 0 & 0 & 0 & a_{8,7} & a_{8,8} & a_{8,9} & 0 & 0 \\
  0 & 0 & 0 & 0 & 0 & 0 & a_{9,7} & a_{9,8} & a_{9,9} & 0 \\
  0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{10,7} & a_{10,8} & a_{10,9} \\
  0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{10,9} & a_{10,10}
\end{pmatrix}
\begin{pmatrix}
  V_1 \\
  V_2 \\
  V_3 \\
  V_4 \\
  V_5 \\
  V_6 \\
  V_7 \\
  V_8 \\
  V_9 \\
  V_{10}
\end{pmatrix}
= \begin{pmatrix}
  b_1 \\
  b_2 \\
  b_3 \\
  b_4 \\
  b_5 \\
  b_6 \\
  b_7 \\
  b_8 \\
  b_9 \\
  b_{10}
\end{pmatrix}. \quad (2-35)
\]

Solving the 1D portion of this system proceeds as before, isolating the 1D block as
This is solved to obtain the equation

\[
\begin{bmatrix}
a_{2,2} & a_{2,3} & 0 & 0 \\
a_{3,2} & a_{3,3} & a_{3,4} & 0 \\
0 & a_{4,3} & a_{4,4} & a_{4,5} \\
0 & 0 & a_{5,4} & a_{5,5}
\end{bmatrix}
\begin{bmatrix}
V_2 \\
V_3 \\
V_4 \\
V_5
\end{bmatrix}
= \begin{bmatrix}
b_2 \\
b_3 \\
b_4 \\
b_5
\end{bmatrix}
- \begin{bmatrix}
a_{2,1} \\
a_{3,1} \\
a_{4,1} \\
a_{5,1}
\end{bmatrix}
\begin{bmatrix}
0 \\
0 \\
0 \\
a_{5,6}
\end{bmatrix}

V_6.
\tag{2-36}
\]

and these results are substituted into the junction equations to obtain

\[
\begin{bmatrix}
V_2 \\
V_3 \\
V_4 \\
V_5
\end{bmatrix}
= \begin{bmatrix}
b_2' \\
b_3' \\
b_4' \\
b_5'
\end{bmatrix}
+ \begin{bmatrix}
c_2',1 \\
c_3',1 \\
c_4',1 \\
c_5',1
\end{bmatrix}
V_1
+ \begin{bmatrix}
c_2',6 \\
c_3',6 \\
c_4',6 \\
c_5',6
\end{bmatrix}
V_6,
\tag{2-37}
\]

Solving the previous two equations gives junction velocities as a linear combination of “3D” velocities as

\[
\begin{bmatrix}
V_1 \\
V_6
\end{bmatrix}
= \begin{bmatrix}
b_1' \\
b_6'
\end{bmatrix}
+ \begin{bmatrix}
c_1',7 \\
c_6',7
\end{bmatrix}
V_7
+ \begin{bmatrix}
c_1',8 \\
c_6',8
\end{bmatrix}
V_8.
\tag{2-40}
\]

These two expressions are substituted into the 3D axial flow equations to obtain a final closed set of equations for the 3D axial velocities (\(V_7\) and \(V_8\)). The current method used to solve this final equation block is described in the next subsection. Once the 3D velocities are known, the 1D network junction velocities (\(V_1\) and \(V_6\)) follow by back-substitution of vessel velocities \(V_7\) and \(V_8\) into Eq. (2-40), and the internal component velocities are obtained in a final stage of the back-substitution of \(V_1\) and \(V_6\) into Eq. (2-37).

A similar solution pattern follows for the pressure equation of the semi-implicit (basic) step and for the stabilizer mass and energy equations.
The Capacitance Matrix Method

The capacitance matrix method is applied in TRACE to provide an efficient numerical solution algorithm for solving the multidimensional vessel-matrix equations. Each vessel-matrix equation combines the multidimensional mesh-cell or interface equations of all vessel components in the modeled system. The external or internal connectivity to the VESSEL component(s) of 1D hydro-component loops introduces nonzero elements into the vessel matrix, coupling the vessel mesh cells or interfaces at the loop source connections to the vessel(s). The vessel-matrix equations that are solved are the semi-implicit pressure vessel-matrix equation in the outer-stage solution and the stabilizer motion $x$-, $r$-, $y$-, or $\theta$-, and $z$-direction vessel-matrix equations in the prepass stage of the solution and the stabilizer mass and energy vessel-matrix equations in the postpass stage of the solution.

The capacitance matrix method is a direct L-U matrix-decomposition solution algorithm like the direct full-matrix L-U matrix-decomposition solution algorithm used in TRAC-PF1/MOD1, but it does the L-U matrix decomposition on the banded portion of the vessel matrix with a more efficient banded-matrix solver routine. The banded portion of the vessel matrix includes the nonzero coupling elements between a vessel mesh cell or interface and its six adjacent (neighboring) mesh cells or interfaces in 3D geometry. Nonzero elements outside the bandwidth of the matrix that couple vessel mesh cells or interfaces to nonadjacent mesh cells or interfaces of the same vessel or a different vessel component (due to 1D hydro-component loop connectivity) will be referred to as nonzero outlying elements. The effect that the nonzero outlying elements have on the matrix-equation solution is accounted for in the capacitance matrix method by a direct full-matrix L-U matrix decomposition of a lower-order capacitance matrix. That solution is used to modify the banded-matrix equation solution to give the desired solution of the vessel matrix with its nonzero outlying elements. The capacitance matrix method was found in a study to be more efficient than a direct full-matrix L-U matrix-decomposition solution of a vessel-matrix equation when fewer than 20% of the vessel-matrix rows have nonzero outlying elements. For most system models (especially those with more than a hundred vessel mesh cells), only a few percent of the vessel-matrix rows have nonzero outlying elements. Thus, for a four-loop plant model with eight rows on nonzero outlying elements, the capacitance matrix method is faster than a full-matrix method by factors of 2, 4, 8, and 12 for vessel matrices of order 100, 200, 300, and 400, respectively. Similar factors apply to computer memory storage for the vessel-matrix equation by the full-matrix method versus the capacitance matrix method.

We can summarize the above description of the method by noting that the capacitance matrix method is a direct two-stage procedure. In the first stage, the banded-matrix portion of the matrix equation is solved with an efficient banded-matrix solver to determine the solution for the vessel-matrix equation with zero-valued outlying elements. Then, if there are nonzero outlying elements in the vessel matrix (1D hydro-component loops that connect back to a nonadjacent vessel location generate nonzero outlying elements), the second stage evaluates a direct full-matrix L-U matrix-decomposition solution of a much lower-order capacitance-matrix equation. Doing this accounts for the effect the nonzero outlying elements have on the vessel-matrix equation solution. This results in a modification of the banded-matrix solution to determine the solution of the vessel-matrix equation with nonzero outlying elements.
The following derivation determines the working equations and presents the four-step solution procedure programmed into the code. Given the vessel-matrix equation

\[ A \cdot x = b, \quad (2-41) \]

where \( A \) is a known (vessel) matrix, \( x \) is an unknown (mass density, velocity, energy, or pressure) vector, and \( b \) is a known vector, let us partition \( A \) as follows into the sum of its banded matrix \( B \) and a matrix product \( E \cdot R \) that has only the nonzero elements lying outside the bandwidth:

\[ A \cdot x = (B + E \cdot R) \cdot x = b. \quad (2-42) \]

Consider the following example of how a simple form for \( A \) would appear when partitioned.

For \( A = \begin{bmatrix} x & x & O & O & O & O \\ x & x & x & O & t & O \\ O & x & x & x & O & O \\ O & O & x & x & x & O \\ r & O & s & x & x & x \\ O & O & O & O & x & x \end{bmatrix} \), a matrix of order \( N \), \( (N \times N) \)

where \( r, s, t, \) and \( x \) are nonzero elements, \( N = 6 \) is the total number of rows and columns in \( A \), and \( M = 2 \) is the number of rows in \( A \) having nonzero elements outside the three-diagonal bandwidth, then define

\[ A = B + E \cdot R \quad (2-44) \]

where

\[ B = \begin{bmatrix} x & x & O & O & O & O \\ x & x & x & O & O & O \\ O & x & x & x & O & O \\ O & O & x & x & x & O \\ O & O & O & x & x & x \\ O & O & O & O & x & x \end{bmatrix}, \quad E = \begin{bmatrix} O & O \\ O & 1 \\ O & O \\ O & O \\ 1 & O \\ O & O \end{bmatrix} \]

\( (N \times N) \) \hspace{2cm} (\hspace{1cm} (N \times M) \)
\[ R = \begin{bmatrix} r & O & s & O & O & O \\ O & O & O & t & O \\ O & O & O & O & O \\ O & O & O & O & O \\ r & O & s & O & O \\ O & O & O & O & O \end{bmatrix}, \quad E \cdot R = \begin{bmatrix} O & O & O & O & O \\ O & O & O & t & O \\ O & O & O & O & O \\ O & O & O & O & O \\ r & O & s & O & O \\ O & O & O & O & O \end{bmatrix}. \] (2-45)

\[(M \times N) \quad (N \times N) \] (2-46)

Note that the nonzero elements in \( E \) are unity and in \( R \) are the actual nonzero outlying elements of \( A \). The term \( A \) is an \( N \times N \) matrix with \( M \) rows having nonzero elements outside its bandwidth, \( B \) is an \( N \times N \) banded matrix, \( E \) is an \( N \times M \) matrix, and \( R \) is an \( M \times N \) matrix.

Multiply Eq. (2-42) by the inverse of the banded matrix, \( B \) to get

\[ (I + B^{-1} \cdot E \cdot R) \cdot x = B^{-1} \cdot b. \] (2-47)

Define \( R \cdot x = y \) and move its term in Eq. (2-47) to the right-hand side of the equation, giving

\[ x = B^{-1} \cdot b - B^{-1} \cdot E \cdot y. \] (2-48)

Substitute Eq. (2-48) for \( x \) into Eq. (2-47) to give

\[ (I + B^{-1} \cdot E \cdot R) \cdot (B^{-1} \cdot b - B^{-1} \cdot E \cdot y) = B^{-1} \cdot b. \] (2-49)

Expand Eq. (2-49), delete the \( B^{-1} \cdot b \) term from both sides of the equation, and multiply the equation by \((B^{-1} \cdot E)^{-1}\) giving

\[ (I + R \cdot B^{-1} \cdot E) \cdot y = R \cdot B^{-1} \cdot b. \] (2-50)

Multiply Eq. (2-50) by the inverse of the matrix on its left-hand side to define \( y \) as follows:

\[ y = (I + R \cdot B^{-1} \cdot E)^{-1} \cdot R \cdot B^{-1} \cdot b. \] (2-51)

To determine \( x = A^{-1} \cdot b \), evaluate Eq. (2-51) for \( y \) and substitute \( y \) into Eq. (2-48) to evaluate \( x \).

This evaluation procedure appears lengthy until we observe that it involves the following four steps with some intermediate results used several times.

**Step 1.** Multiply the vector \( b \) and each of the \( M \) columns of \( E \) by the inverse of \( B \).

\[ \hat{x} = B^{-1} \cdot b \quad \text{and} \quad \hat{E} = B^{-1} \cdot E \] (2-52)

\[(N) \quad (N \times N) \quad (N) \quad (N \times M) \quad (N \times N) \quad (N \times M) \]
Step 2. Multiply $\hat{\vec{x}}$ and $\hat{\vec{E}}$ from Step 1 by $R$.

$$\hat{\vec{b}} = R \cdot \hat{\vec{x}} \quad \text{and} \quad \hat{\vec{R}} = R \cdot \hat{\vec{E}}$$

(2-53)

Step 3. Evaluate Eq. (2-51) for $y$ using $\hat{\vec{b}}$ and $\hat{\vec{R}}$ from Step 2.

$$y = (I + \hat{\vec{R}})^{-1} \cdot \hat{\vec{b}}$$

(2-54)

Step 4. Evaluate Eq. (2-48) for the desired solution vector $\vec{x}$ using $\hat{\vec{x}}$ and $\hat{\vec{E}}$ from Step 1 and $y$ from Step 3.

$$\vec{x} = \hat{\vec{x}} - \hat{\vec{E}} \cdot y$$

(2-55)

Computationally, Eq. (2-51) is solved by performing a single banded-matrix L-U matrix decomposition to determine $B^{-1}$. Then $B^{-1}$ is applied to the $1+M$ column vectors of $\vec{b}$ and $\vec{E}$ by a direct forward-elimination and backward-substitution solution procedure. Equation (2-54) requires that a L-U matrix decomposition be applied to the full (nonbanded), but much smaller, capacitance matrix $I^{+}\hat{\vec{R}}$. The method becomes rapidly less efficient as the size of the capacitance matrix $I^{+}\hat{\vec{R}}$ increases. The remainder of the computation involves matrix multiplications that are performed efficiently on a vector computer.

**Water Packing**

The water-packing logic in the code is triggered under certain conditions (but not all conditions) when the code attempts during a time step to overfill (pack) a liquid-full finite-difference mesh cell or to overextract (stretch) liquid from a liquid-full cell. The physical analog to water-packing event is a water hammer; when cold water surges down a dead-end pipe filled with steam, a large pressure spike occurs when the last steam collapses and the water fills the pipe. This spike has a very short duration because of the low compressibility of liquid water.

In any Eulerian finite-difference scheme, the boundary of a mesh cell behaves like the dead end of a pipe in a water hammer event. This is especially true when condensation is present. Consider a
1D mesh cell with pure liquid entering from the left and pure vapor flowing in from the right to condense on the liquid. It is not possible for a standard finite-difference momentum equation to produce a liquid-mass flow out of the right cell face that exactly balances the flow in the left cell face at the instant when the cell fills with liquid. In fact, when strong condensation is present, the momentum equation generally will predict a liquid velocity into the cell on the right face. This circumstance produces a numerical dead end for the liquid. Unlike the water hammer, the final solution is not to halt the flow, but to push the liquid on through the right cell face. As with a hammer, this is accomplished with an abrupt increase in pressure.

In TRACE, we have adopted a method for mitigating water-packing that is similar in spirit to shock-fitting techniques. Logic has been installed that detects pressure excursions caused by water-packing. When they occur, it is clear that the finite-difference momentum equation is producing invalid results. Therefore, we modify the equation at those locations and times to obtain a better solution. A standard motion equation at a cell edge can be written as

\[ V_{j+1/2}^{n+1} = V_{j+1/2}^n + a + b(P_j^{n+1} - P_{j+1}^{n+1}) \]  \quad (2-56)

Additional force terms are incorporated in the term \( a \), and \( b \) includes the time-step size and inverse of mesh length and density. If packing is detected in cell \( j \), the equation is modified to the form

\[ V_{j+1/2}^{n+1} = V_{j+1/2}^n + a + b(cP_j^{n+1} - P_{j+1}^{n+1}) \]  \quad (2-57)

The constant \( c \) multiplying \( P_j^{n+1} \) is taken to be a large number so that only small changes in the pressure of the \( j^{th} \) cell are required to obtain the appropriate velocity for the liquid outflow. To prevent excessively large vapor velocities, the value of the coefficient \( b \) in the vapor equation is set equal to the corresponding coefficient in the liquid equation.

In a given cell of a 1D component, the code does not consider the water-packing logic if the cell void fraction is greater than 0.08, if the liquid in the cell is superheated, or if the net mass flow is out of the cell. Also, the code cannot make adjustments at a cell interface or test across that interface if the associated flow area is less than or equal to \( 10^{-10} \text{ m}^2 \). Further, TRACE does not consider adjacent cells in which the void fraction is less than 0.1. The code predicts the change in the current cell pressure to give a new pressure; if the predicted pressure change is negative, the code transfers to logic to detect stretching. If the pressure rise is greater than or equal to 0, and if this new pressure does not exceed the maximum of its current value and the adjacent-cell pressures by at least 7\%, with a minimum increase of 50 kPa (one-half bar), the water-packing logic terminates. The void-fraction tests ensure that the water-packing logic will not smooth out a true water-hammer-type phenomenon in the calculation, while the pressure checks prevent the logic from being triggered too often. If, through the tests, more than one interface of a given cell permits the water-packing correction, the code applies the correction only at the interface across which the void fraction is higher. The code does not permit the water-packing correction at the
interface opposite a FILL component if the velocities at both interfaces have the same sign or at the interface at which the PUMP-component source is applied. Also, the code terminates the water-packing logic for a given cell interface if choking is detected at that interface and if the interface is either the first or last interface of a component.

The stretching logic is similar, although the code looks for a pressure drop in the current cell that reduces its pressure to less than the minimum of 95% of its current value or 95% of the neighboring cells, with the additional constraint that the projected pressure must be less than the saturation pressure corresponding to the current liquid temperature minus 20.0 K. The final constraint for stretching is that the test pressure cannot be below the lower pressure limit for the equation of state (see Chapter 11). For a stretch event, the code does not make an adjustment at a given interface if the void fraction on the other side of the interface is less than or equal to 0.1, if the liquid velocity at the interface is into the cell in which the stretch is detected, or if the PUMP-component source is applied at the interface.

The 3D VESSEL water-packing detection logic is very similar. The VESSEL, however, permits packing to occur if the current cell void fraction is greater than 0.1, instead of the 0.08 in the 1D components. Also, in detecting a stretch, the code requires the pressure test to be 0.8 of that in the 1D components.
The nuclear reaction that takes place in the reactor core generates energy inside the fuel. In a PWR, that energy is then transferred to the primary fluid and crosses the steam-generator tubes to the secondary fluid. In a BWR, that energy is deposited directly into the primary fluid, causing steam to be generated, and ultimately driving the turbines. The code must calculate the heat conduction in the fuel and the steam-generator tubes to simulate correctly the heat-transfer processes involved in thermal-energy transport. Also, the passive solid structures, such as piping walls, vessel walls, and the internal vessel structures, represent significant metal masses that can store or release large amounts of thermal energy depending upon the reactor coolant temperature. Therefore, the code needs to model these additional structures. This chapter describes the underlying theory employed by TRACE in order to model these phenomena.

**Nomenclature**

The following nomenclature applies to this chapter

- $A$ = area in radial direction
- $A^*$ = area in axial direction
- $\equiv = \text{coefficient matrix}$
- $\cong = \text{nonzero elements of }A$
- $B = \text{equality vector}$
- $\equiv c_p = \text{specific heat}$
- $C, D, E = \text{nonzero submatrices of }A$
- $f_t, f_{ss} = \text{stability flags}$
- HTC = heat transfer coefficient
- $h = \text{convective HTC}$
\[ h_{gap} = \text{gap conductance} \]
\[ k = \text{thermal conductivity} \]
\[ N_R = \text{number of nodes that segment the radial direction} \]
\[ N_Z = \text{number of nodes that segment the axial direction} \]
\[ \bar{q} = \text{heat flux vector} \]
\[ q'' = \text{heat generation rate per unit volume} \]
\[ q_{total} = \text{total heat flux} \]
\[ R = \text{radius} \]
\[ R^+, R^- = \text{variables defined by Eqs. (3-26) and (3-27)} \]
\[ r = \text{radial coordinate} \]
\[ t = \text{time} \]
\[ T = \text{temperature} \]
\[ \bar{T} = \text{temperature vector} \]
\[ V = \text{cell volume} \]
\[ z = \text{axial distance} \]
\[ z_b = \text{bottom of the fuel rod} \]
\[ z_u = \text{top of the fuel rod} \]
\[ \Delta r = \text{radial increment} \]
\[ \Delta t = \text{time increment} \]
\[ \Delta x = \text{slab thickness} \]
\[ \Delta z = \text{axial increment} \]
\[ \rho = \text{density} \]

**Subscripts**

\[ g = \text{gas} \]
\[ I = \text{inner surface} \]
\[ i, j = \text{finite-difference indices} \]
\[ l = \text{liquid} \]
\[ max = \text{maximum} \]
\[ o = \text{outer surface} \]
Superscripts

\( j \) = axial direction

\( n, n + 1 \) = current-time and new-time values

\( p \) = predicted new-time values

\( +, - \) = refers to material to the right and left of the interface, respectively

\( ' \) = new quantities when a fine mesh is added

**Governing Equations**

Because the heat flux in a solid material is a vector quantity, the following general equation describes the heat-conduction process in an arbitrary geometry:

\[
\frac{\partial (\rho c_p T)}{\partial t} + \nabla \cdot \bar{q} = q'' .
\]  

(3-1)

In practice, the product \( \rho c_p \) is assumed to be constant for purposes of taking the time derivative.

The heat flux \( \bar{q} \) can be expressed in terms of the temperature gradient by Fourier’s law of conduction (Ref. 3-1) as follows:

\[
\bar{q} = -k \nabla T .
\]  

(3-2)

Therefore, Eq. (3-1) becomes

\[
\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + q'' .
\]  

(3-3)

The thermal history of the reactor structure is obtained from a solution of the heat-conduction equation applied to different geometries. The next section discusses the coupling of the heat-conduction field equation in any of its many forms to the thermal-hydraulic field equations representing the fluid. Following this discussion, we present the details concerning the various formulations of the heat-conduction equations that represent particular geometries typically found in reactor systems. These geometries include cylindrical walls, slabs, and core fuel rods. The first model analyzes heat conduction within the walls of the 1D loop components, such as pipe walls. The latter two are associated with heat transfer within structural components of the vessel. They are modeled similarly in the code, differing only in the area and volume calculations used in the finite-difference equations.
**Coupling of Thermal Hydraulics with the Reactor Structure**

The energy transported by convective heat transfer from any structure into the different fluid phases is modeled using Newton’s law of cooling to represent the energy exchange rate between the structure and the fluid phase. These terms appear in the energy equations of the different fluid phases. **Chapter 6** discusses the logic used to determine which heat-transfer regime exists between the wall and fluid and which correlations for the wall heat-transfer coefficient (HTC) are used to represent the different regimes. The coupling algorithm (Figure 3-1) is currently implicit in terms of the wall temperature, liquid and vapor phase temperatures and explicit in terms of the heat transfer coefficient. For each new-time step, the wall HTCs \( h \) of a given structure are evaluated using the surface wall temperatures \( T_w \) and the fluid conditions obtained for the last time step. The new-time fluid-dynamics equations are solved using these HTCs, the new-time surface temperatures, and the new-time fluid temperatures where the sum of the total energy transported into the fluid cell can be written as

\[
q_{\text{total}}^{n+1} = h_l^n(T_w^n - T_l^n) + h_g^n(T_w^n - T_g^n) +
\]

\[
\left[h_l^n\left(\frac{\partial T_w}{\partial T_l} - 1\right) + h_g^n\frac{\partial T_w}{\partial T_l}\right](T_l^{n+1} - T_l^n) +
\left[h_g^n\left(\frac{\partial T_w}{\partial T_g} - 1\right) + h_l^n\frac{\partial T_w}{\partial T_g}\right](T_g^{n+1} - T_g^n)
\]

In general the finite volume approximation for the conduction equation (i.e. Eq. (3-3)) can be written as a set of linear equations for the new time heat structure temperatures:

\[
A \cdot T = B
\]

Given a convective heat transfer boundary condition, then the right-hand side vector \( B \) is a function of the liquid and vapor phase temperatures for the fluid cell associated with the HS. Therefore, the derivative of Eq. (3-5) with respect to a change in the liquid phase temperature, yields:

\[
A \cdot \frac{\partial T}{\partial T_l} = \frac{\partial B}{\partial T_l}
\]

and the derivative of Eq. (3-5) with respect to a change in the vapor phase temperature, yields,

\[
A \cdot \frac{\partial T}{\partial T_g} = \frac{\partial B}{\partial T_g}
\]

The solution of Eq. (3-5) gives the predicted wall temperatures, \( T_w^n \) in Eq. (3-4). The solution of Eq. (3-6) gives how the HS temperatures change given a change in the liquid phase temperature and the solution of Eq. (3-7) gives how the HS temperatures change given a change in vapor
The solution of these three equations is the linearization of the conduction equation about the liquid and vapor phase temperatures.

\[ T^{n+1} = T^n + \frac{\partial T}{\partial T_l} (T_l^{n+1} - T_l^n) + \frac{\partial T}{\partial T_g} (T_g^{n+1} - T_g^n). \]  

(3-8)

Notice that the coefficient matrix is not a function of the liquid or vapor phase temperatures, therefore, the difference between Eq. (3-5), Eq. (3-6), and Eq. (3-7) is the change in the right-hand side vector. The forward elimination developed for the solution of Eq. (3-5) is saved and used to obtain the linearization derivatives in Eq. (3-6) and Eq. (3-7). From the linearization of the heat conduction equation, the two derivatives \( \frac{\partial T_w}{\partial T_l} \) and \( \frac{\partial T_w}{\partial T_g} \) are obtained for the radial HS node that is the wall of the HS. These two derivatives of how the HS wall temperature changes given a change in the liquid phase temperature and how the HS wall temperature changes
given a change in the vapor phase temperature together with Eq. (3-4) determines how the wall heat flux changes given a change in the liquid and vapor phase temperatures. This allows the fluid dynamics solution to be consistent with the linearized conduction equation.

Eq. (3-4) and Eq. (3-8) completely describe a single-side heat structure (i.e. a HS with convective heat transfer boundary condition on either the inside or outside surface of the heat structure). For single-sided heat structures Eq. (3-5) through Eq. (3-7) are solved once and the linearization coefficients saved and used to update the HS temperature distribution each outer iteration (see Figure 3-1).

For double-sided heat structures there are additional linearization terms associated with the change in liquid and vapor phase temperatures on the other side of the heat structure. Experimentation with typical double-sided heat structures in a PWR and BWR power plant model indicate that in most cases the derivative of the wall temperature given a change in the fluid temperatures on the other side of the heat structure was small enough that it could be ignored. Therefore, for double-sided HS that derivatives of the phase temperatures on the other side of the heat structure are ignored in Eq. (3-4). However, for double-sided HS’s, Eq. (3-8) is not used to update the HS temperature distributions each outer iteration. For double-sided HS’s, Eq. (3-5) through Eq. (3-7) are solved for both the inner and outer surface. This ensures that for double-sided HSs the temperature distribution is consistent with the conduction equation and not an approximate linearization of the conduction equation.

![Cylindrical wall geometry](image)

Figure 3-2. Cylindrical wall geometry.
Cylindrical Wall Heat Conduction

The temperature distribution within the walls of the 1D components is obtained from a finite-difference approximation to the 1D conduction equation,

$$\rho c_p \frac{\partial T}{\partial t} = r \frac{\partial}{\partial r} \left( r k \frac{\partial T}{\partial r} \right) + q'''. \quad (3-9)$$

The finite-difference equations are derived by applying an integral method (Ref. 3-2) to the elemental volumes shown in Figure 3-2. The general form of the $i^{th}$ volume ($1 < i < N$) is

$$\frac{r_i}{\Delta r_i} \frac{k}{\Delta T_i} = \left\{ \frac{r_i}{\Delta r_i} \frac{k}{\Delta T_i} + \frac{r_{i+1/2}}{\Delta r_i} \frac{k}{\Delta T_i} \right\} T_{i+1}^{n+1}$$

$$\left( r_i \Delta r_i - \frac{\Delta r_{i-1}^2}{4} \right) (\rho c_p)_{i-1/2} + \left( r_i \Delta r_i + \frac{\Delta r_i^2}{4} \right) (\rho c_p)_{i+1/2} \right\} T_i^n$$

$$\left( r_i \Delta r_i + \frac{\Delta r_i^2}{4} \right) \frac{(\rho c_p)_{i+1/2}}{\Delta t} T_i^n + q''' \right\}$$

where

$$f_i^n = f(t^n, r_i) \quad (3-11)$$

This formulation positions nodal points on material interfaces. Material properties are evaluated between nodes. The boundary conditions applied to the inner ($i = 1$) and outer ($i = N$) surfaces are

$$-k \frac{\partial T}{\partial r} \bigg|_{i=1,N} = \pm [h_i (T_i - T_j) + h_g (T_g - T_j)] \quad (3-12)$$

For example, application of this boundary condition to the inner surface ($i = 1$) yields
The resulting linear equations are solved in a sequential fashion in the axial z-direction. For each axial position, a solution is achieved using Gaussian elimination.

A lumped-parameter solution is available to the user if the number of nodes is set equal to one. For this option the wall temperature is obtained from the equation,

\[
T^{n+1} = \frac{1}{2} \left( 2 \Delta r + \frac{\Delta r^2}{R_I} \right) \left( \frac{\rho cp}{\Delta t} (T^n + q^n) + h_i T_i^{n+1} \right) + h_o T_o^{n+1} + \left( 1 + \frac{\Delta r}{R_I} \right) \left[ h_{i,o} T_{i,o}^{n+1} + h_{o,o} T_o^{n+1} \right]
\]

\[
+ \left\{ \frac{1}{2} \left( 2 \Delta r + \frac{\Delta r^2}{R_I} \right) \left( \frac{\rho cp}{\Delta t} (T^n + q^n) + h_i T_i^{n+1} \right) + h_o T_o^{n+1} + \left( 1 + \frac{\Delta r}{R_I} \right) (h_{i,o} + h_{o,o}) \right\}^{-1}
\]

The subscripts \( I \) and \( o \) refer to the inner and outer radii, respectively.

**Slab and Rod Heat Conduction**

Structures that can exchange heat with the fluid in a reactor vessel include downcomer walls and support plates, modeled as slabs, and vessel rods. These elements are referred to as heat-structure components. Both nuclear and electrically heated rods or slabs can be analyzed. The effects of gap conduction, metal-water reaction, and variable material properties are included (these models are documented in Chapter 8).

Only one rod within a cell may have hydro-cell coupling. This “average” rod is coupled to the fluid by Newton’s law of cooling. Any number of additional user-specified rods may be included in each segment. The rod power factors (that is, relative to the average rod located within each segment) are specified by the user for these supplemental rods. The supplemental rods allow the
The user to include hot rods in the reactor vessel. Such rods do not affect the fluid-dynamics calculation because their contributions are already represented by average rods. They are included separately only for the purpose of determining their temperature response.

More than one slab may be located within a cell. Each slab is coupled to the fluid by Newton’s law of cooling.

The user has four numerical calculation options for computing temperature distribution in slabs and rods. For thin slabs or rods of small diameter where the radial temperature profile is flat and axial conduction is negligible, the user may choose the “lumped-parameter” solution. This option gives the best calculational efficiency and should be used whenever it can be justified.

The second option is a 1D solution with implicit differencing in the radial direction and no conduction in the axial direction. This option is appropriate when steep axial profiles do not exist.

The third option is a 2D solution with implicit differencing in the radial direction and explicit differencing in the axial direction. This allows the very small radial node spacing required by the large radial power variations without severely limiting the time step. The explicit differencing in the axial direction does limit the maximum time-step size for axial spacing. In many cases, however, this maximum time-step size is much greater than that used for the fluid-dynamics calculation and is not restrictive. For those cases, the semi-implicit calculation gives good computational efficiency.

The fourth option is the fully implicit, 2D finite-difference calculation. This is the best choice for cases where the axial temperature gradient is very large, such as in the vicinity of a quench front. Then the very fine axial noding that is required would cause the time step to be severely limited if the semi-implicit calculation was used. These methods are discussed in the following sections.

**The Lumped-Parameter Solution.**

The lumped-parameter equation for cylindrical coordinates is Eq. (3-14). If we choose \( f_t = 0 \) and \( f_{ss} = 1 \) for maximum stability, that equation reduces to

\[
T_{n+1}^i = \left\{ \frac{1}{2} \left( 2\Delta r + \frac{\Delta r^2}{R_f} \right) \left( \frac{\rho c_p}{\Delta t} T_n^i + q_n^i \right) + h_{li} T_{n+1}^i + h_{gi} T_{n+1}^i \right. \\
\left. + \left( 1 + \frac{\Delta r}{R_f} \right) \left[ h_{lo} T_{n+1}^o + h_{go} T_{n+1}^o \right] \right\}^{-1}.
\]

\]

(3-15)
For a solid rod, the axial temperatures are

\[ T^{n+1}_i = \frac{\Delta t}{2} \left[ \frac{\rho c_p}{\Delta t} \right] T^n_i + q^n_i + h_1 T^n_{i+1} + h_g T^n_{g1} \left\{ \frac{\Delta r \rho \Delta c_p}{2 \Delta t} + h_1 + h_g \right\}^{-1} \]  

(3-16)

The lumped-parameter equation for the temperature of a slab is

\[ T^{n+1} = \frac{\rho c_p \Delta x}{\Delta t} T^n_i + q^n \Delta x + h_1 T^n_{i+1} + h_g T^n_{g1} + h_1 T^n_{i+1} + h_g T^n_{g1} \]

(3-17)

\[ \frac{\rho c_p \Delta x}{\Delta t} + h_1 + h_g + h_{l1} + h_{g1} \]

where \( \Delta x \) is the slab thickness.

**The Semi-Implicit Calculation.**

Finite-difference equations are obtained by applying an integral method (Ref. 3-3) to appropriate differential volumes. The axial noding within a rod (see Figure 3-3) is typically the same or at a finer axial noding than the fluid component axial noding.

Consider a general differential volume (that is, the volume labeled \( i, j \) in Figure 3-3). Using explicit differencing in the axial direction and implicit differencing in the radial direction, the finite-difference equation for this volume is

\[
\left\{ \rho c_p \right\}_{ij} \left[ T^{n+1}_{ij} - T^n_{ij} \right] = \frac{1}{2} \left[ \left( r_i \Delta r_i + \frac{\Delta r^2_i}{4} \right) + \left( r_i \Delta r_{i-1} - \frac{\Delta r^2_{i-1}}{4} \right) \right] \left[ \frac{\Delta z_j + \Delta z_{j-1}}{2} \right] \]

(3-18)

\[
= \left\{ \begin{array}{c}
\frac{T^{n+1}_{i+1,j} - T^n_{ij}}{\Delta r_i} + r_{i+1/2,j} \frac{k}{\Delta r_i} \left( T^{n+1}_{i+1,j} - T^n_{ij} \right)
+ r_{i-1/2,j} \frac{k}{\Delta r_i} \left( T^{n+1}_{i-1,j} - T^n_{ij} \right)
+ k_{i,j+1/2} \frac{\Delta z_j}{\Delta z_j} \left( T^n_{i,j+1} - T^n_{ij} \right)
+ k_{i,j-1/2} \frac{\Delta z_{j-1}}{\Delta z_{j-1}} \left( T^n_{i,j-1} - T^n_{ij} \right)
+ \frac{1}{2} \left[ \left( r_i \Delta r_i + \frac{\Delta r^2_i}{4} \right) + \left( r_i \Delta r_{i-1} - \frac{\Delta r^2_{i-1}}{4} \right) \right]
\end{array} \right. \]
where \( f_{ij} = f(t^n, r_i, z_j) \). In Figure 3-3, the locations of nodes within the volumes located at the boundaries differ (i.e., boundary nodes are typically located at the volume edge, while interior nodes are located in the middle of the volume. This difference should be considered when values are assigned for the relative power densities at each node.

The boundary conditions normally applied to the fuel rods are

- the top \((z = z_u)\) and bottom \((z = z_b)\) of the rods are assumed to be insulated,

\[
\frac{\partial T}{\partial z} \bigg|_{z = z_b, z_u} = 0; \tag{3-19}
\]

- the rod centerline \((r = 0)\) is a line of symmetry,
\[ \frac{\partial T}{\partial r} \bigg|_{r=0} = 0; \quad (3-20) \]

- heat transfer at the inner and outer gap surfaces \((r = r_{gap}^{-}, \ r_{gap}^{+})\) and at the cladding surface \((r = r_{o})\) is specified using Newton’s law,

\[ k \frac{\partial T}{\partial r} \bigg|_{r=r_{gap}^{\pm}} = -h_{gap}^{\pm}(T_{r_{gap}^{\pm}} - T_{r_{gap}^{\pm}}), \quad (3-21) \]

\[ k \frac{\partial T}{\partial r} \bigg|_{r=r_{o}} = -h_{fluid}(T_{r_{o}} - T_{fluid}), \quad (3-22) \]

where \(h_{gap}^{+} = h_{gap}^{-}(r_{gap}^{-}/r_{gap}^{+})\) to conserve energy.

All properties (that is, \(\rho, \ cp,\) and \(k\)) required by the difference equations are stored at the node locations. Linear interpolation is used to obtain properties between nodes (that is, at cell surfaces). A node located at the interface between two dissimilar materials requires two sets of properties. Application of an integral technique to the differential volume in Figure 3-4 results in the differential equation (after dividing through by the volume),

\[
\left(\rho c_p\right)\text{ij} \left(\frac{T_{ij}^{n+1} - T_{ij}^{n}}{\Delta t}\right) - q_{ij}^{m} = \left\{ \begin{array}{c}
T_{i+1/2,j}^{n+1} \times \frac{k_{i+1/2,j}}{\Delta r_{i}} \left(\frac{r_{i} \Delta r_{i} + \frac{\Delta r_{i}^{2}}{4}}{2}\right) + r_{i-1/2,j}^{n} \frac{k_{i-1/2,j}}{\Delta r_{i}} \times \left(\frac{T_{i-1,j}^{n+1} - T_{ij}^{n+1}}{\Delta r_{i-1}}\right) \right. \\
\left. + \left\{ \begin{array}{c}
\bar{k}_{i,j+1/2} \left(\frac{T_{i,j+1}^{n} - T_{ij}^{n}}{\Delta z_{j}}\right) + \bar{k}_{i,j-1/2} \left(\frac{T_{i,j-1}^{n} - T_{ij}^{n}}{\Delta z_{j-1}}\right) \right) \left(\frac{\Delta z_{j} + \Delta z_{j-1}}{2}\right)^{-1}, \quad (3-23) 
\end{array} \right. 
\end{array} \right.
\]
In the above equations,
\[ R_i^+ \equiv \left( r_i + \frac{\Delta r}{2} \right) \Delta r_i \]  
(3-26)  
and  
\[ R_i^- \equiv \left( r_i - \frac{\Delta r_{i-1}}{2} \Delta r_{i-1} \right). \]  
(3-27)  
The superscripts "+" and "−" refer to the material to the right and left of the interface.

The semi-implicit finite-difference formulation for the slab is identical to that of the rod except for the obvious geometric differences.
The Fully Implicit Calculation.

With the cell noding shown in Figure 3-3, the fully implicit finite-difference equation for 2D heat conduction is (Ref. 3-4)

\[
\left(p c_p\right)_{i,j} \left[\frac{T_{i,j}^{n+1} - T_{i,j}^n}{\Delta t}\right] V_{i,j} = q_{ij} + k_{i+1/2,j} \left[\left(\frac{T_{i+1,j}^{n+1} C - T_{i,j}^{n+1}}{\Delta r_j}\right) A_{i+1/2}ight]
\]

\[
+ k_{i-1/2,j} \left[\left(\frac{T_{i-1,j}^{n+1} - T_{i,j}^{n+1}}{\Delta r_{i-1}}\right) A_{i-1/2}\right]
\]

\[
+ k_{i,j+1/2} \left[\left(\frac{T_{i,j+1}^{n+1} - T_{i,j}^{n+1}}{\Delta z_j}\right) A_{i}^j\right]
\]

\[
+ k_{i,j-1/2} \left[\left(\frac{T_{i,j-1}^{n+1} - T_{i,j}^{n+1}}{\Delta z_{j-1}}\right) A_{i}^j\right],
\]

(3-28)

where \( V \) = cell volume, \( A \) = area in radial direction, \( A_i^j \) = area in axial direction, and \( \Delta r \) = cell length in radial or \( x \) direction.

Note that this equation applies to both the slab and rod geometries, providing the areas and volumes of the cells are calculated correctly. Eq. (3-28) can be written (Ref. 3-4) as

\[
a_{1,i,j} T_{i-1,j}^{n+1} + a_{2,i,j} T_{i,j}^{n+1} + a_{3,i,j} T_{i+1,j}^{n+1} + a_{4,i,j} T_{i,j-1}^{n+1} + a_{5,i,j} T_{i,j+1}^{n+1} = b_{i,j},
\]

(3-29)

where

\[
a_{1,i,j} = -\frac{k_{i-1/2,j} A_{i-1/2}}{\Delta r_{i-1}},
\]

(3-30)

\[
a_{2,i,j} = \left(p c_p\right)_{i,j} \frac{V_{i,j}}{\Delta t} + \frac{k_{i+1/2,j} A_{i+1/2}}{\Delta r_j} + \frac{k_{i-1/2,j} A_{i-1/2}}{\Delta r_{i-1}}
\]

\[
+ \frac{k_{i,j+1} A_i^j}{\Delta z_j} + \frac{k_{i,j-1/2} A_i^j}{\Delta z_{j-1}},
\]

(3-31)
\[ a_{3, i, j} = \frac{-k_{i+1/2, j} A_{i+1/2}}{\Delta r_i}, \quad (3-32) \]

\[ a_{4, i, j} = \frac{k_{i, j-1/2} A_i^j}{\Delta z_{j-1}}, \quad (3-33) \]

\[ a_{5, i, j} = \frac{-k_{i, j+1/2} A^j_i}{\Delta z_j}, \quad \text{and} \quad (3-34) \]

\[ b_{i, j} = \left\{ \left( \frac{\rho c_p}{\Delta t} \right) T^n_{i, j} \right\} V_{i, j}, \quad (3-35) \]

Eq. (3-29) is rewritten in matrix notation as

\[ A \cdot T = B \quad (3-36) \]

or

\[
\begin{pmatrix}
D(1) & E(1) \\
C(2) & D(2) & E(2) \\
C(3) & D(3) & E(3) \\
0 & \ldots & \ldots \\
0 & \ldots & \ldots \\
C(NZ - 1) & D(NZ - 1) & E(NZ - 1) \\
C(NZ) & D(NZ) & E(NZ) \\
0 & \ldots & \ldots \\
\end{pmatrix}
\begin{pmatrix}
T(1) \\
T(2) \\
T(3) \\
\vdots \\
T(NZ - 1) \\
T(NZ) \\
\end{pmatrix}
= 
\begin{pmatrix}
B(1) \\
B(2) \\
B(3) \\
\vdots \\
B(NZ - 1) \\
B(NZ) \\
\end{pmatrix}, \quad (3-37)
\]

where

\[ T^{(j)} = \begin{pmatrix} T_{1, j} \\ T_{2, j} \\ \vdots \\ T_{NR, j} \end{pmatrix} \quad (j = 1, NZ), \quad \overline{B}^{(j)} = \begin{pmatrix} b_{1, j} \\ b_{2, j} \\ \vdots \\ b_{NR, j} \end{pmatrix} \quad (j = 1, NZ) \quad (3-38) \]
Matrix $A$ is a symmetrical banded matrix. To solve for the temperatures, matrix $A$ is inverted by a modified Cholesky method. Then the temperatures are computed from

$$T = A^{-1} B.$$  \hfill (3-42)

Note that Eq. (3-42) yields the predicted temperature distribution for the fully implicit 2D HS that appears in Eq. (3-4). The linearization coefficients for the fully implicit 2D HS are:

$$\frac{\partial T}{\partial T_l} = A^{-1} \frac{\partial B}{\partial T_l}.$$ \hfill (3-43)

$$\frac{\partial T}{\partial T_g} = A^{-1} \frac{\partial B}{\partial T_g}.$$ \hfill (3-44)
**Fine-Mesh Algorithm.**

The reflood phase of a postulated LOCA is characterized by a sequence of heat-transfer and two-phase-flow regimes advancing rapidly through the vessel core. A correctly predicted thermal response from the fuel/heater rods during reflood requires a numerical technique that can model the quenching phenomena associated with the quench-front motion.

The leading edge of the quenching region is characterized by large variations of temperatures and heat fluxes within small axial distances ($\Delta z \sim 1$ mm) (Ref. 3-5). The front advancement is controlled by two heat-removal mechanisms, the first being axial conduction from the post-CHF region ahead of the quenched region to the nucleate-boiling region behind the advancing film. The rod conduction model contains the necessary physics to analyze such phenomena. The second is the precursory rod cooling associated with heat transfer to the slugs and droplets entrained in the vapor field downstream of the quench front. The convective heat transfer discussed in Chapter 6 contains the physics necessary to describe this phenomenon.

To model the inherently nonstationary, Lagrangian quench-front motion and to resolve the related thermal gradients, a fine-mesh rezoning technique (Ref. 3-6) is used during the reflood conduction calculations. The axial gradients encountered within the quenching region are resolved by the insertion of rows of transitory nodes (see Figure 3-5). These nodes are added whenever the surface temperature difference between adjacent nodes exceeds a heat transfer regime dependent value ($\Delta T_{max}$). If the heat transfer regime is film boiling, then $\Delta T_{max}$ is given by:

$$\Delta T_{max} = Max\left(25, 5 + 0.067\Delta T_s + 0.000028(\Delta T_s)^2\right),$$

(3-45)

If the heat transfer regime is transition boiling, then $\Delta T_{max}$ is given by:

$$\Delta T_{max} = Min\left(25, 5 + 0.067\Delta T_s\right),$$

(3-46)

If the heat transfer regime is nucleate boiling, then $\Delta T_{max}$ is given by:

$$\Delta T_{max} = Min\left(5, \frac{25}{\Delta T_s}\right),$$

(3-47)

For all other heat transfer regimes, $\Delta T_{max}$ is given by:

$$\Delta T_{max} = 25,$$

(3-48)
The number of permanent rows inserted within each fluid level is specified by the user. The rows are uniformly spaced (that is, $\Delta z$ is constant) within each fluid level. The temperature values at the supplemental nodes are determined from linear interpolation. The permanent nodes added in this fashion remain during the entire TRACE calculation, since reflood is either on or off at the beginning of a TRACE calculation.

Insertion of a fine mesh axial node row is illustrated in Figure 3-6. If the surface temperature axial gradient exceeds $\Delta T_{max}$ given by Eq. (3-45) through Eq. (3-48), then a new transitory node row is inserted. If the original two axial levels $j_o$ and $j_o + 1$ are within the same coarse mesh node, then the temperature of the node row at $j' = j_o + 2$ is equal to the old temperature at $j_o + 1$ and $j' = j_o$ temperature is equal to the old temperature at $j_o$. The new temperature at $j' = j_o + 1$ is given by Eq. (3-49), which conserves energy assuming heat structure densities do not vary significantly in the axial direction.

$$T_{i, j+1} = \frac{c_{p(i, j)} T_{i, j} + c_{p(i, j+2)} T_{i, j+2}}{c_{p(i, j)} + c_{p(i, j+2)}}$$

(3-49)

When the two old conduction node rows are in different coarse mesh axial levels, then the cell edge between the coarse mesh axial levels cannot move. For this case, either the node row below the coarse mesh cell edge will be split according to 2/3 and 1/3 or the node row above the coarse mesh cell edge will be split according to 1/3 and 2/3. The fine mesh logic picks the largest axial
level of the two axial levels at the coarse mesh boundary to split into two axial node rows. For this case the new temperatures are based on the linear interpolation based on the original un-modified noding and temperatures. Since it is a single axial level that is split into two axial levels (i.e., one at 1/3 the height of the original axial level and the other at 2/3 the height of the original axial level), it is not necessary to do any averaging to ensure that energy is conserved with the new noding.

When the axial surface temperature gradient between two node rows becomes less than one-half of $\Delta T_{max}$ given by Eqs. (3-45) through (3-47), then two node rows are merged into one node row. Inserting an axial node row based on $\Delta T_{max}$ and removing an axial node row based on $(\Delta T_{max})/2$ ensures that the fine mesh logic will not consistently insert and remove the same transitory axial level every time step.

The above algorithm can analyze multiple quench fronts simultaneously. Both quenching and dryout are modeled automatically.

During the reflood phase, a number of surface conduction nodes are located within each fluid cell. Therefore, total heat transfer rate is obtained by summing the surface heat flux for each fine mesh axial level associated with a fluid cell.

$$Q = \sum_j \left( q_j + \frac{\partial q_j}{\partial T_l}(T_{l_{n+1}} - T_{l_n}) + \frac{\partial q_j}{\partial T_g}(T_{g_{n+1}} - T_{g_n}) \right) A_j \quad (3-50)$$

It already has been noted that, for a given time step ($\Delta t$), a minimum spacing ($\Delta z$) between rows of conduction nodes exists because of the explicit axial differencing. For reflood
calculations, this axial spacing can be violated, resulting in stability problems. To avoid such problems, the time step is limited internally by a diffusion number. The user also can specify minimum spacing ($\Delta z_{min}$) beyond which supplemental rows of conduction nodes will not be added. This additional advantage can prevent excessively large computer costs.

**References**


Drag Models

As shown in Chapter 1, the liquid- and gas-field momentum equations each include terms for the interfacial shear force and the wall drag force. Closure of these equations thus requires that we specify the interfacial drag coefficient, \( C_i \), and the phasic wall drag coefficients, \( C_{wl} \) and \( C_{wg} \), for wall-liquid and wall-gas shear respectively. Typically, only one of the wall drag coefficients has a non-zero value. For example, in either bubbly/slug or annular/mist flow, all of the wall drag is applied to the liquid phase and \( C_{wg} \) is set to zero. Both the models for the interfacial drag coefficient and the wall drag coefficients are dependent upon the flow regime. These flow regime dependent closure models are discussed below, first for the interfacial drag and then for the wall drag.

Nomenclature

The following nomenclature applies to this chapter:

- \( a \) = minor radius of prolate ellipsoid
- \( A \) = flow area (m\(^2\))
- \( A_k \) = flow area of phase \( k \) in stratified flow (m\(^2\))
- \( A''_i \) = interfacial area per unit volume (m\(^{-1}\))
- \( A''_p \) = projected area per unit volume (m\(^{-1}\))
- \( b \) = major radius of prolate ellipsoid
- \( C_D \) = particle drag coefficient
- \( C_i \) = interfacial drag coefficient
- \( C_0 \) = distribution parameter used in drift flux model