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A NUMERICAL PROCEDURE FOR CALCULATING STEADY/UNSTEADY, SINGLE-PHASE/TWO-PHASE THREE-DIMENSIONAL FLUID FLOW WITH HEAT TRANSFER

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Components Technology Division
Argonne National Laboratory

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* Consultant, Professor of Mechanical Engineering, University of Minnesota, Minneapolis, Minnesota 55455

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NOMENCLATURE

A	convection-diffusion function, Eq. [5.3]
a_B, a_E, a_e, a_N, a_{nb}, a_p, a_S, a_T, a_W	finite-difference coefficients
a_e°, a_p°,	finite-difference coefficients arising from the unsteady term
b	"constant" term in the finite-difference method
c_p	specific heat at constant pressure
c_μ	turbulence constant
D	diffusion strength, Eq. [5.5]
d	pressure coefficient, Eq. [6.8]
E	wall-law constant
F	flow rate, Eq. [5.4]
G	source in turbulence energy due to buoyancy (Table 1)
g	turbulence quantity, Eq. [2.8]
g_j	gravitational acceleration in the jth direction
h	enthalpy
J	total (convection + diffusion) flux
K	interfacial drag coefficient
k	turbulence kinetic energy
M	a large number, Eq. [9.8]
P	resistance of laminar sublayer, Eq. [9.4]; source in turbulence energy (Table 1)
P_g	source term in scalar energy g (Table 1)
p	pressure
p^*	guessed value of pressure

p'	pressure correction
Pr	laminar Prandtl number
Pr_t	turbulent Prandtl number
Q	heat generation per unit volume, Eq. [2.5]
R	interfacial heat transfer coefficient, Eq. [2.5]
r	r-coordinate in cylindrical and spherical coordinate systems (Appendices A and B)
S	source term, Eq. [2.9]
S_C, S_P	parts of the linearized source term, Eq. [4.15]
S_g, S_k, S_ε	source terms for g, k, ε
S_1, S_2	positive and negative parts of S, Eq. [11.7]
T	temperature
t	time
u, v, w	velocity components
u^*, v^*, w^*	velocities based on p^*
$\hat{u}$, $\hat{v}$, $\hat{w}$	pseudo-velocities, Eq. [6.7]
V	viscous source term; volume
v_r, v_θ, v_z	velocity components (cylindrical coordinates, Appendix A)
v_r, v_θ, v_ϕ	velocity components (spherical coordinates, Appendix B)
x_1, x_2, x_3	coordinate directions
y^+	dimensionless distance from wall, Eq. [9.2]
α	under-relaxation factor; thermal diffusivity; defined in Eq. [8.7]; void fraction in Appendices A and B.
Γ	diffusion coefficient, Eq. [2.9]
Γ_g, Γ_h, Γ_k, Γ_ε	diffusion coefficients for g, h, k, ε
Δt	time step
Δx, Δy, Δz	control-volume dimensions
Δx	distances fhown in Fig. 4.3

NOMENCLATURE

δ	distance from wall
ε	dissipation rate
κ	turbulence constant
λ	thermal conductivity
μ	viscosity
ρ	density
ρ_P	"new" density at point P
ρ°	old value
β	defined in Eq. [8.7]
ϕ	general dependent variable, Eq. [2.9]; ϕ-coordinate in spherical coordinate system (Appendix B)
ϕ_P	"new" value of ϕ at point P
ϕ_P°	"old" value of ϕ at point P
ϕ_P^*	last-iteration value of ϕ_P
θ	θ-coordinate in cylindrical and spherical coordinate systems (Appendices A and B)
θ_1, θ_2	void fractions for phase 1, phase 2
γ	volume porosity
γ_x, γ_y, γ_z	surface permeability in x, y, and z-directions
Ω, Ω_m, Ω_h	source due to phase change (evaporation or condensation) in the continuity, momentum, and energy equations
Φ	viscous dissipation, Eq. [2.5]
ν	kinematic viscosity

Subscripts

1,2	phase 1, phase 2
P,E,N,W S,T,B	grid positions (i,j,k), i+1, j+1, i-1, j-1, k+1, k-1
e,n,w,s, t,b	grid positions i+1/2, j+1/2, i-1/2, j-1/2, k+1/2, k-1/2

NOMENCLATURE

Superscripts

*	last iteration value; guessed value

ABSTRACT

This report describes a general numerical procedure for the calculation of steady/unsteady, single-phase/two-phase, three-dimensional fluid flow. The procedure is based on the control-volume approach, which enables the derivation of physically meaningful finite-difference equations. The conservation equations employed are based on a two-fluid model. This permits the analyses of nonhomogeneous and nonequilibrium flow conditions. In addition, surface permeabilities and volume porosities are included in the finite-difference formulations to account for dispersed solid objects in a flow domain. The derivation of the equations and the required iteration scheme are presented, and flow charts are provided for the planning and design of a computer program.

1. INTRODUCTION

This report describes a general numerical method for the solution of the governing equations for three-dimensional, single-phase/two-phase, steady/unsteady flow with heat transfer. The method outlined here has been developed and refined over a number of years, and already a large number of computations for complex single-phase flow situations have been performed. In the present report, this method has been extended to two-phase flow. The description here starts with the differential equations and deals with the numerical method and its possible incorporation into a computer program.

Section 2 is devoted to the set of governing equations for the situation considered. In Section 2.5, the general form of all the governing equations is recognized; this generalization facilitates a unified development of the numerical method and the construction of the computer program.

The conservation equations for quasi-continuum regime are presented in Section 3. We define the quasi-continuum regime as a flow regime which contains finite, dispersed, stationary heat generating (or absorbing) solid objects. The effects of solid objects in a flow regime are accounted by introducing surface permeabilities, volume porosities and distributed resistances and heat sources.

In Section 4 we present some preliminary considerations before we start assembling the finite difference equations. The finite difference formulation of the general equation is presented in Section 5. As we use a staggered grid system, the control volumes for momentum equations are different and require special considerations. The special features of the finite-difference equations for momentum are discussed in Section 6. In Section 7 we have presented the finite difference forms of the continuity equations.

Section 8 contains the derivation of pressure and pressure correction equations. In the present report we have presented two methods for deriving the pressure and pressure correction equations from the continuity and momentum equations. The first procedure is an extension of the single-phase numerical procedure [1], known as SIMPLER (Semi-Implicit Method for Pressure Linked Equation - Revised). In this procedure we use the two-phase continuity equations to determine the void fractions, and use the combined continuity equation to derive the pressure correction equation. In the second procedure also we use both of the phase continuity equations to determine the void fractions; the difference lies in the derivation of the pressure

correction equation. In this procedure we differentiate the phase continuity equations and momentum equations and then combine them to obtain the pressure correction equation. This is analogous to the numerical procedure [2] known as Inter Phase Slip Analyser [IPSA].

Section 9 deals with the boundary conditions for the different dependent variables. A discussion of the ways of handling irregular geometries is included in Section 9.5.

A line-by-line procedure for solving the finite-difference equations is presented in Section 10. This procedure has been found to be superior to the usual point-by-point procedure.

In Section 11, we take an overall view of the entire calculation sequence. The various steps in the iteration scheme are listed in Section 11.1, while the remainder of Section 11 is devoted to matters that enhance the chances of obtaining a converged solution.

The incorporation of the numerical method into a computer program requires careful planning and design. The flow charts given in Section 12 are intended to contribute to this process.

Although all formulations in the report are for Cartesian co-ordinate system, we have provided tables in the Appendices A and B showing all the necessary changes needed to apply these formulations to cylindrical and spherical co-ordinate systems.

2. DIFFERENTIAL EQUATIONS: CONTINUUM

The governing equations for a single-phase/two-phase, three-dimensional, unsteady flow with heat transfer are given here in Cartesian tensor notation. For two-phase flow, we use the two-fluid model of Harlow and Amsden [3] to describe the conservation equations of mass, momentum and energy. The three coordinate directions, x, y, z, are denoted by x_i, and the three velocity components, u, v, and w are denoted by u_i. A repeated index implies the sum of three terms; that is:

$$\frac{\partial u_i}{\partial x_i} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \quad . \tag{2.1}$$

The subscripts 1 and 2 are used to denote phase 1 and phase 2. However, when the formulation is applicable to both phases, we have avoided the subscripts 1 or 2. In the Appendices A and B, we have provided tables to apply the formulations to cylindrical and spherical co-ordinate systems.

2.1 Continuity Equations

For phase 1:

$$\frac{\partial[\rho_1\theta_1]}{\partial t} + \frac{\partial}{\partial x_i}[\rho_1\theta_1 u_{1i}] = \Omega_1 \quad . \tag{2.2a}$$

Here, Ω_1 is the source term due to phase change [evaporation or condensation] and θ is the void fraction. The continuity equation for phase 2 is similar. By combining the two continuity equations, we eliminate the source terms, because $\Omega_1 = -\Omega_2$, and obtain

$$\frac{\partial}{\partial t}[\rho_1\theta_1 + \rho_2\theta_2] + \frac{\partial}{\partial x_i}[\rho_1\theta_1 u_{1i} + \rho_2\theta_2 u_{2i}] = 0 \quad . \tag{2.2b}$$

2.2 Momentum Equations

For phase 1 and for the j direction:

$$\frac{\partial}{\partial t}[\rho_1\theta_1 u_{1j}] + \frac{\partial}{\partial x_i}[\rho_1\theta_1 u_{1i} u_{1j}] = -\theta_1 \frac{\partial p}{\partial x_j} + \frac{\partial}{\partial x_i}\left(\mu_1\theta_1 \frac{\partial u_{1j}}{\partial x_i}\right)$$

$$+ \rho_1\theta_1 g_j + V_{1j} + \Omega_{mlj} + K[u_{2j} - u_{1j}] \quad . \tag{2.3}$$

The subscript j can take the values 1, 2, or 3 depending on the momentum direction chosen. The subscript i is a repeated index and implies the summation convention outlined in Eq. [2.1]. The term Ω_m is a source to the momentum field due to phase change and K is the interfacial drag coefficient. The viscous contribution to the momentum equation is expressed by two terms:

$$\frac{\partial}{\partial x_i}\left[\mu_1\theta_1 \frac{\partial u_{1j}}{\partial x_i}\right] ,$$

and V_{1j}, which is given by

$$V_{1j} = \frac{\partial}{\partial x_i}\left[\mu_1\theta_1\left(\frac{\partial u_{1i}}{\partial x_j}\right)\right] \quad . \qquad [2.4]$$

For turbulent flow, all quantities in Eqs. [2.2] and [2.3] are considered time averaged values and the viscosity μ is interpreted as the effective viscosity.

2.3 Energy Equations

For phase 1:

$$\frac{\partial}{\partial t}[\rho_1\theta_1 h_1] + \frac{\partial}{\partial x_i}[\rho_1\theta_1 u_{1i} h_1] = \frac{\partial}{\partial x_i}\left(\Gamma_{h1}\theta_1\frac{\partial h_1}{\partial x_i}\right) + \theta_1\left(\frac{\partial p}{\partial t}\right)$$

$$+ \Omega_{h1} + R\,[T_2 - T_1] + \Phi_1 + Q_1 \quad . \qquad [2.5]$$

Here, Ω_h stands for λ/c_p, where λ is the thermal conductivity, and c_p is the specific heat at constant pressure. The heat generation rate per unit volume, the source due to phase change, the interfacial heat transfer coefficient, and viscous dissipation are denoted by Q, Ω, R, and Φ, respectively. The term $\partial p/\partial t$ accounts for the fact that the internal energy [rather than enthalpy] is stored in a fluid.

For turbulent flow, Γ_h is interpreted as the effective transport coefficient for enthalpy.

2.4 Turbulence Equations

Calculation of the effective viscosity and the effective transport coefficient for the enthalpy often requires additional differential equations. One such proposal for single-phase is the k-ε-g model described in [4]. As far as we know, no generalized turbulence model exists for two-phase flows. We are assuming here that the turbulence equations for two-phase flows have the same general form as those for single-phase. We further assume that all terms containing interaction between the phases can be considered as part of the source term. With these assumptions, the equations for the turbulence quantities k, ε, and g can be written as:

For phase 1:

$$\frac{\partial}{\partial t}[\rho_1\theta_1 k_1] + \frac{\partial}{\partial x_i}[\rho_1\theta_1 u_{1i} k_1] = \frac{\partial}{\partial x_i}\left(\Gamma_{k1}\theta_1\frac{\partial k_1}{\partial x_i}\right) + S_{k1} \quad ; \qquad [2.6]$$

$$\frac{\partial}{\partial t}[\rho_1\theta_1\varepsilon_1] + \frac{\partial}{\partial x_i}[\rho_1\theta_1 u_{1i}\varepsilon_1] = \frac{\partial}{\partial x_i}\left(\Gamma_{\varepsilon 1}\theta_1 \frac{\partial \varepsilon_1}{\partial x_i}\right) + S_{\varepsilon 1} \quad . \qquad [2.7]$$

$$\frac{\partial}{\partial t}[\rho_1\theta_1 g_1] + \frac{\partial}{\partial x_i}[\rho_1\theta_1 u_{1i} g_1] = \frac{\partial}{\partial x_i}\left(\Gamma_{g1}\theta_1 \frac{\partial g}{\partial x_i}\right) + S_{g1} \quad . \qquad [2.8]$$

Here, the quantities Γ_k, Γ_ε, and Γ_g are the diffusion coefficients for k, ε, and g, respectively, and S_k, S_ε, and S_g are the corresponding source terms. The actual expressions for these Γ's and S's depend on the particular details of the turbulence model. The turbulence equations for phase 2 can be described in a similar manner.

It is to be noted here that we require additional auxiliary equations which relate k, ε, and g to effective viscosity and transport coefficient for enthalpy appearing in Eqs. [2.4] and [2.5], respectively.

2.5 General Form

Equations [2.3], [2.5], [2.6], [2.7], and [2.8] can be seen to possess a common form. If the general dependent variable for phase 1 is denoted by ϕ_1, the corresponding differential equation has the form:

$$\frac{\partial}{\partial t}[\rho_1\theta_1\phi_1] + \frac{\partial}{\partial x_i}[\rho_1\theta_1 u_{1i}\phi_1] = \frac{\partial}{\partial x_i}\left(\Gamma_{\phi 1}\theta_1 \frac{\partial \phi}{\partial x_i}\right) + S_{\phi 1} \quad , \qquad [2.9]$$

where the four terms can be referred to as: the unsteady term, the convection term, the diffusion term, and the source term. The density ρ and the velocity components u_i satisfy the continuity equation [2.2]. The diffusion coefficient Γ_ϕ and the source term S_ϕ are specific to each meaning of ϕ. Source terms for all conservation equations are given in Table 1.

The recognition of this general form of the governing differential equations is the first important step toward formulation of a general numerical scheme and construction of an efficient computer program. For, much of the formulation can be completed by reference to Eq. [2.9] alone, and a single sequence of computer instructions is all that may be needed for solving any number of equations possessing the general form.

Table 1. Source terms for continuity, momentum, energy and turbulence equations.

Equation	Variable	ϕ	Source Term $S_\phi = S_{c\phi} + S_{p\phi}\phi$ S_c	S_p
Continuity	Void fraction (phase 1)	θ_1	Ω_1	-
Momentum	Velocity phase 1, j direction	u_{1j}	$\rho_1\theta_1 g_j + V_{1j} + \Omega_{mlj} + Ku_{2j} - \theta_1 \frac{\partial p}{\partial x_j}$	$-Ku_{1j}$
Energy	Enthalpy (phase 1)	h_1	$\theta_1 \frac{\partial p}{\partial t} + \Omega_{h_1} + \Phi_1 + Q_1 + RT_2$	$-RT_1$
Turbulence equation for k_1	Turbulence kinetic energy $\left(\frac{\overline{u'_{1i}\, u'_{1i}}}{2}\right)$	k_1	$\rho_1\theta_1 (P_1 + G_1) + I_{k1}$	$-\rho_1\theta_1\varepsilon_1/k_1$
Turbulence equation for ε_1	Kinematic dissipation rate of turbulence energy $\left[\nu_1 \frac{\partial u'_{1i}}{\partial x_k}\left(\frac{\partial u'_{1i}}{\partial x_k} + \frac{\partial u'_{1k}}{\partial x_i}\right)\right]$	ε_1	$\frac{\theta_1\rho_1\varepsilon_1\left[\left(C_1\right)_{\varepsilon 1} P_1 + \left(C_3\right)_{\varepsilon 1} G_1\right]}{k_i} + I_{\varepsilon 1}$	$-(C_2)_{\varepsilon 1} \frac{\rho_1\varepsilon_1\theta_1}{k_1}$

Table 1. Source terms for continuity, momentum, energy and turbulence equations. (contd.)

Equation	Variable	ϕ	S_c	S_p
Turbulence equation for g_1	Scalar energy $\frac{1}{2} T'^2$	g_1	$\rho_1 \theta_1 P_{g1} + \frac{\partial}{\partial x_i}\left(\alpha_1 \rho_1 \theta_1 \frac{\partial g_1}{\partial x_1}\right) + I_{g1}$	$-\frac{\varepsilon_1}{k_1 R_1}$

In the above table:

P: Generation rate of turbulence energy due to mean velocity gradient.

P_g: Generation rate of g by mean temperature gradients

I: Source due to interaction between two phases.

G: Generation rate of turbulence energy due to buoyant effects.

α: Thermal diffusivity, and

$(C_1)_\varepsilon$, $(C_2)_\varepsilon$, and $(C_3)_\varepsilon$ are empirical coefficients.

Definitions of generation terms P, P_g and G and the values of empirical coefficients $(C_1)_\varepsilon$, $(C_2)_\varepsilon$, and $(C_3)_\varepsilon$ are given in [3].

3. CONSERVATION EQUATIONS: QUASI-CONTINUUM

3.1 Flow Domain with Solid Objects

The presence of solid objects in a flow domain has two effects on fluid flow. One is the geometrical effect; here the presence of solid objects influences the flow by reducing the available space. This effect is taken into account by including volume porosity and surface permeabilities in the governing equations. The second is the physical effect; here, the solid objects influence the momentum and heat transfer to fluid flow. This effect is taken into account by considering solid objects within a control volume as distributed resistances to momentum transfer and distributed sources [or sinks] for heat transfer.

In applying the concept of volume porosity and surface permeability, we are assuming that a real system containing numerous solid objects can be replaced by an idealized system having distributed solid objects such that both systems have the same volumetric porosities, same surface permeabilities, and same interactions [momentum and heat transfer] between fluid and solid surfaces.

3.2 Volume Porosity and Surface Permeability

We consider a fixed finite region of volume V in space with enveloping surface A. There are finite numbers of dispersed, fixed heat generating solids inside V, some may be cut through by A as illustrated in figure 3.1. Clearly, $V = V_f + V_s$, where V_f is the total fluid volume and V_s is the total solid volume. Only a fraction of the enveloping surface A is unobstructed to fluid flow.

We define γ_v as the local volume porosity, i.e., fraction of the local volume inside V that is occupied by the fluid. It may take on value between 0 and 1. If the local volume under consideration is completely inside a dispersed solid, $\gamma_v = 0$; if it is completely in the fluid, $\gamma_v = 1$. If the local volume is partly in a dispersed solid and partly in fluid, then $0 \leq \gamma_v \leq 1$. Hence, in general, $0 \leq \gamma_v \leq 1$.

The local surface permeability γ_a is defined as the fraction of the local surface in A that is unobstructed to fluid flow. It is easy to see that, in general, $0 \leq \gamma_a \leq 1$. We define the average volume porosity as:

$$\gamma_v = \frac{1}{V} \int_V \gamma_v \, dv \qquad [3.1]$$

and the average surface permeability as

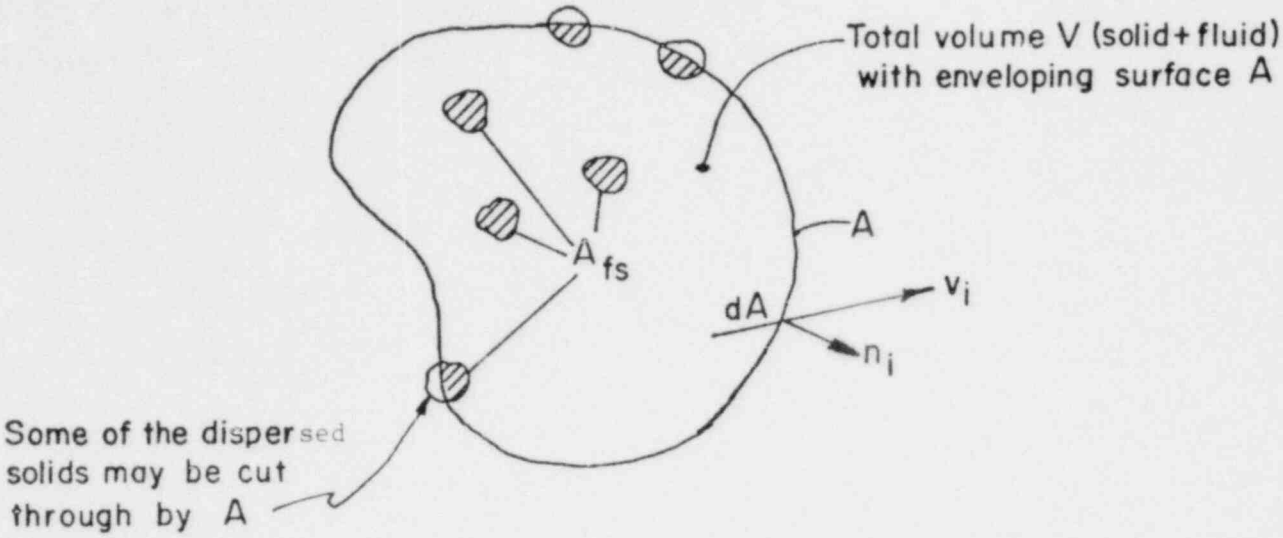

Fig. 3.1 Domain containing dispersed solid objects

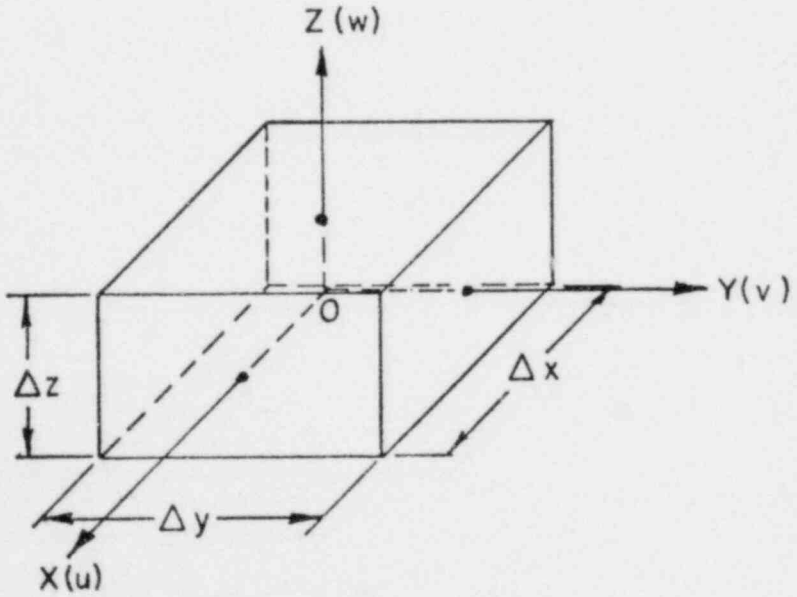

Fig. 3.2 Finite control volume in Cartesian co-ordinates

$$\gamma_{x_i} = \frac{1}{A_{x_i}} \int_{A_{x_i}} \bar{\gamma}_{x_i} \, da_{x_i} \qquad [3.2]$$

Here, the subscript x_i refers to direction normal to surface area under consideration. Since, the unobstructed area A_{x_i} that is available for free fluid flow is

$$(A_f)_{x_i} = \int_{A_{xi}} \gamma_{x_i} \, da, \qquad [3.3]$$

it follows immediately, that

$$(A_f)_{x_i} = \gamma_{x_i} A_{x_i} \quad . \qquad [3.4]$$

Similarly,

$$V_f = \gamma_v V. \qquad [3.5]$$

3.3 Continuity Equations

The formulations of the conservation equations for quasi-continuum flow regime are given in [5]. We are presenting here only the final equations.

We consider a stationary volume element

$$\Delta V = \Delta x \, \Delta y \, \Delta z, \qquad [3.6]$$

through which fluid is flowing (see figure 3.2). It's enveloping surface

$$\Delta A = 2(\Delta y \Delta z + \Delta z \Delta x + \Delta x \Delta y).$$

The centroid of V is located at 0 (x,y,z). The velocity components in the x,y and z directions are u,v, and w respectively. The continuity equation for phase 1 is:

$$\gamma_v \frac{\partial(\rho_1 \theta_1)}{\partial t} + \frac{\Delta(\rho_1 \theta_1 u_1 \gamma_x)}{\Delta x} + \frac{\Delta(\rho_1 \theta_1 v_1 \gamma_y)}{\Delta y}$$

$$+ \frac{\Delta(\rho_1 \theta_1 w_1 \gamma_z)}{\Delta z} = \Omega_1 \gamma_v \qquad [3.7]$$

Here, Ω_1 is the source per unit fluid volume and we define,

$$\frac{\Delta(\,)}{\Delta x_j} = \frac{(\,)_{x_j + \Delta x_j/2} - (\,)_{x_j - \Delta x_j/2}}{\Delta x_j} \qquad [3.8]$$

The continuity equation for phase 2 is similar.

3.4 Momentum Equations

The momentum equation for phase 1 in x-direction is:

$$\frac{\partial}{\partial t}\left[\rho_1\theta_1 u_1\gamma_v\right] + \frac{\Delta[\rho_1\theta_1 u_1^2\gamma_x]}{\Delta x} + \frac{\Delta[\rho_1\theta_i u_1 v_1\gamma_y]}{\Delta y} + \frac{\Delta(\rho_1\theta_1 u_1 w_1\gamma_z)}{\Delta z} = (\rho_1\theta_1 g_x\gamma_v) - \theta_1\gamma_v\frac{\Delta p}{\Delta x} + \frac{\Delta\left(\theta_1\tau_{xx}\gamma_x\right)}{\Delta x} + \frac{\Delta\left(\theta_1\tau_{xy}\gamma_y\right)}{\Delta y} + \frac{\Delta\left(\theta_1\tau_{xz}\gamma_z\right)}{\Delta z} + \gamma_v K (u_2 - u_1) - R_x \qquad [3.9]$$

Here, R_x is the distributed frictional resistance per unit volume in x-direction. Equations for second phase and for other directions are similar.

3.5 Energy Equations

Energy equations for phase 1:

$$\frac{\partial}{\partial t}[\rho_1\theta_1 h_1\gamma_v] + \frac{\Delta\left(\rho_1\theta_1 u_1 h_1\gamma_x\right)}{\Delta x} + \frac{\Delta\left(\rho_1\theta_1 v_1 h_1\gamma_y\right)}{\Delta y} + \frac{\Delta\left(\rho_1\theta_1 w_1 h_1\gamma_z\right)}{\Delta z} = \gamma_v\frac{d\left(p\theta_1\right)}{dt} + \gamma_v\left[\dot{Q}_{ls} + \dot{Q}_1 + \Phi_1 + R\,(T_2 - T_1) + \Omega_{h_1}\right] + \left[\frac{\Delta\left(\theta_1\gamma_x\lambda_1\frac{\partial T_1}{\partial x}\right)}{\Delta x} + \frac{\Delta\left(\theta_1\gamma_y\lambda_1\frac{\partial T_1}{\partial y}\right)}{\Delta y} + \frac{\Delta\left(\theta_1\gamma_z\lambda_1\frac{\partial T_1}{\partial z}\right)}{\Delta z}\right] \qquad [3.10]$$

Here, $\dot{Q}_1$ is the distributed heat source per unit fluid volume and $\dot{Q}_{ls}$ is the rate of heat transfer between fluid and dispersed solid objects per unit fluid volume. The energy equation for phase 2 is similar.

4. PRELIMINARY CONSIDERATIONS

The numerical solution of the governing differential equations is accomplished by constructing a grid and obtaining the values of the dependent variables at the grid points. Although the principles used can be applied to a grid in any coordinate system, only a Cartesian-coordinate grid is employed here.

The finite-difference equations are derived by integrating the differential equation over a control volume surrounding each grid point. Thus, the derivation process and the resulting equations have direct physical meaning, and the consequent solution satisfies the conservation principles (such as the conservation of mass, the conservation of momentum,) over any group of control volumes and, of course, over the whole calculation domain. This desirable feature of the present method exists for any number of grid points, and not just in the limit of a very fine grid.

4.1 Construction of Control Volumes.

The control volumes around the grid points can be defined in a number of ways. Two practices for this will be described here. Any one of these practices can be employed, depending on the taste and convenience of the user. In the first practice, the control volume faces are located midway between neighboring grid points. Figure 4.1 shows the grid points by dots and the control-volume boundaries by dashed lines. Although only a two-dimensional view is shown, the three-dimensional configuration can be easily imagined. It is not necessary for the grid lines to be uniformly spaced.

In the second practice, one decides the locations of the control-volume faces first and then places a grid point in the geometrical center of each control volume. Again, the control volumes can have nonuniform sizes. This type of construction is shown in Figure 4.2.

This may be a convenient place to remark on the use of nonuniform grids. A misconception seems to prevail that the nonuniform grids lead to lower accuracy than do the uniform grids. This is simply not true. The grid spacing should be directly linked to the way the dependent variable changes in the domain. Obviously, a fine grid is sufficient where the changes are steep, and a coarse grid is sufficient where the changes are rather flat. Indeed, a nonuniform grid enables us to deploy the computing power in an effective way. For most problems, it is desirable to compute exploratory coarse-grid solutions, from which useful guidance can be obtained for designing an appropriate nonuniform grid.

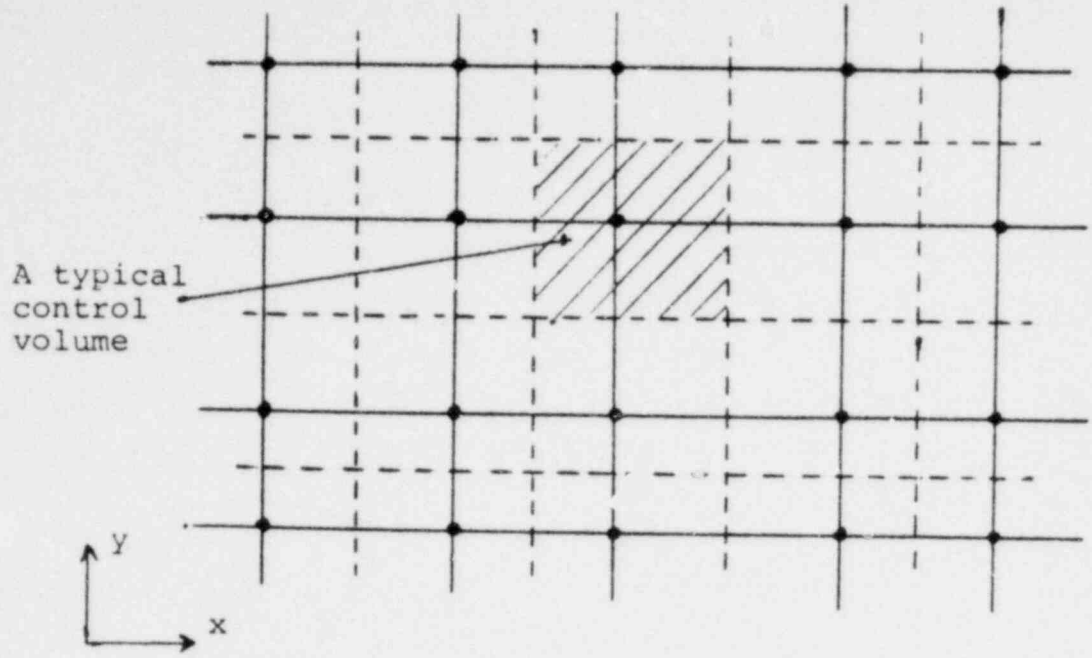

Fig. 4.1 Construction of control volumes (first practice)

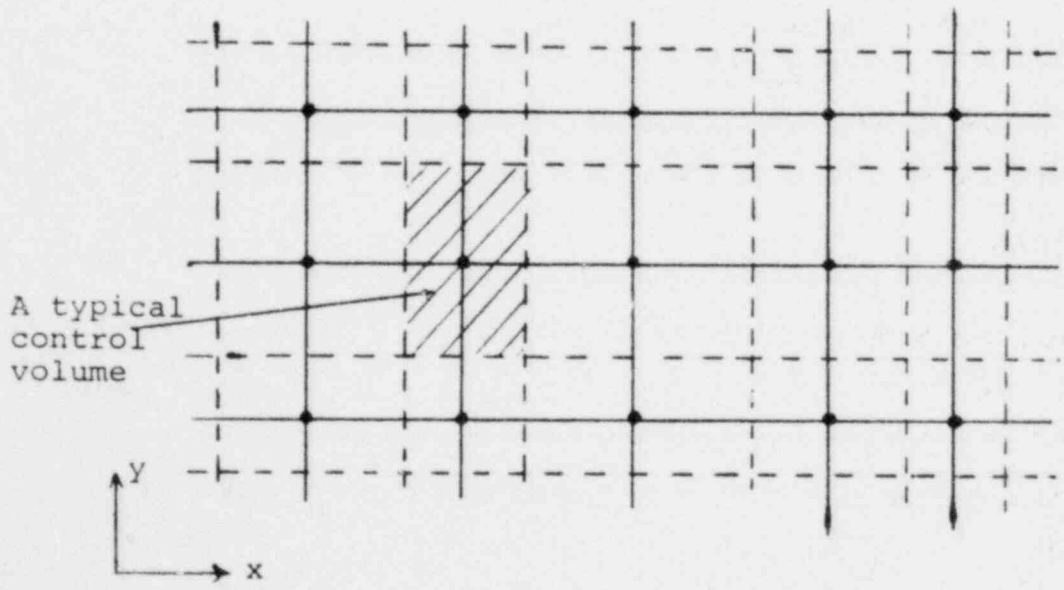

Fig. 4.2 Construction of control volumes (second practice)

4.2 Unsteady Situations

The solution for an unsteady situation is obtained by marching in time. For every time step, the values of the dependent variables at the beginning of the time step are supposed to be known, and those at the end of the step are to be calculated. A fully implicit scheme is recommended in this report. This means that the "new" values govern the entire time step, and the "old" values appear only through the term $\partial[\rho\theta\phi]/\partial t$. When the time step Δt is made very large, the calculation procedure automatically reverts to the steady-state formulation.

4.3 Convection and Diffusion Terms

If the total convection + diffusion flux of phase 1 is expressed by $J_{\phi 1}$:

$$\left(J_{\phi 1}\right)_i = \rho_1\theta_1 u_{1i}\phi_1 - \Gamma_{\phi,1}\left(\frac{\partial \phi_1}{\partial x_i}\right) \qquad [4.1]$$

the convection and diffusion terms in Eq. [2.9] can be written as:

$$\frac{\partial}{\partial x_i}\left[\rho_1\theta_1 u_{1i}\phi_1\right] - \frac{\partial}{\partial x_i}\left[\Gamma_{\phi 1}\theta_1 \frac{\partial \phi_1}{\partial x_i}\right] = \frac{\partial (J_{\phi 1})_i}{\partial x_i} \qquad [4.2]$$

Integration of these terms over the control volume will lead to the balance of the total fluxes entering and leaving the control volume at its faces.

Figure 4.3 shows a control-volume face between grid points P and E. The face is normal to the x-direction and has an area $[\gamma_x \Delta y \Delta z]$. The expression for the total flux $J_{\phi e}$ can be based on the exact solution for a one-dimensional problem, given in [6].

For a one-dimensional case

$$\frac{d}{dx}\left[\rho\theta u\phi\right] = \frac{d}{dx}\left[\Gamma_\phi \frac{d\phi}{dx}\right] \qquad [4.3]$$

with the boundary conditions

$$\begin{aligned} x = o;\quad & \phi = \phi_o \\ x = L;\quad & \phi = \phi_L \end{aligned} \qquad [4.4]$$

the solution is

$$\frac{\phi - \phi_o}{\phi_L - \phi_o} = \frac{\exp[Pe\ x/L] - 1}{\exp[Pe] - 1} \quad . \qquad [4.5]$$

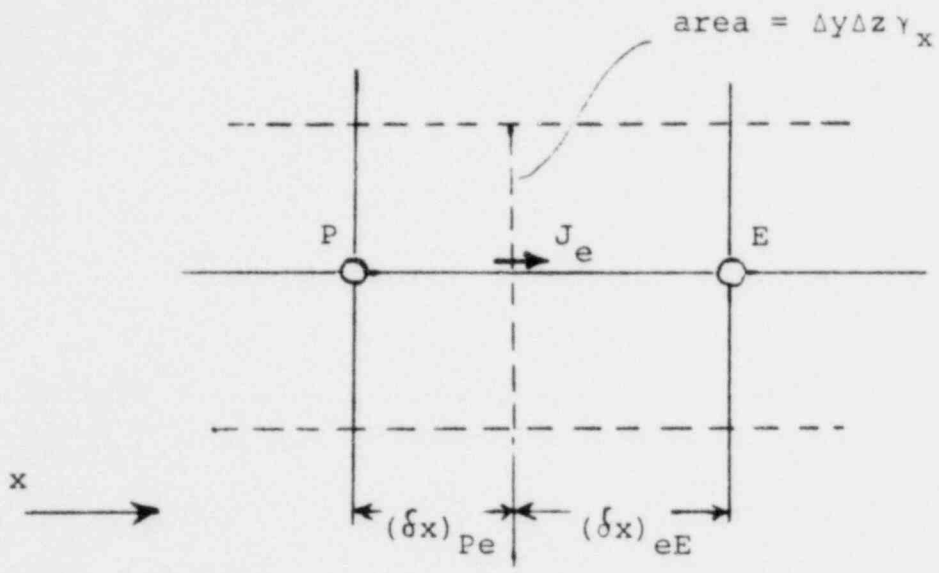

Fig. 4.3 Total flux across a control-volume face

Here, $Pe = (\rho uL/\Gamma_\phi)$ is the Peclet number. Equation [4.5] leads to:

$$J_e(\gamma_x \Delta y \Delta z) = a_E(\phi_p - \phi_E) + F_e\phi_p \quad . \qquad [4.6]$$

where

$$a_E = \left\{ F_e/[\exp[F_e/D_e] - 1] \right\} \quad , \qquad [4.7]$$

$$F_e = [\rho\theta u]_e \gamma_x \Delta y \Delta z \quad , \qquad [4.8]$$

and

$$D_e = [\gamma_x \Delta y \Delta z] \Big/ \left[(\delta x)_{Pe} \Big/ (\Gamma_{\phi P}\phi_P) + (\delta x)_{eE} \Big/ (\Gamma_{\phi E}\phi_E) \right] \quad . \qquad [4.9]$$

Here, F_e is the flow rate across the control-volume face, while D_e represents the strength of diffusion. The ratio F_e/D_e is the local Peclet number. We can see from Fig. 4.4 that Eq. [4.7] reduces to the central-difference scheme at low values of the Peclet number and progressively takes on an "upwind" character as the Peclet number is increased.

The definition of D_e, given in Eq. [4.9], is based on the model that the value Γ_P prevails in control volume around point P, and the value Γ_E rules the behavior in the control volume around E. That this representation leads to more realistic and accurate solutions has been shown in [7]; also the formulation makes it easy to handle irregular geometries or obstacles, as we shall explain later.

Since the computation of the exponential in Eq. [4.7] is time-consuming, an approximation to the equation has been devised, which, for all practical purposes, would perform almost identically to Eq. [4.7]. This approximation is:

$$J_{\phi e}[\gamma_x \Delta y \Delta z] = a_E[\phi_p - \phi_E] + F_e\phi_p \qquad [4.10]$$

or

$$J_{\phi e}[\gamma_x \Delta y \Delta z] = a_p[\phi_p - \phi_E] + F_e\phi_E \quad , \qquad [4.11]$$

where

$$a_E = \left\{ D_e \left[\!\left[0, \; [1 - 0.1|F_e/D_e|]^5 \right]\!\right] + \left[\!\left[-F_e, 0 \right]\!\right] \right\}, \qquad [4.12]$$

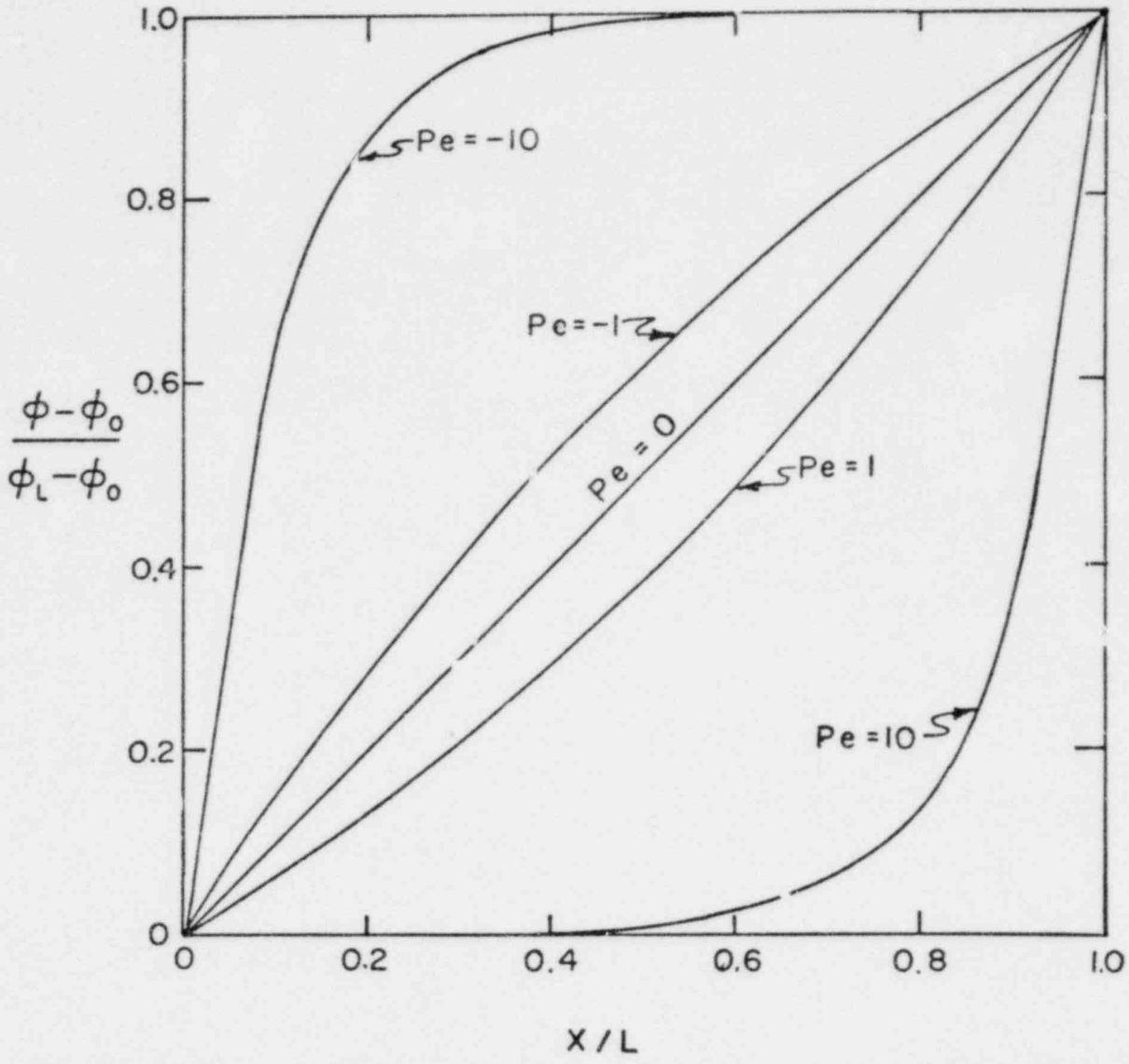

Fig. 4.4 Effect of Peclet number on the variation of ϕ

and

$$a_p = \left\{ D_e [\![0, [1 - 0.1 |F_e/D_e|]^5]\!] + [\![F_e, 0]\!] \right\} \qquad [4.13]$$

Figure 4.5 shows comparison of various finite difference schemes for convection and diffusion terms. We can see that the approximation [4.12] is very close to the exact solution.

Here, the new operator $[\![\quad]\!]$ is to be interpreted as $[\![A, B]\!]$ = the greater of A and B. [4.14]

It should be noted that $[\![A, B]\!]$ is equivalent to AMAX1 [A,B] in the computer language FORTRAN.

4.4 Source Term

For the finite-difference representation of the source term S in Eq. [2.9], it is convenient to express S as:

$$S_\phi = S_{c\phi} + S_{p\phi} (\phi_p) \qquad [4.15]$$

where the quantities $S_{c\phi}$, $S_{p\phi}$ and ϕ_p would be assumed to prevail over the control volume surrounding point P. This "linearization" of the source term is an effective device for stability and convergence. The exact expressions for $S_{c\phi}$ and $S_{p\phi}$ will depend on the actual form of S_ϕ. Some advice on this linearization will be presented later. Here it may be noted that $S_{p\phi}$ must always be kept equal to or less than zero, or else instability, divergence or physically unrealistic solutions would result. When the expression for S_ϕ is rather complicated, one may set $S_{p\phi}$ equal to zero, and $S_{c\phi}$ equal to S_ϕ. When the S_ϕ - ϕ variation is nonlinear, $S_{c\phi}$ and $S_{p\phi}$ can themselves be functions of ϕ_p; then they should be iteratively recalculated until convergence is achieved.

4.5 Unsteady Term

For the representation of the term $\partial[\rho\theta\phi]/\partial t$, we shall assume that the values ρ_p, θ_p, and ϕ_p prevail over the control volume surrounding point P. The integration of the unsteady term over the control volume would then give:

$$\int_{c.v.} \partial[\rho\theta\phi]/\partial t \; dxdydz = [\rho_p\theta_p\phi_p - \rho^o_p\theta^o_p\phi^o_p] \gamma_v \Delta x\Delta y\Delta z/\Delta t \qquad [4.16]$$

where the superscript o denctes the known values at the beginning of the time step.

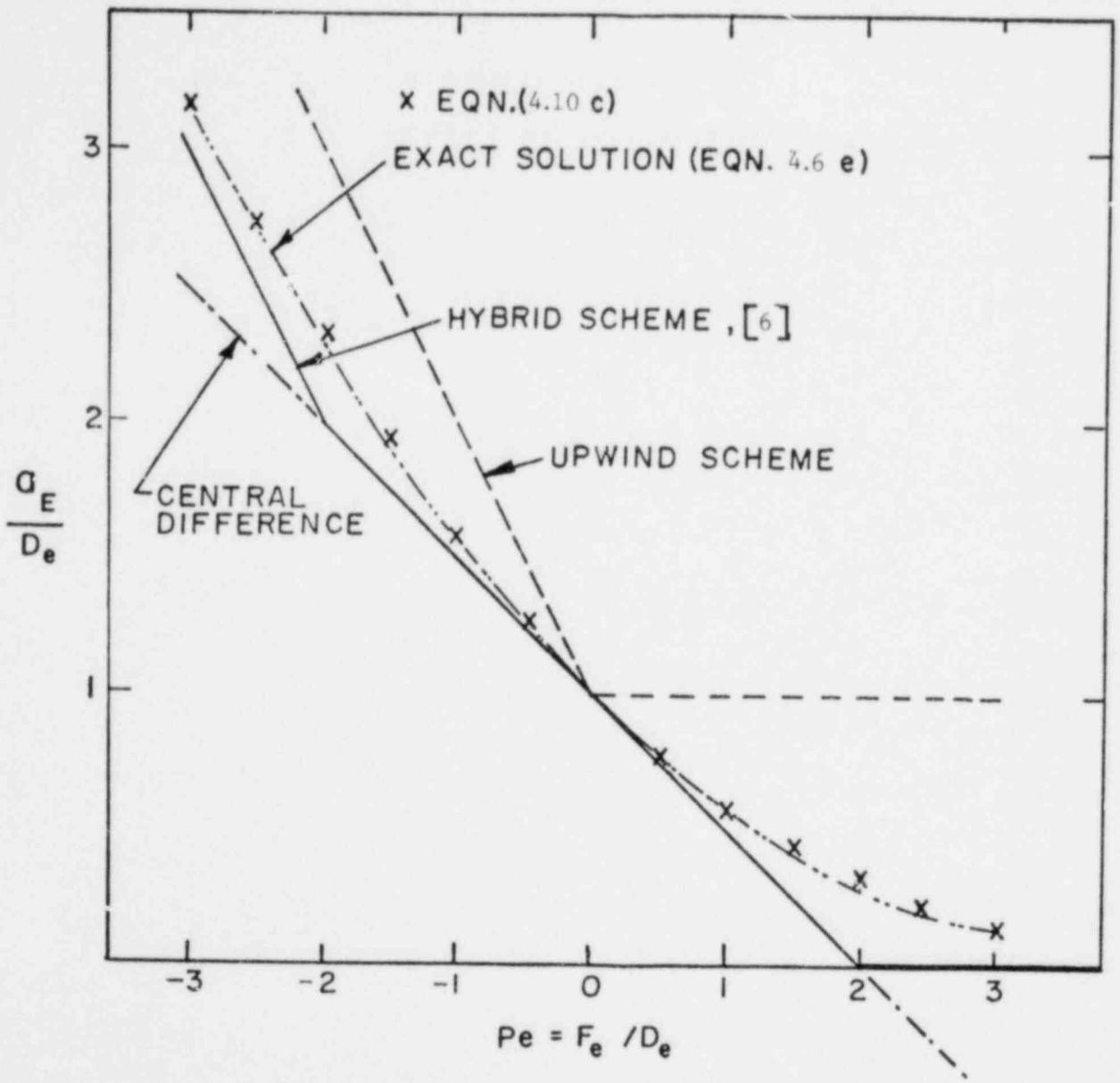

Fig. 4.5 Comparison of various finite difference schemes for convection and diffusion terms

5. GENERAL FINITE-DIFFERENCE EQUATION

5.1 General Form

The basic details outlined so far enable us to obtain the finite-difference form of the general differential equation [2.9]. Let us consider the control volume shown in Fig. 5.1. It is constructed around point P, which has E and W as its east and west neighbors, N and S as the north and south neighbors, and T and B as the top and bottom neighbors representing the z-direction. The control-volume faces are denoted by e, w, n, s, t, and b.

The general finite-difference equation for variable ϕ can be arranged as:

Phase 1 or Phase 2

$$a_P\phi_P = a_E\phi_E + a_W\phi_W + a_N\phi_N + a_S\phi_S + a_T\phi_T + a_B\phi_B + a_P^o\phi_P + b \qquad [5.1]$$

where:

$$a_E = A_e + [\![-F_e, 0]\!] , \qquad [5.2a]$$

$$a_W = A_w + [\![F_w, 0]\!] , \qquad [5.2b]$$

$$a_N = A_n + [\![-F_n, 0]\!] , \qquad [5.2c]$$

$$a_S = A_s + [\![F_s, 0]\!] , \qquad [5.2d]$$

$$a_T = A_t + [\![-F_t, 0]\!] , \qquad [5.2e]$$

$$a_B = A_b + [\![F_b, 0]\!] , \qquad [5.2f]$$

$$a_P^o = \rho_P^o \theta_P^o \gamma_v \Delta x \Delta y \Delta z / \Delta t , \qquad [5.2g]$$

$$b = S_{c\phi} \gamma_v \Delta x \Delta y \Delta z \qquad [5.2h]$$

and

$$a_P = a_E + a_W + a_N + a_S + a_T + a_B + a_P^o - S_{P\phi} \gamma_v \Delta x \Delta y \Delta z . \qquad [5.2i]$$

The quantities A_e, A_w, A_n, A_s, A_t, and A_b are defined in an identical manner. For example:

$$A_e = D_e [\![0, \ (1 - 0.1 |F_e/D_e|)^5]\!] , \qquad [5.3]$$

where F_e and D_e are given by Eqs. (4.8) and (4.9). For any other face, appropriate definitions of F and D are to be used, such as:

$$F_t = [\rho\theta w]_t \ \gamma_z \Delta x \Delta y , \qquad [5.4]$$

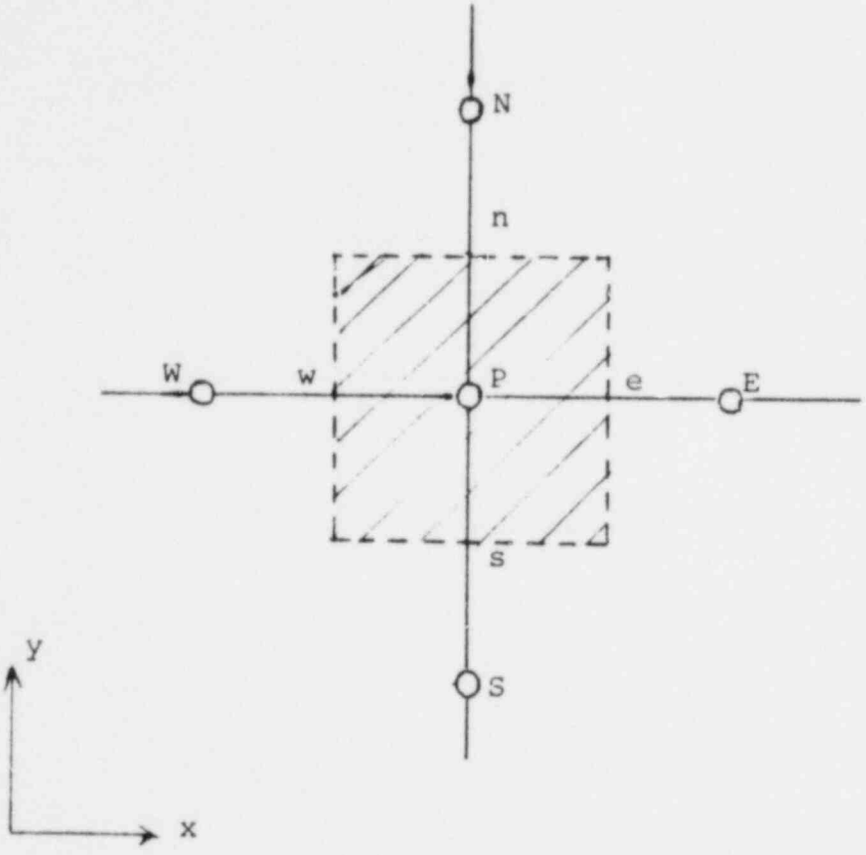

Fig. 5.1 Control volume around point P

and

$$D_t = (\gamma_x \Delta x \Delta y) \; / \; [(\delta z)_{Pt}/(\Gamma_{\phi P}\theta_P) + (\delta z)_{tT}/(\Gamma_{\phi T}\theta_T)] . \qquad [5.5]$$

Therefore,

$$A_t = D_t [\![0, (1 - 0.1 |F_t/D_t|)^5]\!] . \qquad [5.6]$$

The derivation of Eq. (5.2i) is as follows. If we combine equations (4.6), (5.2a), and (5.3), we get:

$$J_e (\gamma_x \Delta y \Delta z) = \{ A_e + [\![-F_e, 0]\!] \}(\phi_P - \phi_E) + F_e \phi_P . \qquad [5.7]$$

From the definition of a_E (Eq. 5.2), we can now write Eq. (5.7) as:

$$J_e (\gamma_x \Delta y \Delta z) = a_E (\phi_P - \phi_E) + F_e \phi_P . \qquad [5.8]$$

Similar expressions would hold for J_n and J_t. For the remaining fluxes, the corresponding expressions are:

$$J_w (\gamma_x \Delta y \Delta z) = \{ A_w + [\![-F_w, 0]\!] \} (\phi_W - \phi_P) + F_w \phi_W , \qquad [5.9]$$

which is obtained from Eq. (5.7) by replacing ϕ_P and ϕ_E by ϕ_W and ϕ_P respectively. A further rearrangement gives:

$$J_w (\gamma_x \Delta y \Delta z) = \{ A_w + [\![F_w, 0]\!] \} (\phi_W - \phi_P)$$
$$+ \{ [\![-F_w, 0]\!] - [\![F_w, 0]\!] \} (\phi_W - \phi_P) + F_w \phi_W . \qquad [5.10]$$

Noting that:

$$[\![-F_w, 0]\!] - [\![F_w, 0]\!] = -F_w , \qquad [5.11]$$

we obtain:

$$J_w (\gamma_x \Delta y \Delta z) = \{ A_w + [\![F_w, 0]\!] \} (\phi_W - \phi_P) + F_w \phi_P . \qquad [5.12]$$

With a_W defined by Eq. (5.2b), we write:

$$J_w (\gamma_x \Delta y \Delta z) = a_W (\phi_W - \phi_P) + F_w \phi_P . \qquad [5.13]$$

Similar expressions can be written for J_s and J_b. With all these flux expressions for the control-volume faces, and with the contributions from Eq. (4.15) and (4.16), the coefficient of ϕ_p can be written as:

$$a_p = a_E + F_e + a_W - F_w + a_N + F_n + a_S - F_s$$
$$+ a_T + F_t + a_B - F_b - S_{p\phi} \gamma_v \Delta x \Delta y \Delta z$$
$$+ \rho_p \theta_p \gamma_v \Delta x \Delta y \Delta z / \Delta t . \qquad [5.14]$$

Substitution of Eq. (5.2g) into this leads to:

$$a_P = a_E + a_W + a_N + a_S + a_T + a_B + a_P^o - S_{p\phi}\gamma_v\Delta x\Delta y\Delta z \quad [5.15]$$

$$+ \left\{(\rho_p\theta_p - \rho_p^*\theta_p^o)\gamma_v\Delta x\Delta y\Delta z/\Delta t + F_e - F_w + F_n - F_s + F_t - F_b\right\} .$$

The terms in the curly brackets can be recognized as the discretized form of the continuity equation (see Eq. 7.1, for example), and hence can be regarded as equal to zero. With the contents of the curly brackets in Eq. (5.15) set equal to zero, we obtain Eq. (5.2i).

5.2 Formulations in i,j,k, Notations

Consider the control volume shown in Fig. (5.2). It is constructed around grid point P (i,j,k) which has E (i+1, j, k) and W (i-1, j, k) as its east and west neighbors, N(i, j+1, k) and S (i, j-1, k) as the north and south neighbors, and T (i, j, k+1) and B (i, j, k-1) as the top and bottom neighbors representing the z-direction. The control volume is formed by six planes $x_{i-1/2}$, $x_{i+1/2}$, $y_{j-1/2}$, $y_{j+1/2}$, $z_{k-1/2}$, and $z_{k+1/2}$. For simplicity, the indices i, j, and k are suppressed. Therefore,

$\phi_{i+1/2} = \phi_{i+1/2,\,j,\,k}$; $\phi_{j+1} = \phi_{i,j+1,k}$ and so on.

The general finite difference equation can be arranged as

$$a_{ijk}\phi_{ijk} = a_{i+1}\phi_{i+1} + a_{i-1}\phi_{i-1} + a_{j+1}\phi_{j+1} + a_{j-1}\phi_{j-1}$$
$$+ a_{k+1}\phi_{k+1} + a_{k-1}\phi_{k-1} + a^o_{ijk}\phi^o_{ijk} + b_{ijk} \quad [5.16]$$

Here,

$$a_{i+1} = A_{i+1/2} + [\![\, -F_{i+1/2},\, 0 \,]\!] , \quad [5.17a]$$

$$a_{i-1} = A_{i-1/2} + [\![\, F_{i-1/2},\, 0 \,]\!] , \quad [5.17b]$$

$$a_{j+1} = A_{j+1/2} + [\![\, -F_{j+1/2},\, 0 \,]\!] , \quad [5.17c]$$

$$a_{j-1} = A_{j-1/2} + [\![\, F_{j-1/2},\, 0 \,]\!] , \quad [5.17d]$$

$$a_{k+1} = A_{k+1/2} + [\![\, -F_{k+1/2},\, 0 \,]\!] , \quad [5.17e]$$

$$a_{k-1} = A_{k-1/2} + [\![\, F_{k-1/2},\, 0 \,]\!] , \quad [5.17f]$$

$$a^o_{ijk} = (\rho^o\theta^o)_{ijk}(\gamma_v\Delta x_i\Delta y_j\Delta z_k)/\Delta t , \quad [5.17g]$$

$$b_{ijk} = S_{c\phi}\gamma_v\Delta x_i\Delta y_j\Delta z_k , \quad [5.17h]$$

and

$$a_{ijk} = a_{i+1} + a_{i-1} + a_{j+1} + a_{j-1} + a_{k+1} + a_{k-1}$$
$$+ a^o - S_{p\phi}\gamma_v\Delta x_i\Delta y_j\Delta z_k . \quad [5.17i]$$

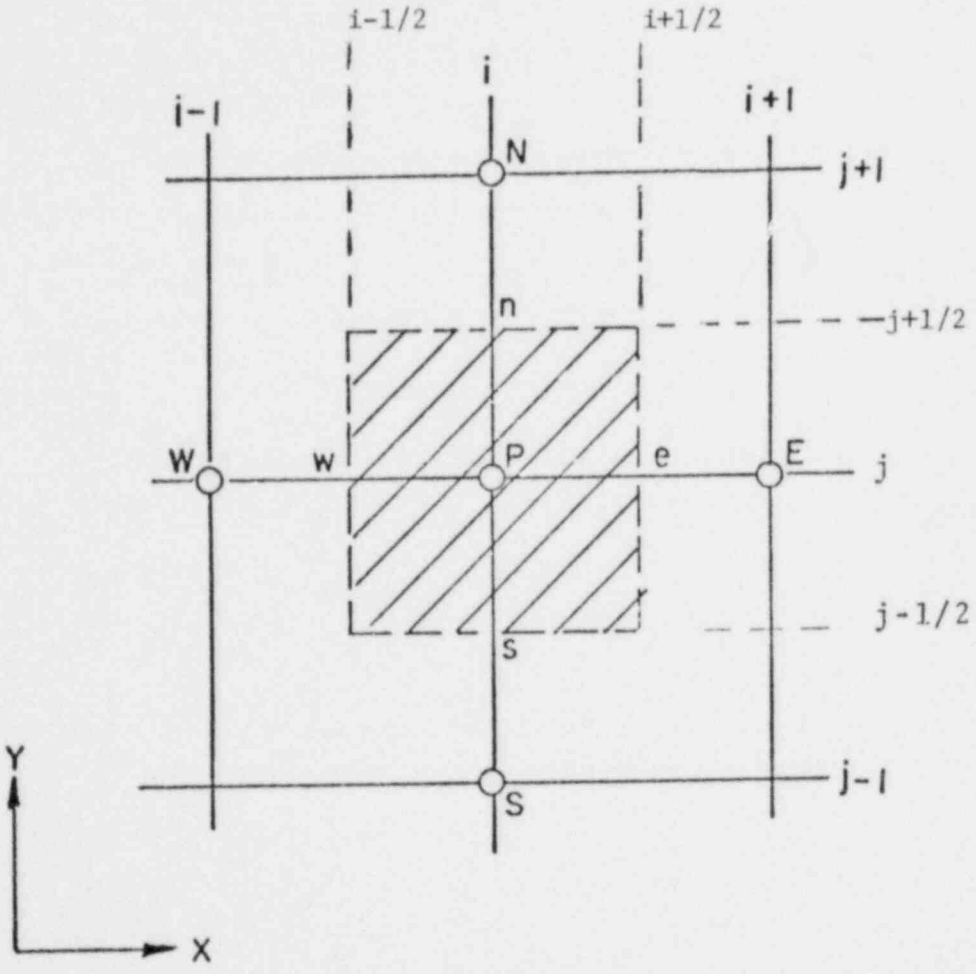

Fig. 5.2 Control volume around point P in ijk notation

The quantities $A_{i+1/2}$, $F_{i+1/2}$, etc., in Eqs. (5.17a) to (5.17f) are defined in the following manner:

$$A_{i+1/2} = D_{i+1/2} \left[\!\left[0, \ (1 - 0.1 \, |F_{i+1/2}/D_{i+1/2}|)^5 \right]\!\right] , \qquad [5.18]$$

$$D_{i+1/2} = \frac{(\Delta y_j \, \Delta z_k) \ (\gamma_x)_{i+1/2}}{\left[\dfrac{\Delta x_i}{2(\Gamma_\phi \theta)_{ijk}} + \dfrac{\Delta x_{i+1}}{2\Gamma_{\phi,i+1}\theta_{i+1}} \right]} , \qquad [5.19]$$

and

$$F_{i+1/2} = (\rho \theta u \gamma_x)_{i+1/2} \Delta y_j \Delta z_k . \qquad [5.20]$$

Similarly for other faces, e.g.

$$A_{k-1/2} = D_{k-1/2} \left[\!\left[0, \ (1 - 0.1 \, |F_{k-1/2}/D_{k-1/2}|)^5 \right]\!\right] , \qquad [5.21]$$

$$D_{k-1/2} = \frac{\Delta x_i \Delta y_j (\gamma_z)_{k-1/2}}{\left[\dfrac{\Delta z_k}{2(\Gamma_\phi \theta)_{ijk}} + \dfrac{\Delta z_{k-1}}{2\Gamma_{\phi,k-1}\theta_{k-1}} \right]}$$

and

$$F_{k-1/2} = (\rho \theta w \gamma_z)_{k-1/2} \Delta x_i \Delta y_j . \qquad [5.23]$$

6. THE FINITE-DIFFERENCE FORM OF MOMENTUM EQUATIONS

Since the momentum equations conform to the general ϕ equation, no separate derivation of their finite-difference form should be necessary. However, because it is desirable to calculate the velocity components for "staggered" locations, as will be explained shortly, some differences of detail arise in constructing the momentum finite-difference equations.

6.1 Staggered Grid

Although all dependent variables are calculated for the grid points, the velocity components u, v, and w of both phases constitute an exception. They are calculated for displaced or "staggered" locations, and not for the grid points. The displaced locations of the velocity components are such that they are placed on the faces of the control volumes. Thus, the x-direction velocity u is calculated at the faces which are normal to the x direction.

Figure 6.1 shows the locations of u and v, by short arrows, on a two-dimensional grid; the three-dimensional counterpart can be easily imagined. With respect to the grid points, the u locations are displaced only in the x direction, the v locations only in the y direction, and so on. The location for u thus lies on the x-direction link joining two adjacent grid points. It is the pressure difference between these grid points that will be used to "drive" the velocity u located between them. This is the main consequence of the staggered grid.

Whether the staggered velocity locations lie exactly midway between the adjacent grid points depends on how the control volumes are defined. The velocity components are located on the control-volume faces, but the latter may or may not be midway between the grid points, as outlined in Section 4.1.

6.2 The Momentum Control Volumes.

A direct consequence of the staggered grid is that the control volumes to be used for the conservation of the momentum must also be staggered. The control volumes shown in Figs. 4.1 and 4.2 will now be referred to as the main control volumes. The control volumes for momentum will be staggered in the direction of the momentum such that its faces normal to that direction pass through the grid points (see figure 6.1). Thus, the pressures at these grid points can be directly used for calculating the pressure force on the momentum control volume. Figure 6.2 shows the control volumes for the x-direction momentum.

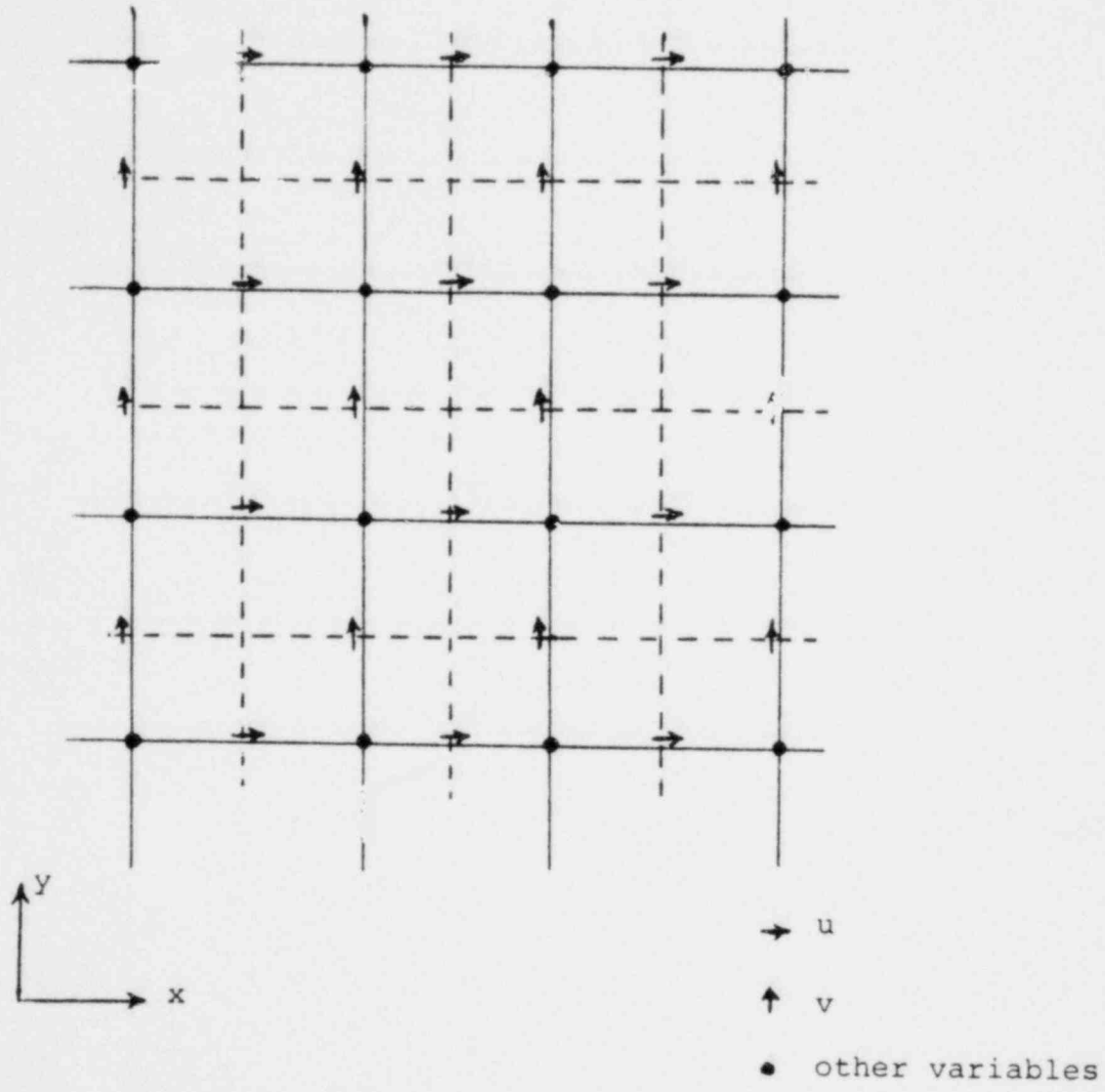

Fig. 6.1 Staggered grid

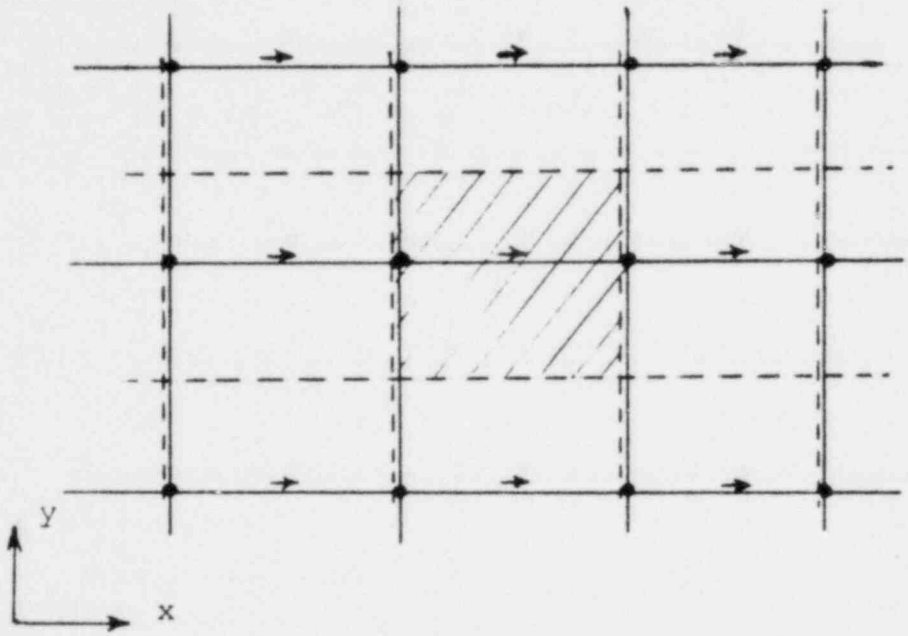

Fig. 6.2 Momentum control volume in x-direction

6.3 The Finite-Difference Equation for Momentum.

All the basic concepts developed in Section 4 and implemented in Section 5 can now be applied to the staggered control volumes for momentum. The differences are mainly geometrical and involve the appropriate calculation of the flow rates and diffusion strengths for the faces of the momentum control volume.

Consider the situation shown in Fig. 6.3. Let F_n and F_{nE} denote the flow rates for the two main control volumes which contribute to the momentum control volum around e. It will be assumed that the calculation of F_n and F_{nE} is already performed. The part of F_n that contributes to the y-direction flow rate at the upper face of the momentum control volume is:

F_n x (distance Pe) / (distance we).

Similarly, the contribution of F_{nE} is:

F_{nE} x (distance eE) / (distance e-eE),

where eE is the point on the right side of E where an arrow is shown in Fig. 6.3. Thus, the total y-direction flow rate at the upper face of the momentum control volume is:

$$F_n \cdot \frac{\text{distance Pe}}{\text{distance we}} + F_{nE} \cdot \frac{\text{distance eE}}{\text{distance e-eE}} .$$

The diffusion quantity for the same face is calculated from

$$D_n \cdot \frac{\text{distance Pe}}{\text{distance we}} + D_{nE} \cdot \frac{\text{distance eE}}{\text{distance e-eE}} .$$

The evaluation of the main-control-volume diffusion strengths D_n and D_{nE} is to be performed in the manner stated in Eq. (4.9).

The x-direction flow rate entering the momentum control volume at P is obtained by linear interpolation:

$$F_p = F_w \cdot \frac{\text{distance Pe}}{\text{distance we}} + F_e \cdot \frac{\text{distance wP}}{\text{distance we}} .$$

The x-direction flow rate entering the momentum control volume at P can be obtained by a linear interpolation between F_w and F_e. The diffusion strength at P is wholly governed by $\Gamma_{\phi p}$ and hence calculated as:

$$D_p = \gamma_x \Delta y \Delta z \Gamma_{\phi p} \partial_p / (\delta x)_{we} . \qquad [6.1]$$

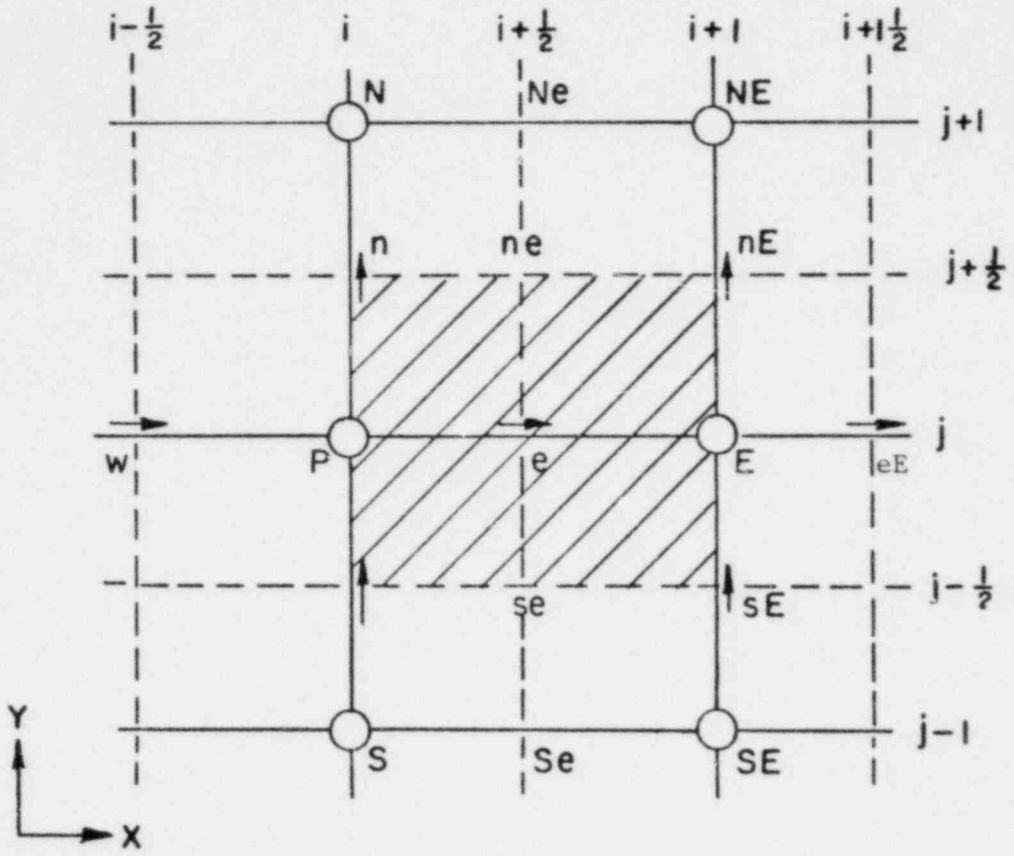

Fig. 6.3 Momentum control volume in relation to the main control volumes

The quantity $(\rho_p^o \theta_p^o \gamma_v \Delta x \Delta y \Delta z)$ in Eq. (5.5g) stands for the mass of fluid contained in the main control volume around point P. The corresponding quantity for the momentum control volume shown in Fig. 6.3 can be obtained by taking the appropriate mass contributions from the main control volumes surrounding points P and E.

With these details, the momentum finite-difference counterpart of Eq. (5.1) can be constructed. One additional feature, however, should now be introduced. As seen from Eq. (2.3), the pressure gradient appears in the momentum equation, but the pressure field is neither known beforehand nor directly obtainable from some sort of "conservation equation for pressure." Thus, pressure must be regarded as unknown and determined indirectly from the constraint that the velocity field satisfies the continuity equation (2.2). For this reason, it is necessary to display separately the pressure-containing terms in the finite-difference form of the momentum equation.

From these considerations, we write the finite-difference equation for the control volume shown in Fig. 6.3 as:

$$a_e u_e = \Sigma a_{nb} u_{nb} + a_e^o u_e^o + b + (\gamma_x \theta \Delta y \Delta z)\ (p_p - p_E) \quad , \qquad [6.2]$$

where the subscript nb denotes a neighbor u and the summation is to be taken over the six neighbors surrounding u_e. The term $a_e^o u_e^o$ arises from the unsteady term in the differential equation; a_e^o is to be calculated similar to a_p^o, as already defined. The definitions of the neighbor coefficients a_{nb} and the center coefficient a_e are identical to those in Eq. (5.2), with appropriate calculations of the flow rates F and diffusion strength D. However, in order to aid computer programming, a few of the coefficients of the finite difference momentum equation are presented here in i,j,k notation.

$$a_{Ne} = a_{i+1/2,j+1} = A_{i+1/2,j+1/2} + [\![-F_{i+1/2,j+1/2}, 0]\!], \qquad [6.3a]$$

$$a_w = a_{i-1/2} = A_{i,j,k} + [\![F_{i,j,k}, 0]\!], \qquad [6.3b]$$

$$a_{Se} = a_{i+1/2,\, j-1} = A_{i+1/2,j-1/2} + [\![F_{i+1/2,j-1/2}, 0]\!], \qquad [6.3c]$$

$$A_{ne} = A_{i+1/2,j+1/2} =$$

$$= D_{i+1/2,j+1/2}\ [\![0,\ (1 - 0.1|F_{i+1/2,j+1/2}/D_{i+1/2,j+1/2}|)^5]\!] \qquad [6.4]$$

$$F_{ne} = F_{i+1/2,j+1/2} =$$

$$= \frac{1}{2} (\rho\theta v)_{i+1/2,j+1/2} \left[\gamma_{y_{j+1/2}} \Delta x_i + \gamma_{y_{i+1,j+1/2}} \Delta x_{i+1} \right] \Delta z_k \qquad [6.5]$$

$$D_{ne} = D_{i+1/2,j+1/2} =$$

$$= \frac{1}{2} \left(\Delta x_i \gamma_{y_{j+1/2}} + \Delta x_{i+1} \gamma_{y_{i+1,j+1/2}} \right)$$

$$\left[\frac{\Delta x_i}{(\mu\theta + \mu_{i+1}\theta_{i+1})} + \frac{\Delta x_{i+1}}{(\mu_{j+1}\theta_{j+1} + \mu_{i+1,j+1}\theta_{i+1,j+1})} \right] \qquad [6.6]$$

The contributions of the source term that enter a_e and b do not contain the pressure gradient; the effect of the pressure gradient is expressed by the last term in Eq. (6.2), where $(\gamma_x \Delta y \Delta z)$ is the area on which the pressure drop $(p_p - p_E)$ acts. The momentum equations for the y- and z- directions can be obtained in a similar manner.

6.4 Velocity-Pressure Relationships.

In order to convert the indirect specification of pressure contained in the continuity equation into a direct algorithm for calculating pressure, we need to establish relationships between the velocity components and corresponding pressure drops. For this purpose, let us define a pseudo-velocity by:

$$\hat{u}_e \equiv [\Sigma a_{nb} u_{nb} + a_e^o u_e^o + b]/a_e \quad . \qquad [6.7]$$

This enables us to write Eq. (6.2) as:

$$u_e = \hat{u}_e + d_e [p_p - p_E], \qquad [6.8]$$

where

$$d_e \equiv [\gamma_x \theta \Delta y \Delta z]/a_e \quad . \qquad [6.9]$$

Pseudo-velocities $\hat{v}$ and $\hat{w}$ can be similarly obtained from the corresponding momentum equations.

If we now imagine that the pressure changes from a guessed value p* to a new value p, the corresponding change in the velocity can be expressed as:

$$u_e - u_e^* = d_e [(p_p - p_p^*) - (p_E - p_E^*)] \qquad [6.10]$$

where we have assumed that the change in $\hat{u}_e$ is unimportant. If the change in pressure is denoted by the "pressure correction" p', i.e.,

$$p = p^* + p' \quad , \qquad [6.11]$$

we can derive a velocity-correction formula from Eq. (6.10) as:

$$u_e = u_e^* + d_e [p'_p - p'_E] \quad . \qquad [6.12]$$

Here u_e^* is the value of u_e given by Eq. (6.2) when the guessed value p* is substituted for the pressure p.

The similarity between Eqs. (6.8) and (6.12) should be noted.

7. FINITE-DIFFERENCE FORMS OF THE CONTINUITY EQUATIONS

7.1 Phase Continuity Equation

We can see that the phase continuity equation has the same form as the general Eq. (2.9) without the diffusion term. We can therefore, make $\Gamma_\theta = 0$ and use the formulations described in Section 5. It may be noted here that due to the absence of the diffusion turn, the final finite-difference equations that we obtain correspond to the equations that we obtain by upwind differencing.

The finite-difference equation for void fraction θ_1 of phase 1 can be arranged as:

$$a_p\theta_{1p} = a_{ijk}(\theta_1)_{ijk} = a_{i+1}(\theta_1)_{i+1} + a_{i-1}(\theta_1)_{i-1} + a_{j+1}(\theta_1)_{j+1} + a_{j-1}(\theta_1)_{j-1} + a_{k+1}(\theta_1)_{k+1} + a_{k-1}(\theta_1)_{k-1} + a^o_{ijk}(\theta_1)^o_{ijk} + b, \quad [7.1]$$

where

$$a_{i+1} = [\![-F_{i+1/2},\ 0\ ]\!], \quad [7.2a]$$

$$a_{i-1} = [\![\ F_{i-1/2},\ 0\ ]\!], \quad [7.2b]$$

$$a_{j+1} = [\![-F_{j+1/2},\ 0\ ]\!], \quad [7.2c]$$

$$a_{j-1} = [\![\ F_{j-1/2},\ 0\ ]\!], \quad [7.2d]$$

$$a_{k+1} = [\![-F_{k+1/2},\ 0\ ]\!], \quad [7.2e]$$

$$a_{k-1} = [\![\ F_{k-1/2},\ 0\ ]\!], \quad [7.2f]$$

$$a^o_{ijk} = [\rho^o_1\gamma_v]_{ijk}[\Delta x_i\Delta y_j\Delta z_k]\ /\ \Delta t, \quad [7.2g]$$

$$b_{ijk} = \Omega_1\gamma_v\Delta x_i\Delta y_j\Delta z_k, \quad [7.2h]$$

$$\bar{a}_{i+1} = [\![\ F_{i+1/2},\ 0\ ]\!], \quad [7.2i]$$

$$\bar{a}_{i-1} = [\![-F_{i-1/2},\ 0\ ]\!], \quad [7.2j]$$

$$\bar{a}_{j+1} = [\![\ F_{j+1/2},\ 0\ ]\!], \quad [7.2k]$$

$$\bar{a}_{j-1} = [\![-F_{j-1/2},\ 0\ ]\!], \quad [7.2\ 1]$$

$$\bar{a}_{k+1} = [\![\ F_{k+1/2},\ 0\ ]\!], \quad [7.2m]$$

$$\bar{a}_{k-1} = [\![-F_{k-1/2},\ 0\ ]\!], \quad [7.2n]$$

$$\bar{a}^o_{ijk} = (\rho_v\gamma_v)_{ijk}(\Delta x_i\Delta y_j\Delta z_k)/\Delta t, \quad [7.2\ o]$$

and

$$a_{ijk} = \bar{a}_{i+1} + \bar{a}_{i-1} + \bar{a}_{j+1} + \bar{a}_{j-1} + \bar{a}_{k+1} + \bar{a}_{k-1} + \bar{a}^{o} \quad . \qquad [7.2p]$$

The coefficients without overscore represent "inflows" while the coefficients with overscore represent "outflows". The quantities F appearing in equation (7.2) are as defined previously but without void fraction. Thus

$$F_{i+1/2} = (\rho_1 u_1 \gamma_x)_{i+1/2} \Delta y_j \Delta z_k \quad . \qquad [7.3]$$

The finite-difference equation for void fraction θ_2 is similar.

7.2 Combined Continuity Equation

The combined continuity equation, Eq. (2.2b) is integrated over the control volume as shown in Fig. 5.1 to yield:

$$\begin{aligned} &\left\{\left[(\rho_1\theta_1 u_1 + \rho_2\theta_2 u_2)\gamma_x\right]_w - \left[(\rho_1\theta_1 u_1 + \rho_2\theta_2 u_2)\gamma_x\right]_e\right\} (\Delta y \Delta z) \\ &+ \left\{\left[(\rho_1\theta_1 v_1 + \rho_2\theta_2 v_2)\gamma_y\right]_s - \left[(\rho_1\theta_1 v_1 + \rho_2\theta_2 v_2)\gamma_y\right]_n\right\} (\Delta z \Delta x) \\ &+ \left\{\left[(\rho_1\theta_1 w_1 + \rho_2\theta_2 w_2)\gamma_z\right]_b - \left[(\rho_1\theta_1 w_1 + \rho_2\theta_2 w_2)\gamma_z\right]_t\right\} (\Delta x \Delta y) \\ &+ \left[(\rho_1\theta_1 + \rho_2\theta_2)^{o} - (\rho_1\theta_1 + \rho_2\theta_2)\right] (\gamma_v \Delta x \Delta y \Delta z/\Delta t) = 0 \end{aligned} \qquad [7.4]$$

We use the two phase continuity equations to compute the void fractions, and the combined continuity equation (7.4) for determining the pressure correction. Since the pressure or the pressure correction do not appear here, further manipulation is needed to derive the finite-difference equations for p and p'.

8. PRESSURE AND PRESSURE CORRECTION EQUATIONS

8.1 Pressure Equation

Substitution of the velocity-pressure relations such as Eq. [6.8] into Eq. [7.4] leads to:

$$a_p P_p = a_E P_E + a_W P_W + a_N P_N + a_S P_S + a_B P_B + b \ , \qquad [8.1]$$

where

$$a_E = \left\{ \left(\rho_1 \theta_1 d_1 + \rho_2 \theta_2 d_2 \right) \gamma_x \right\}_e \quad (\Delta y \Delta z) \ , \qquad [8.2a]$$

$$a_W = \left\{ \left(\rho_1 \theta_1 d_1 + \rho_2 \theta_2 d_2 \right) \gamma_x \right\}_w \quad (\Delta y \Delta z) \ , \qquad [8.2b]$$

$$a_N = \left\{ \left(\rho_1 \theta_1 d_1 + \rho_2 \theta_2 d_2 \right) \gamma_y \right\}_n \quad (\Delta x \Delta z) \ , \qquad [8.2c]$$

$$a_S = \left\{ \left(\rho_1 \theta_1 d_1 + \rho_2 \theta_2 d_2 \right) \gamma_y \right\}_s \quad (\Delta x \Delta z) \ , \qquad [8.2d]$$

$$a_B = \left\{ \left(\rho_1 \theta_1 d_1 + \rho_2 \theta_2 d_2 \right) \gamma_z \right\}_b \quad (\Delta x \Delta y) \ , \qquad [8.2e]$$

$$a_T = \left\{ \left(\rho_1 \theta_1 d_1 + \rho_2 \theta_2 d_2 \right) \gamma_z \right\}_t \quad (\Delta x \Delta y) \ , \qquad [8.2f]$$

$$a_p = a_E + a_W + a_N + a_S + a_T + a_B \ , \qquad [8.2g]$$

and,

$$\begin{aligned} b = & \left\{ \left[(\rho_1 \theta_1 \hat{u}_1 + \rho_2 \theta_2 \hat{u}_2) \gamma_x \right]_w - \left[(\rho_1 \theta_1 \hat{u}_1 + \rho_2 \theta_2 \hat{u}_2) \gamma_x \right]_e \right\} (\Delta y \Delta z) \\ & + \left\{ \left[(\rho_1 \theta_1 \hat{v}_1 + \rho_2 \theta_2 \hat{u}_2) \gamma_y \right]_s - \left[(\rho_1 \theta_1 \hat{u}_1 + \rho_2 \theta_2 \hat{u}_2) \gamma_y \right]_n \right\} (\Delta x \Delta z) \\ & + \left\{ \left[(\rho_1 \theta_1 \hat{w}_1 + \rho_2 \theta_2 \hat{w}_2) \gamma_z \right]_b - \left[(\rho_1 \theta_1 \hat{w}_1 + \rho_2 \theta_2 \hat{w}_2) \gamma_z \right]_t \right\} (\Delta x \Delta y) \\ & + \left[(\rho_1 \theta_1 + \rho_2 \theta_2)^o - (\rho_1 \theta_1 + \rho_2 \theta_2) \right] (\gamma_v \Delta x \Delta y \Delta z / \Delta t) \end{aligned} \qquad [8.2h]$$

8.2 Pressure Correction Equation 1

In this section we have derived the pressure correction equation for two-phase flow by extending the 'SIMPLER' procedure for single phase. If we sub-titute Eq. [6.12] (and similar velocity-correction formulas for v and w) into Eq. [7.4], we get the pressure correction equation

$$a_P p'_P = a_E p'_E + a_W p'_W + a_N p'_N + a_S p'_S + a_T p'_T + a_B p'_B + b \quad , \qquad [8.3]$$

where a_E, a_W, a_N, a_S, a_T, a_B, and a_p are given by Eqs. [8.2a] to [8.2g], and b is given by

$$\begin{aligned} b = &\left\{ \left[(\rho_1\theta_1 u^*_1 + \rho_2\theta_2 u^*_2)\gamma_x \right]_w - \left[(\rho_1\theta_1 u^*_1 + \rho_2\theta_2 u^*_2)\gamma_x \right]_e \right\} (\Delta y \Delta z) \\ &+ \left\{ \left[(\rho_1\theta_1 v^*_1 + \rho_2\theta_2 v^*_2)\gamma_y \right]_s - \left[(\rho_1\theta_1 v^*_1 + \rho_2\theta_2 v^*_2)\gamma_y \right]_n \right\} (\Delta x \Delta z) \\ &+ \left\{ \left[(\rho_1\theta_1 w^*_1 + \rho_2\theta_2 w^*_2)\gamma_z \right]_b - \left[(\rho_1\theta_1 w^*_1 + \rho_2\theta_2 w^*_2)\gamma_z \right]_t \right\} (\Delta x \Delta y) \\ &+ \left[(\rho_1\theta_1 + \rho_2\theta_2)^o - (\rho_1\theta_1 + \rho_2\theta_2) \right] (\gamma_v \Delta x \Delta y \Delta z / \Delta t). \end{aligned} \qquad [8.4]$$

The similarity between Eqs. [8.2h] and [8.4] should be noted. The only difference between the two equations is that, whereas the b for the pressure equation is calculated in terms of $\hat{u}$, $\hat{v}$, and $\hat{w}$, the corresponding quantity for the pressure correction equation is obtained in terms of u^*, v^*, and w^*.

8.3 Pressure Correction Equation 2

The pressure correction equation derived in this section is based on the procedure very similar to the numerical procedure known as IPSA[2]. In this procedure we differentiate the phase continuity equations and momentum equations and combine them with the condition

$$\theta_1 + \theta_2 = 1 \qquad [8.5]$$

to obtain the pressure correction equation.

Let us assume that we have an estimated pressure field p^*. We can then solve the momentum equations to obtain velocity fields u^*_1, v^*_1 and w^*_1 for phase 1 and u^*_2, v^*_2 and w^*_2 for phase 2. These velocity fields can be used in the continuity equations to obtain void fractions θ^*_1 and θ^*_2. As the void fractions are based on estimated pressure field p^*, they will, in general, not add up to 1. We, therefore, require the corrections to void fractions θ'_1 and θ'_2 such that

$$\left(\theta^*_1 + \theta'_1\right) + \left(\theta^*_2 + \theta'_2\right) = 1 \quad , \qquad [8.6]$$

or

$$\theta'_1 + \theta'_2 = 1 - \theta^*_1 - \theta^*_2 \quad . \qquad [8.6a]$$

Now from Eq. [7.1], the void fraction for phase 1 is given by

$$\theta_1^* = \frac{\left(\sum_{n=1}^{n=6} a_{1n}\theta_{1n}^*\right)_{inflow} + a_1^o\theta_1^o + b_1}{\left(\sum_{n=1}^{n=6} \bar{a}_{1n}\right)_{outflow} + \bar{a}_{1o}} = \frac{\beta_1}{\alpha_1} \quad . \qquad [8.7]$$

Here the subscript n refers to six neighboring points. From Eq. [8.7] we derive a void fraction correction formula.

$$\theta_1' = \frac{\alpha_1\left(\sum_{n=1}^{n=6} a_{1n}'\theta_{1n}^*\right)_{inflow} - \beta_1\left(\sum_{n=1}^{n=6} \bar{a}_{1n}'\right)_{outflow}}{\alpha_1^2} \quad , \qquad [8.8a]$$

or

$$\theta_1' = \frac{\left(\sum_{n=1}^{n=6} a_{1n}'\theta_{1n}^*\right)_{inflow} - \theta_1^*\left(\sum_{n=1}^{n=6} \bar{a}_{1n}'\right)_{outflow}}{\alpha_1} \quad . \qquad [8.8b]$$

Here a_{1n}' and $\bar{a}_{1n}'$ are the changes in coefficients due to pressure correction p'.

In order to determine a_{1n}' and $\bar{a}_{1n}'$ we look at the coefficients $(a_1)_{i+1}$ and $(\bar{a}_1)_{i+1}$ (Eq. [7.2]) making note that the coefficients a_{1n} and $\bar{a}_{1n}$ exist only for inflows and outflows, respectively (Eq. [7.2]);

$$(a_1)_{i+1} = |F_{i+1/2}|_{inflow} = -(\rho_1)_{i+1}(u_1^*\gamma_x)_{i+1/2}\Delta y_j\Delta z_k \quad , \qquad [8.9a]$$

and

$$(\bar{a}_1)_{i+1} = (F_{i+1/2})_{outflow} = \rho_{1i}(u_1^*\gamma_x)_{i+1/2}\Delta y_j\Delta z_k \quad . \qquad [8.9b]$$

Combining Eq. [8.9] with Eq. [6.12] we get

$$(a_1')_{i+1} = (\rho_1)_{i+1}(\gamma_x d_1)_{i+1/2}\Delta y_j\Delta z_k\,(p_{i+1}' - p_i') \quad , \text{ (inflow only)} \qquad [8.10a]$$

and

$$(\bar{a}_1')_{i+1} = (\rho_1)_i(\gamma_x d_1)_{i+1/2}\Delta y_j\Delta z_k\,(p_i' - p_{i+1}') \quad \text{(outflow only)} \qquad [8.10b]$$

Equations for other neighboring coefficients and for phase 2 can be obtained in an identical manner. We now substitute all these coefficients in Eqs. [8.7] and [8.8a]. After simplification we get

$$\theta_1' = \frac{1}{\alpha_1}\left\{\underset{\substack{\text{inflow}\\ \text{only}}}{\sum_{n=1}^{n=6}} (\rho_1 Ad_1 \theta_1^*)_n \quad (p_n' - p_p') \right.$$

$$\left. -(\rho_1\theta_1^*)_{ijk} \underset{\substack{\text{outflow}\\ \text{only}}}{\sum_{n=1}^{n=6}} (Ad_1)_n \ (p_p' - p_n') \right\} , \qquad [8.11a]$$

$$\theta_2' = \frac{1}{\alpha_2}\left\{\underset{\substack{\text{inflow}\\ \text{only}}}{\sum_{n=1}^{n=6}} (\rho_2 Ad_2 \theta_2^*)_n \quad (p_n' - p_p') \right.$$

$$\left. - (\rho_2\theta_2^*)_{ijk} \underset{\substack{\text{outflow}\\ \text{only}}}{\sum_{n=1}^{n=6}} (Ad_2)_n \ (p_p' - p_n') \right\} , \qquad [8.11b]$$

and

$$\left\{1 - (\theta_1^* + \theta_2^*)\right\} = \underset{\substack{\text{inflow}\\ \text{only}}}{\sum_{n=1}^{n=6}} \left\{\left[\frac{(\rho_1 Ad_1 \theta_1^*)_n}{\alpha_1} + \frac{(\rho_2 Ad_2 \theta_2^*)_n}{\alpha_2}\right]\right.$$

$$+ \left[\frac{(Ad_1)_n}{\alpha_1} (\rho_1\theta_1^*)_{ijk} + \frac{(Ad_2)_n}{\alpha_2} (\rho_2\theta_2^*)_{ijk} \right] \Bigg\} \quad p_n'$$

outflow only

$$- p'_{ijk} \Bigg\{ \sum_{n=1}^{n=6} \left[\frac{(\rho_1 Ad_1\theta_1^*)_n}{\alpha_1} + \frac{(\rho_2 Ad_2\theta_2^*)_n}{\alpha_2} \right]$$

inflow only

$$+ \sum_{n=1}^{n=6} \left[\frac{(Ad_1)_n}{\alpha_1} (\rho_1\theta_1^*)_{ijk} + \frac{(Ad_2)_n}{\alpha_2} (\rho_2\theta_2^*)_{ijk} \right] \Bigg\} \quad . \qquad [8.12]$$

outflow only

Here A represents the cross sectional area, e.g.

$$A_{i+1} = (\gamma_x)_{i+1/2} \Delta y_j \Delta z_k \ , \qquad [8.13a]$$

$$A_{i-1} = (\gamma_x)_{i-1/2} \Delta y_j \Delta z_k \ . \qquad [8.13b]$$

Eq. [8.12] is our final pressure correction equation. After solving for pressure corrections (Eq. [8.12]) we use Eqs. [8.11] for computing void fraction corrections. The velocities and void fractions are then modified to account for these corrections.

9. BOUNDARY CONDITIONS

9.1 Preliminary Considerations

Within the general framework outlined in this report, a variety of boundary-condition practices can be used. The practices that are suggested in this section have been found to be convenient, but the general numerical method is in no way restricted to these particular practices.

At first, it will be assumed that the calculation domain has the shape of a rectangular box. The boundary-condition treatment for such a domain will be outlined. Later, it will be explained how actual boundaries internal to this nominal domain can be accommodated.

Design of Control Volumes

The calculation domain will be divided such that the control volumes fill the entire domain. The boundaries of the domain will be both control-volume faces and the grid-point locations. The scheme is illustrated in Fig. 9.1. An advantage of this design is that it can be conveniently used whether the boundary value of ϕ or the corresponding boundary flux is specified. Further, since the control volumes fill the entire domain, the integral conservation is always satisfied. Lastly, the presence of a grid point on the boundary surface enables us to use the values of Γ and ρ there directly for the calculation of diffusion flux mass-flow rate across the boundary.

9.2 Initial Conditions

Generally, before the solution sequence can begin, all values of variables must be assigned. This can be accomplished by either continuing a previous run via the restart capability or by specifying the initial temperature, pressure, and velocity distribution throughout the interior points of the space under consideration. When the initialization is not a restart, density and enthalpy can be calculated from equations of state, using the specified pressures and temperatures. If the determination of these distributions and their subsequent input into the code are found to be tedious, certain options[8] can be provided to ease the initialization task. When a steady-state solution is being sought, an initialization as close as possible to the expected solution should be used to reduce computer running time.

Pressure Initialization for Static Head

When gravity is acting along any of the three principal coordinate axes and there is either constant or one-dimensional temperature variation in that same direction, an option can be used to reduce the initialization task. This

option can be exercised by specifying a pressure at a point and either the constant or one-dimensional temperature variation. The entire temperature field can be generated from the input temperature information. The density field can then be computed by the equation of state. With this density field and the point pressure, a pressure field can be generated to account for the static head. From the pressure and temperature fields, the enthalpy can be obtained, thus completing this initialization option.

Pressure-drop Initialization

A linear variation or constant-pressure-gradient initialization option can also be used as in COMMIX-1[8]. This can be used when the constant pressure gradient is along any one of the three principal axes. It is accomplished by specifying the constant pressure gradient as either $\partial P/\partial x$, $\partial P/\partial y$, or $\partial P/\partial z$, and a point pressure. This option can be used along with the static-head initialization. However, if the constant pressure gradient is along the same axis as gravity, the pressure gradient due to gravity must be included in the specification of the constant pressure gradient.

Initial Values for Turbulence Quantities

For the correct specification of the mathematical problem, the initial values of all the dependent variables, which include the turbulence quantities such as k, ε, must be specified.

Often, however, this information is unavailable and must be guessed. It is usually reasonable to assume that the turbulence kinetic energy at a point is about 1% to 10% of the mean-motion kinetic energy at that point. The value of ε is harder to guess. One may be able to estimate the mixing length for a given situation and derive the value of ε from it. If L is the mixing length, the corresponding value of ε is given by

$$\varepsilon = c_\mu^{3/4} \, k^{3/2}/L \qquad [9.1]$$

where c_μ is a constant ($c_\mu = 0.09$ usually). Alternatively, one may adjust ε such that the Reynolds number based on the turbulent viscosity μ_t (where $\mu_t = c_\mu \rho k^2/\varepsilon$) and a characteristic length scale is of the order of 500.

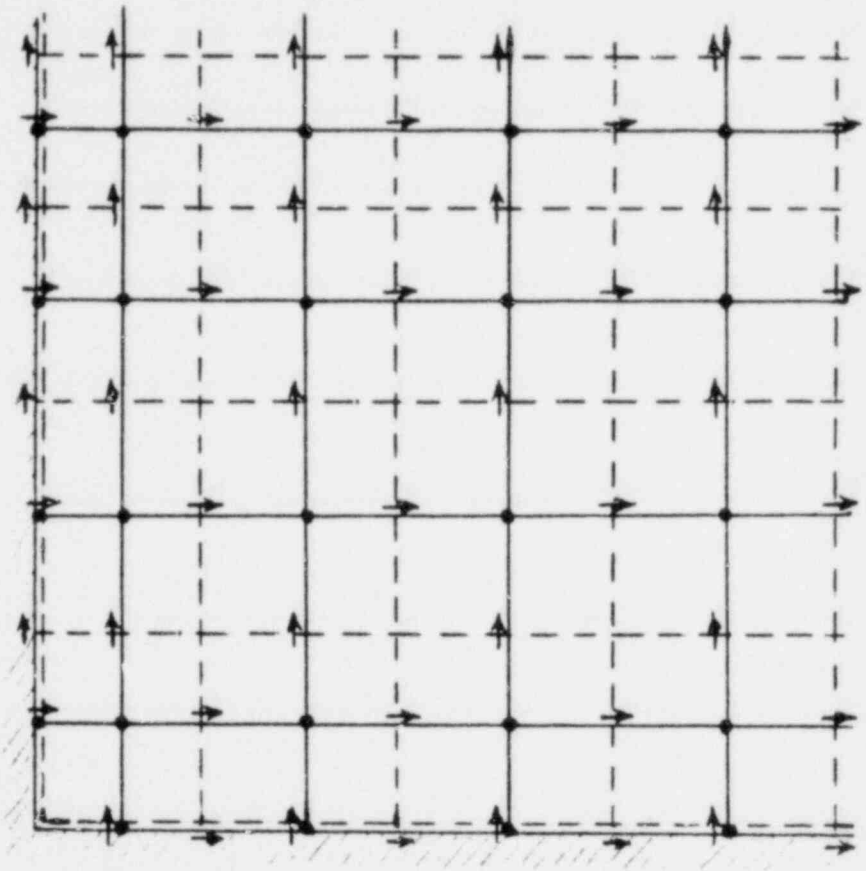

Fig. 9.1 Design of near-boundary control volumes

9.3 Boundary Conditions for the General ϕ Equation

Given Value of the Dependent Variable

The simplest treatment of the boundary condition is available when the value of the dependent variable is specified at the boundary. This occurs at the walls of known temperature, and at the inflow boundaries. When fluid enters a calculation domain, we normally know the values of ϕ it brings with it. If this information is not obtainable, the problem is not properly posed. A no-slip wall simply indicates that the velocity at the wall is known to be zero. No special treatment is needed when the value of ϕ at the boundary is known. The boundary value will simply appear as one of the neighbors of the near-boundary grid point, and its influence will be correctly felt in the solution.

Given Flux at the Boundary

Since for the near-boundary control volume, a face of the control volume coincides with the boundary, the known flux at the boundary surface can be incorporated as an additional source term for the control volume. At the same time, the coefficient connecting the unknown boundary value of ϕ should be set equal to zero.

The given flux situation arises when the heat flux at a wall is given. Also, any surface of symmetry represents a zero-flux situation. Further, an outflow boundary can be treated as a zero-flux situation, as will be explained below.

At an outflow boundary, the boundary value of ϕ is normally not known. Further, there is no need to know it since the value lies on the downstream side of the calculation domain and is thus unable to influence the solution. Thus, setting the coefficient of that boundary value to zero is all that is needed to treat an outflow boundary. Since this is all that we do at a zero-flux boundary, the treatment for an outflow boundary turns out to be identical to that of a zero-flux boundary.

Lastly, a slip wall is also to be treated by setting the boundary-value coefficient equal to zero.

Incorporation of Wall Functions

When the flow is turbulent, and the turbulence model accounts for only the fully turbulent region, the near-wall region (where the laminar and turbulent transports are comparable) is usually handled by way of wall functions. The use of wall functions for the k-ε model is described in [7]. The computational aspects of wall functions are illustrated here.

The wall functions described here have been based on a rather simple situation, namely a zero-pressure-gradient, uniform-property-flow near an impermeable wall. That they can often be used in more complex situations with reasonable success is a consequence of the thinness of the wall layer to which they apply. In a thin layer, the effects of pressure gradient, property variation or mass transfer are likely to have only a second-order importance. By the same argument, the curvature of the wall can be ignored, for the purpose of the wall functions, in the immediate vicinity of the wall. Thus, the wall functions for a flat plate can often be used near a pipe wall without modification.

The purpose of the wall functions is to provide the correct value of the relevant diffusion flux at the wall boundary. This can be accomplished either by specifying an additional source term for the near-wall control volume or by using an appropriate value of Γ at the boundary.

Let B denote a boundary location and P the grid point in the near-boundary control volume. The distance, normal to the wall, between P and B is given by δ.

The requirement that the velocity distribution near the wall conform to the "law of the wall" can be expressed via the following expression for the boundary Γ for the velocity.

$$\left.\begin{aligned} \Gamma_B &= \mu && \text{for } y^+ \leq 11.5 \\ &= \mu y^+ \kappa / \ln(Ey^+) && \text{for } y^+ > 11.5 \end{aligned}\right\} \qquad [9.2]$$

Here μ is the laminar viscosity, κ and E are constants (usually taken as: $\kappa = 0.4$, $E = 9.0$), and y^+ is defined by

$$y^+ \equiv \rho k_p^{1/2} c_\mu^{1/4} \delta / \mu \ , \qquad [9.3]$$

where k is the turbulence kinetic energy, and c_μ is a constant ($c_\mu = 0.09$).

For the energy equation, the corresponding wall value of Γ is given by

$$\left.\begin{aligned} \Gamma_B &= \mu/Pr && \text{for } y^+ \leq 11.5 \\ &= \mu y^+ \Big/ \left\{ Pr_t \left[(1/\kappa) \ln(Ey^+) + P \right] \right\} && \text{for } y^+ > 11.5 \end{aligned}\right\} \qquad [9.4]$$

where Pr and Pr_t stand for the laminar and turbulent Prandtl numbers respectively, and P is the so-called resistance of the laminar sublayer, given by

$$P = 9.0(Pr/Pr_t - 1)\ (Pr/Pr_t)^{-1/4} \qquad [9.5]$$

There is insufficient evidence and well-coordinate knowledge about the variation of the turbulent Prandtl number in complex situations. If a constant value of the turbulent Prandtl number Pr_t is to be used, a value around 0.9 is found to be appropriate for flow near walls, while $Pr_t = 0.5$ seems to be applicable to free jets and wakes.

Calculation of Boundary Coefficients

For the situation shown in Fig. 9.2, the calculation of the coefficient a_W in the finite-difference equation for ϕ_P will now be explained.

a_W is still defined by Eq. [5.2b], but the flow rate F_w is now to be calculated from the density and velocity stored at point W. Thus,

$$F_w = \rho_W u_W \gamma_x \Delta y \Delta z \quad . \tag{9.6}$$

Also, the diffusion conductance D_w should be calculated from Γ_W alone. That is,

$$D_w = (\gamma_x \Delta y \Delta z)\, \Gamma_W / (\delta_x)_{WP} \quad . \tag{9.7}$$

9.4 Boundary Conditions for the Press[illegible]d Pressure-Correction Equations

Since the continuity equation has been reformulated as the pressure equation and the pressure-correction equation, special attention should be given to the boundary conditions for these equations. Normally, either the velocity normal to the boundary is specified or the pressure at the boundary is given.

Given Normal Velocity at the Boundary

A control volume adjacent to a boundary is shown in Fig. 9.2. If the velocity u_W entering the control volume at the boundary face is known, then, in the derivation of the pressure and pressure-correction equations, we would not substitute u_W in terms of $\hat{u}_W$ or u_W^*; we would directly use the known value of u_W. Thus, p_W or p'_W would not appear in the p or p' equations. In other words, the coefficient a_W will be zero in these equations. Since this boundary coefficient is zero, no information about the boundary pressure is needed.

The given velocity boundary condition occurs at walls, symmetry planes, and inflow boundaries with known flow rate. Even the outflow boundaries can be treated as known-velocity boundaries by specifying the normal velocity there by reference to overall mass conservation. Only when the flow rates are unknown, but the pressure drop is specified, do we need to turn to the given-pressure boundary condition.

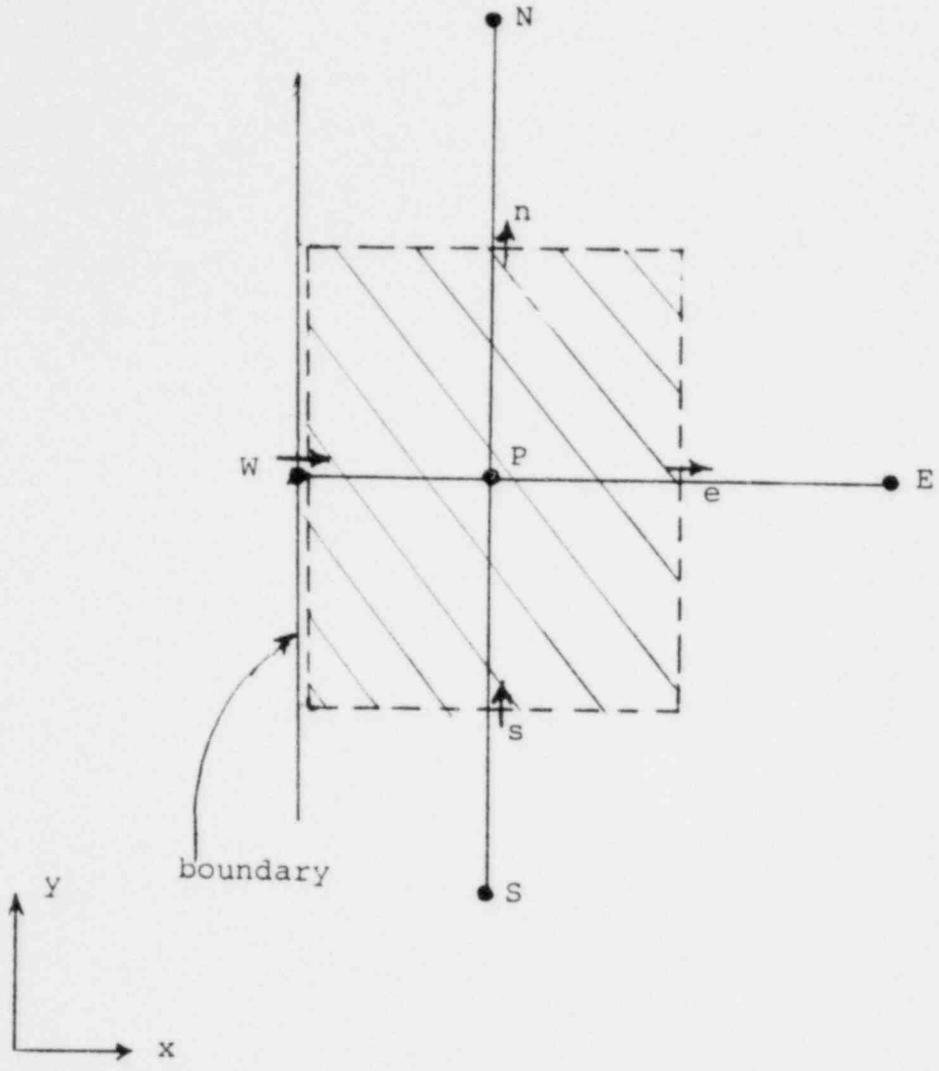

Fig. 9.2 Near-boundary control volume

Given Pressure at the Boundary

When the pressure at the boundary point W in Fig. 9.2 is known, the situation is straightforward. For the pressure equation, the known value p_W is to be used in the appropriate neighbor term. Further, if p_W^* is set equal to p_W, we shall have $p_W' = 0$, which serves as the known boundary value for the pressure-correction equation.

9.5 Boundary Values for Turbulence Quantities

For the boundary values of all the turbulence quantities such as k, ε, the correct specification of the values at all inflow boundaries must be given so that we know what turbulence level and scale are brought into the calculation domain by the incoming streams. Many a times, this information is unavailable and must be guessed.

Fortunately, in many situations the flow within the calculation domain is so complex that it is insensitive to the boundary values of k and ε convected by the inflow streams. The reason is that a complex flow causes substantial generation of k and ε within the domain. The distribution of k and ε is thus largely governed by the source terms and only very weakly by the convection terms. It is then sufficient to assume that the inflow streams bring rather small values of k and ε and show that the results are independent of the exact magnitude of these small values.

9.6 Irregular Geometries

When the actual boundaries of the calculation domain do not coincide with the boundaries of the nominal (rectangular) domain, special treatment is needed to incorporate the "internal" boundaries. Two practices are suggested below, which could be used in combination if desired. When the boundary is internal to the nominal calculation domain, the grid should be so designed that the actual boundary is suitably approximated by a succession of control-volume faces. Figure 9.3 illustrates this for a solid obstacle projecting into the nominal calculation domain. The dashed lines indicate the control-volume faces, while the shaded area denotes the obstacle.

The treatment of irregular boundaries through appropriate choice of the Γ's is described in [6]. When ϕ stands for velocity, the corresponding values of Γ for the control volumes that lie in the solid can be made very large. This results in very small (essentially zero) values of velocity predicted for

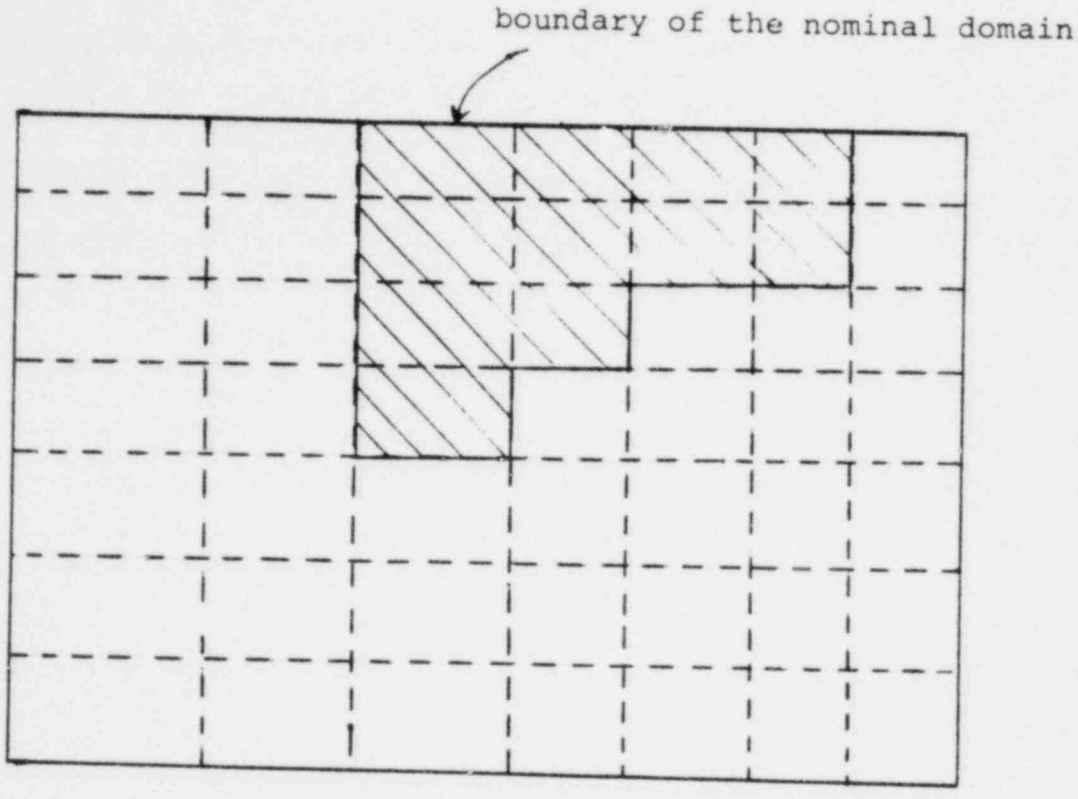

Fig. 9.3 Design of control volumes for irregular geometry

the solid region. A given value of ϕ, such as temperature, can also be arranged at the internal boundary by making the Γ values for the solid large and by specifying the given value of ϕ at the nominal boundary adjacent to the solid. An adiabatic surface, on the other hand, can be simulated by the use of a very low Γ_h for the solid.

An alternative practice for the treatment of internal boundaries works through the use of the source term. The given fluxes at the actual boundary can be incorporated as additional sources into the appropriate near-boundary control volumes. If the boundary values of the dependent variable are given, they can be established at the desired grid points by the following specification of S_C and S_p for those points

$$S_C = M\phi_{given} \quad , \qquad [9.8]$$

$$S_p = -M \quad , \qquad [9.9]$$

where M is a large number (say, 10^{30}). The consequence of these large sources is that they alone dominate the finite-difference equation which then reduces to

$$\phi_p \approx \phi_{given} \quad . \qquad [9.10]$$

10. SOLUTION OF THE FINITE-DIFFERENCE EQUATIONS

The finite-difference equations derived in Section 5-8 (for the general variable ϕ, for the velocity components, for pressure, and for the pressure correction) have a common form. They all relate the value of the variable at P to the values at the six neighbor points. It is, therefore, sufficient to describe the method of solution for the algebraic equations of the general form.

Although the general finite-difference equation contains seven unknowns, the equations for the near-boundary control volumes have fewer unknowns. This results from the fact that either the boundary values are known or their influence has been set equal to zero through our boundary-condition practice. Thus, we may always regard the boundary values as known for the purpose of solving the equations.

10.1 Tri-Diagonal-Matrix Algorithm

The primary building block in the solution method is the Tri-Diagonal-Matrix Algorithm (TDMA). It enables us to solve directly for all the values along one line.

Let the system of equations be represented by

$$A_i\phi_i = B_i\phi_{i+1} + C_i\phi_{i-1} + D_i \quad , \qquad [10.1]$$

for $i = 2, 3, \ldots, N$, with ϕ_1 and ϕ_{N+1} being the known values.

The first step is to calculate the transformed coefficients P_i and Q_i from

$$P_2 = B_2/A_2 \quad , \quad Q_2 = (C_2\phi_1 + D_2)/A_2 \quad , \qquad [10.2]$$

and, for $i = 3, 4, \ldots, N$

$$P_i = B_i/(A_i - C_iP_{i-1}) \quad ,$$

$$Q_i = (D_i + C_iQ_{i-1})/(A_i - C_iP_{i-1}) \quad , \qquad [10.3]$$

The second and final step is the "back substitution", i.e., the calculation of ϕ_i from

for $i = N, N-1, N-2, \ldots, 4,3,2$:

$$\phi_i = P_i\phi_{i+1} + Q_i \quad . \qquad [10.4]$$

This step gives the solution of the system of equations [10.1].

10.2 Line-By-Line Scheme

The line-by-line procedure for solving the finite-difference equations can be seen as the logical extension of the Gauss-Seidel point-by-point method. Instead of visiting a point and solving for the value there by the use of the available values at the neighbor points, we choose a line and solve for all the values along it by the TDMA.

The procedure is schematically illustrated in Fig. 10.1. A grid line is chosen for the application of the TDMA. In the finite-difference equations for all the points along this line will appear the values of the variable along the four neighboring lines (two of which are shown in Fig. 10.1; the other two contain the z-direction neighbors). If these neighbor-line values are assumed to be known, then the finite-difference equations along the chosen line will take the form of Eq.[10.1] and can be solved by the TDMA. The main advantage of this procedure is that the boundary-condition information from the ends of the line is at once transmitted to the interior of the domain, no matter how many grid points lie on the line. In the point-by-point procedure, on the other hand, the influences from the boundary travel only one grid interval per iteration.

When all the lines in a given direction are visited, the basic operation of the line-by-line procedure is complete.

10.3 Traverse and Sweep Directions

The basic operation just mentioned does not, however, give the final solution of the algebraic equations. The reason is that guessed values from neighboring lines were used in the procedure. Only after many repetitions of the basic operation, we get the correct solution of the equations. Of course, it is desirable to seek ways of reducing the number of required repetitions.

The direction of the line chosen for the TDMA is called the traverse direction. In many problems, geometrical and other factors result in a situation where the coefficients in a particular direction are much larger than those in other directions. In this situation, a TDMA traverse in the direction of large coefficients is particularly effective; because the guessed values from the neighboring lines enter with only weak coefficients. When such a preferred traverse direction is not available, it is best to conduct three successive repetitions of the basic operation by choosing a new traverse direction each time.

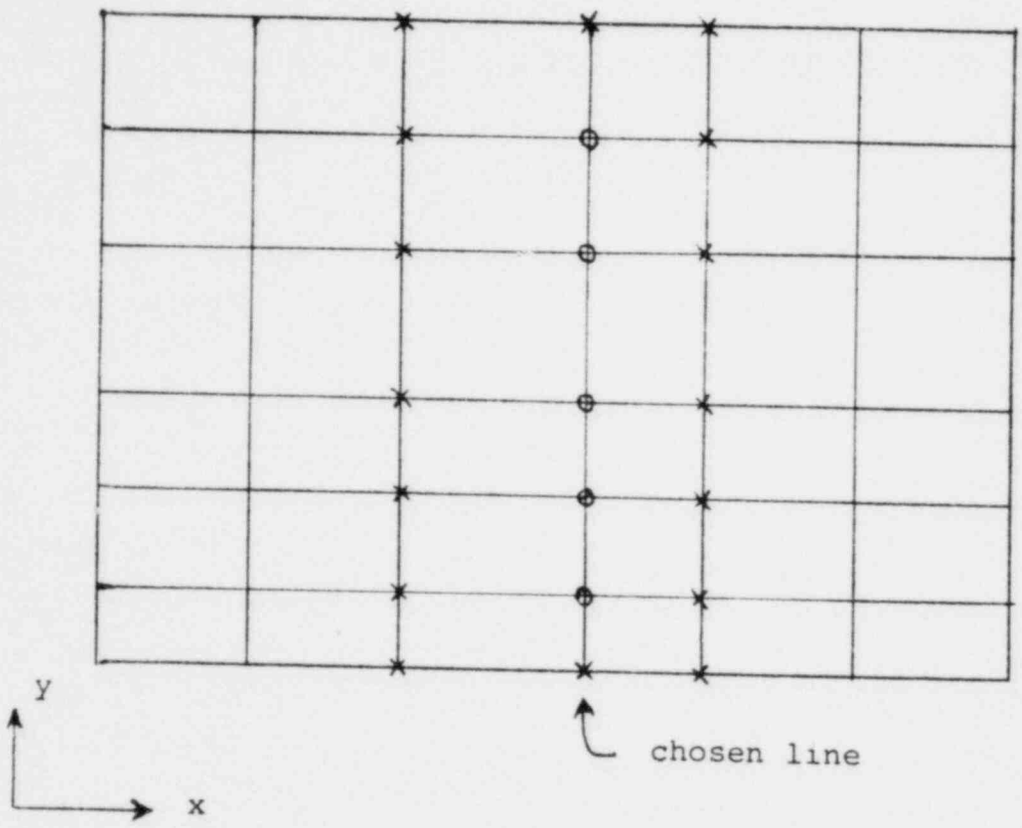

Fig. 10.1 Illustration of the line-by-line scheme

Having chosen the direction of traverse, we need to decide the sequence in which the lines are visited. This will be called the sweep direction. It is convenient to start at one end of the calculation domain and proceed to the other end, so that the boundary-condition influence is quickly brought in. If the fluid flow in the domain has a predominant direction, it is very beneficial to make the sweep direction the same as the predominant flow direction. Then the upstream information rapidly gets conveyed to the downstream locations. In absence of a major flow direction, it is best to alternate the sweep direction in the successive repetitions of the algorithm.

10.4 Optimization of the Equation-Solving Effort

The equation-solving algorithm described so far is to be used for one variable at a time. Further, it regards the finite-difference equations as linear. The nonlinearity of the equations and the interlinkage between the variables are to be handled by the iteration scheme outlined in the next section. During any given iteration we have only tentative values of the coefficients in the finite-difference equations. The coefficients must be recalculated for every iteration to reflect the changes that have occurred in the relevant dependent variables. Therefore, the repetitions of the line-by-line procedure, which is working on merely the tentative values of the coefficients, need not be carried to ultimate convergence. It is sufficient to obtain a reasonably good solution of the algebraic equations before the coefficients are recalculated. The optimum equation-solving effort should be determined by experience and experimentation, but a simple rule is that the work required for calculating the coefficients should be roughly comparable to the work involved in solving the equations.

11. ITERATION SCHEME

For every time step in an unsteady situation, a number of iterations must be performed to account for the interlinkages and nonlinearities. Also, the solution for a steady-state problem is achieved after a number of iterations. A given iteration starts with a set of values of all the dependent variables (obtained from an initial guess for the first iteration and from the previous iteration for subsequent iterations) and proceeds to obtain a new set of values. When subsequent iterations cease to produce any significant change in the values, the iteration sequence is said to have reached convergence.

11.1 Suggested Sequence of Operations

(1) Start with an initial guess for all the dependent variables.

(2) Calculate the density field from the equations of state.

(3) Calculate the coefficients in the x-direction momentum equations. Hence obtain the values of $\hat{u}_1$ and $\hat{u}_2$ (Eq. [6.7]).

(4) Similarly, obtain the coefficients in the y- and z-direction momentum equations. Hence evaluate $\hat{v}_1$, $\hat{v}_2$, $\hat{w}_1$, and $\hat{w}_2$.

(5) Set up and solve the pressure equation [8.1] to obtain the values of p.

(6) Using this pressure field as p^*, solve the momentum equations (Eq. [6.2] for u and similar equations for v and w) to yield u_1^*, u_2^*, v_1^*, v_2^*, w_1^*, and w_2^*.

(7) Solve phase continuity equation [7.1] for θ_1^* and similar equation for θ_2^* for computing phase void fractions, θ_1^* and θ_2^*.

(8) If $\theta_1^* + \theta_2^* = 1$, go to Step 12.

(9) Set up and solve the pressure-correction equation, Eq. [8.3] -- (note that only b needs to be recalculated) -- to obtain the values of p'.

(10) Use the velocity-correction formula, Eq. [6.12] (and similar equations for v and w) to obtain the corrected velocity field u, v, w.

(11) Solve phase continuity equations to obtain θ_1 and θ_2.

(12) Set up and solve the general finite-difference equation, Eq. [5.1], for ϕ, with ϕ standing for enthalpies h_1 and h_2 and the turbulence quantities k_1, k_2, ε_1, ε_2, g_1 and g_2, in a sequential manner.

(13) Perform integral balances on mass flow of gas and liquid. Correct gas and liquid flows, and pressure.

(14) Return to Step (2) with the new values obtained during this iteration as improved guesses and continue the procedure until convergence.

The above described sequence of operations is based on the extension of the "SIMPLER" procedure. In regard to the procedure analogous to "IPSA", the above sequence of operations remain the same except that Steps (9) and (11) are replaced by the following two steps:

(9a) Set up and solve the pressure correction equation, Eq. [8.12] to obtain the values of p'.

(11a) Use the void fraction-correction formulae, Eqs. [8.11] to obtain corrected void fractions.

11.2 Under-Relaxation

The finite-difference equations and the line-by-line scheme have been constructed such that, if there were no interlinkages and nonlinearities, convergence will be certain. However, because the equations of interest here would almost always contain nonlinear and interlinked influences, care must be taken to prevent divergence. One simple strategy is to slow down the changes in the coefficients that would occur from iteration to iteration. This is accomplished via under-relaxation.

Under-Relaxation of the Dependent Variables

The general finite-difference equation, Eq. [5.1] can be written as

$$a_p \phi_p = \sum a_{nb} \phi_{nb} + a_p^o \phi_p^o + b \quad , \qquad [11.1]$$

where the subscript nb denotes the neighbor points. This equation can be modified as follows: From Eq. [11.1] we can write

$$\phi_p = \sum \frac{a_{nb}}{a_p} \phi_{nb} + \frac{a_p^o \phi_p^o}{a_p} + b/a_p \quad . \qquad [11.1a]$$

Also, let

$$\phi_p^{new} = \alpha \phi_p^{nur} + (1 - \alpha) \phi_p^* \quad , \qquad [11.1b]$$

where ϕ_p^* denotes the last iteration value of ϕ_p, ϕ_p^{nur} denotes the value obtained directly if Eq. [11.1] is solved; and α is the under-relaxation factor. Substitution of Eq. [11.1a] in Eq. [11.1b] and rearrangement gives

$$(a_p/\alpha)\phi_p = \Sigma a_{nb}\phi_{nb} + a_p^o\phi_p^o + b + (1 - \alpha)(a_p/\alpha)\phi_p^* \quad . \qquad [11.2]$$

It is easy to see that, when ϕ_p becomes equal to ϕ_p^* (i.e., the iterations converge), Eq. [11.2] becomes identical to Eq. [11.1]. In the meantime, however, Eq. [11.2] would have a tendency to keep the resulting ϕ_p closed to ϕ_p^* (than Eq. [11.1] would do) provided the relaxation factor ϕ is less than 1. A value of α close to zero would indicate a very heavy under-relaxation.

A value of $\alpha = 0.5$ usually provides sufficient under-relaxation for most variables. For the velocity components, a value of $\alpha \simeq 0.7$ may be used. The pressure equation may be under-relaxed by using $\alpha = 0.8$. These values should be regarded as only initial suggestions; a proper set of α values should be obtained by actual experience for a given class of problems.

Under-Relaxation of Auxiliary Quantities

In addition to under-relaxing the dependent variables, a number of other quantities can be under-relaxed with advantage. For example, the density ρ and the diffusion coefficient Γ can be calculated from

$$\rho = \alpha\,\rho_{new} + (1 - \alpha)\rho_{old} \quad , \qquad [11.3]$$

$$\Gamma = \alpha\,\Gamma_{new} + (1 - \alpha)\Gamma_{old} \quad . \qquad [11.4]$$

Often the source terms can be a cause of divergence. Under-relaxation of the source terms in the form

$$S = \alpha\,S_{new} + (1 - \alpha)S_{old} \quad , \qquad [11.5]$$

can be helpful to prevent divergence. Even some boundary values can be introduced in a controlled manner via

$$\phi_B = \alpha\,\phi_{B,given} + (1 - \alpha)\phi_{B,old} \quad , \qquad [11.6]$$

where ϕ_B denotes a boundary value.

It should be obvious that the values of α appearing in Eqs. [11.2] to [11.6] can all be different; indeed, it is permissible, though inconvenient, to choose a separate value of α for each grid point. Further, the values of α can be changed as the iterations proceed.

11.3 Linearization of the Source Term

In the derivation of the finite-difference equations, we have expressed the source term S via Eq. [4.15] in a linearized form. This form is an attempt to anticipate the change in S resulting from the change in the value of ϕ_p. A proper linearization of S is often the key to obtaining a converged solution. It has already been mentioned that S_p in Eq. [4.15] should not be allowed to become positive. Another general recommendation pertains to those dependent variables which because of their physical significance must always remain positive. The turbulence quantities k, ε and g belong to this category. Such variables often have positive and negative source terms, and their imbalance could often lead to negative values of k, ε and g, which are not physically meaningful. These negative values can be entirely prevented if the source term is linearized according to the following practice.

Let S_1 and S_2 denote the positive and negative parts of the source term such that

$$S = S_1 - S_2 \qquad (S_1 > 0,\ S_2 > 0) \quad . \tag{11.7}$$

Set S_C and S_p according to

$$S_C = S_1 \quad , \tag{11.8}$$

and

$$S_p = -(S_2/\phi_p^*) \quad , \tag{11.9}$$

where ϕ_p denotes the last-iteration value of ϕ_p.

11.4 Distinction Between Steady and Unsteady Situations

The calculation method outlined in this report makes only a small distinction between the steady and unsteady problems. The suggested calculation sequence for one time step in an unsteady situation is almost identical to the sequence for obtaining the steady-state solution. If the time step Δt is made very large, our finite-difference equations for an unsteady problem reduce to those for a steady problem.

The main difference between the two situations turns out to be in the number of the required iterations. In an unsteady situation, the "initial" values of ϕ for any time step are either given or known from the previous time step. If the value of Δt is reasonable, we do not expect the ϕ values to

change very drastically within one time step. Thus, the values ϕ_r^o at the start of the time step serve as good guesses for the new values ϕ_p, and therefore, only a few iterations may be sufficient to attain convergence for the time step. On the other hand, the guesses available for a steady-state problem are often rather "wild", and it is then expected that many iterations would be necessary before convergence is obtained.

There is another difference between the two situations; it pertains to the computer-storage requirement. For an unsteady problem, two sets of values of the dependent variables, ϕ_p^o and ϕ_p, must be given computer storage. For a steady-state problem, ϕ_p^o has no relevance, and a single set of ϕ_p values represents the storage requirement for the dependent variables.

11.5 Performance of Integral Balances

During the iterative process, because of partial convergence of the continuity equations, it is possible that the total (or individual phase) mass flow out of a slab of cells is not equal to the known, correct value. In order to make the solution at subsequent slabs of cells more accurate, it is advantageous to correct the velocity and pressure fields to satisfy the integral mass balance. This section explains such a practice, and describes its merits.

Consider first a flow in which there is a predominant flow direction (e.g., pipe flow). For a pipe flow, we recognize that the total flow outwards of any plane perpendicular to the pipe axis must be equal to the inflow at the entrance of the pipe. Mathematically, this means

$$\sum_i \sum_j \rho_{ij} w_{ij} A_{ij} = \dot{m} \qquad [11.10]$$

where ρ is density, w is the axial velocity, and A is the area perpendicular to the pipe axis. The summation is made over all cells in the cross-sectional plane. Since the above equation is not always satisfied until convergence, we wish to correct w_{ij} by an amount Δw_{ij} to meet this criteria. There are a few different ways to perform the corrections to the w field and associated pressure field; here two methods found often superior to others will be described.

Uniform Pressure Correction

Let Δp be a uniform correction (over the cross-section) to the pressure affecting the w velocity at the given plane. Also, let D_w be $\frac{\partial w}{\partial p}$ for each cell. We can then write

$$\Delta p \sum_i \sum_j \rho_{ij} (D_w)_{ij} A_{ij} = \Delta \dot{m} \quad , \qquad [11.11]$$

where $\Delta \dot{m}$ is the error (required-actual). This leads to the relation for Δp, as follows:

$$\Delta p = \frac{\Delta \dot{m}}{\sum \sum \rho_{ij} (D_w)_{ij} A_{ij}} \quad , \text{ and} \qquad [11.12]$$

$$\Delta w_{ij} = (D_w)_{ij} \, \Delta p \quad . \qquad [11.13]$$

Note that the Δp correction is uniform, but Δw is different for each cell.

The above expressions can be extended to two-phase flows, considering the total mass flow as the quantity to be balanced. Thus,

$$\sum_i \sum_j (\theta_1 \rho_1)_{ij} (w_1)_{ij} A_{ij} + \sum_i \sum_j (\theta_2 \rho_2)_{ij} (w_2)_{ij} A_{ij} = \dot{m}_1 + \dot{m}_2 = \dot{m}_t \quad . \qquad [11.14]$$

We can derive in a straightforward way, that

$$\Delta p = \frac{(\dot{m}_t)_{req} - (\dot{m}_t)_{actual}}{\sum_i \sum_j \left[\left(\theta_1 \rho_1 D_{w_1} \right)_{ij} + \left(\theta_2 \rho_2 D_{w_2} \right)_{ij} \right] A_{ij}} \quad , \qquad [11.15]$$

$$(\Delta w_1)_{ij} = \left(D_{w_1} \right)_{ij} \Delta p \quad , \text{ and} \qquad [11.16]$$

$$(\Delta w_2)_{ij} = \left(D_{w_2} \right)_{ij} \Delta p \quad . \qquad [11.17]$$

For multiphase flows, the same practice will also hold good if extension is made for all of the phases.

Uniform Velocity Correction

Let Δw be a uniform correction (over the cross-section) to the axial velocity at a given plane. We can then write

$$\Delta w \sum_i \sum_j \rho_{ij} A_{ij} = \Delta \dot{m} \quad , \qquad [11.18a]$$

or

$$\Delta w = \frac{\Delta \dot{m}}{\sum \sum \rho_{ij} A_{ij}} \quad . \qquad [11.18b]$$

Having computed Δw, we can easily derive the relation for Δp_{ij}.

$$\Delta p_{ij} = \frac{\Delta w}{(D_w)_{ij}} = \frac{1}{(D_w)_{ij}} \frac{\Delta \dot{m}}{\sum_i \sum_j \rho_{ij} A_{ij}} \qquad [11.19]$$

It should be noted that in this procedure, we have uniform Δw for all cells in a plane, but Δp is different for each cell.

We can extend this procedure to two phase flows in the following way. Let $\Delta\dot{m}_1$ and $\Delta\dot{m}_2$ be the errors in mass flow rates and Δw_1 and Δw_2 be the velocity corrections of phase 1 and phase 2, respectively. We then have

$$\Delta w_1 = \frac{\Delta\dot{m}_1}{\sum_i \sum_j \left(\rho_1 \theta_1 A_1\right)_{ij}} \quad , \qquad [11.20]$$

and

$$\Delta w_2 = \frac{\Delta\dot{m}_2}{\sum_i \sum_j \left(\rho_2 \theta_2 A_2\right)_{ij}} \quad . \qquad [11.21]$$

The pressure correction Δp_{ij} can be obtained by averaging the pressure corrections required for balancing of each phase of the two phases. Thus

$$\Delta p_{ij} = \frac{1}{2}\left((\Delta p_{ij})_1 + (\Delta p)_{ij_2}\right) = \frac{1}{2}\left[\frac{\Delta\dot{m}_1}{D_{w_{ij}} \sum_{ij}\sum \left(\rho_1 \theta_1 A_i\right)_{ij}} + \frac{\Delta\dot{m}_2}{D_{w_{ij}} \sum_i \sum_j \left(\rho_2 \theta_2 A_{ij}\right)}\right] \qquad [11.22]$$

The Δw corrections are applied at the slab concerned, but the Δp corrections are made to all downstream planes in the domain. This practice avoids creation of artificial pressure gradients at subsequent planes.

12. SUGGESTED FLOW CHARTS

The calculation method described so far can be visualized through the flow charts presented in this section. It should be recognized that a number of decisions taken while designing the computer program would have some effect on the details of the flow charts, but their main framework would continue to remain useful. The description here is given for an unsteady situation; the specialization to a steady-state problem has already been dealt with.

12.1 Time-Step and Iteration Loops

The main structure of the computer program can be seen from Fig. 12.1. We begin by specifying the grid and, if desired, calculating a number of geometrical quantities which will be frequently needed in later work. Next, the initial values of all variables are specified. The output, which will consist of the initial values at this stage, can be arranged just before we begin the time step. The iteration sequence, for which further details will be given shortly, is then repeated a number of times until convergence is obtained. This completes one time step, after which we return to the beginning of the output section and proceed to the next time step. When the required number of time steps have been performed, the computation is terminated.

12.2 Iteration Sequence

The details of the iteration sequence are shown in Fig. 12.2. They follow the steps listed in Section 11.1. More information about the general ϕ equation sequence follows in Section 12.3. The sequences for the momentum equations, and for the pressure and pressure-correction equations should also follow the general pattern for the ϕ equation.

12.3 General ϕ Equation Sequence

The flow chart for the sequence of setting up and solving the finite-difference equations for ϕ is given in Fig. 12.3. We begin by calculating the values of Γ_ϕ, and the source-term quantities $(S_C)_\phi$ and $(S_p)_\phi$ for the particular ϕ under consideration. The modifications necessary for introducing the boundary conditions are performed next. This sets the stage for the calculation of the finite-difference coefficients, for under-relaxation and subsequent solution of the algebraic equations by the line-by-line method.

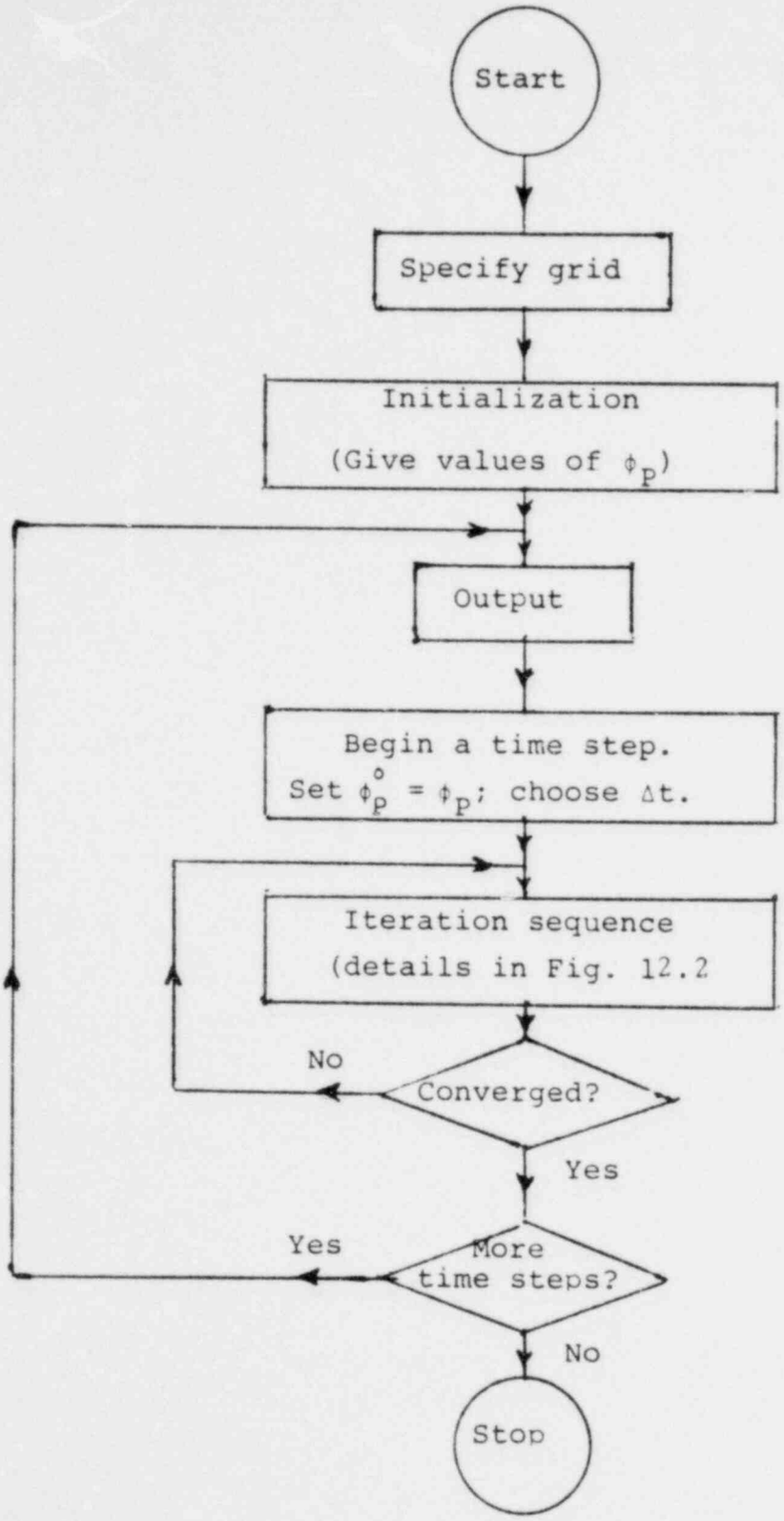

Fig. 12.1 The overall flow chart

(1) Calculate densities ρ_1 and ρ_2

(2) x-momentum coefficients for both phases. Calculate $\hat{u}_1$; $\hat{u}_2$

(3) y-momentum coefficients for both phases. Calculate $\hat{v}_1$; $\hat{v}_2$

(4) z-momentum coefficients for both phases. Calculate $\hat{w}_1$; $\hat{w}_2$

(5) Set up and solve the pressure equation

(6) Solve the momentum equations for both phases to get u_1^*, u_2^*, v_1^*, v_2^*, w_1^*, and w_2^*

(7) Solve the phase continuity equations to get θ_1^* and θ_2^*

(8) Set up and solve the pressure correction equation (Eq. [8.3] or Eq. [8.12])

(9) Correct the velocities to get u_1, v_1, w_1, u_2, v_2 and w_2

(10) Solve the phase continuity equations to get θ_1 and θ_2 or use the correction equations to correct the void fractions

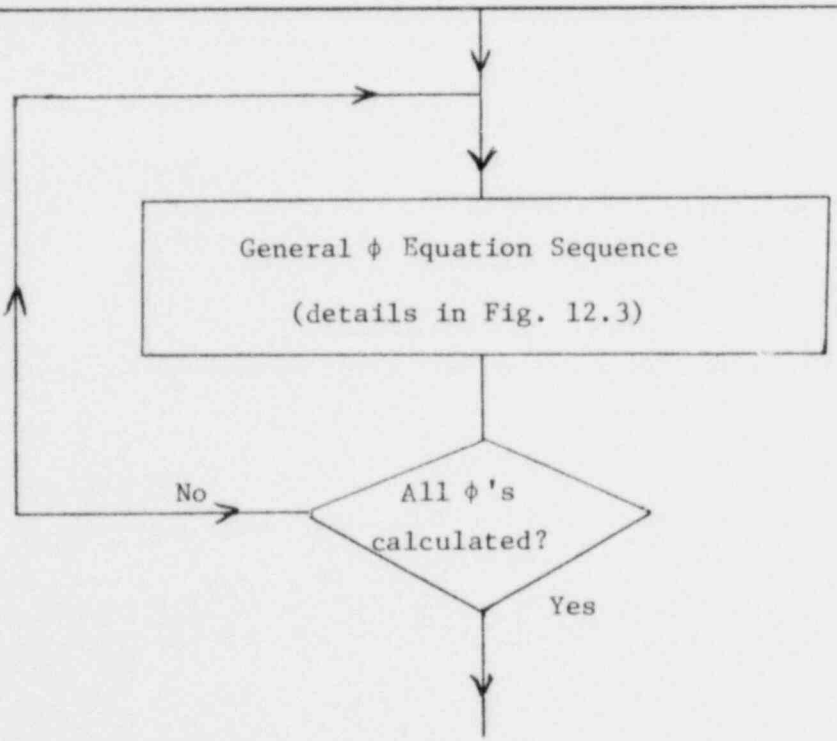

Fig. 12.2 Iteration Sequence

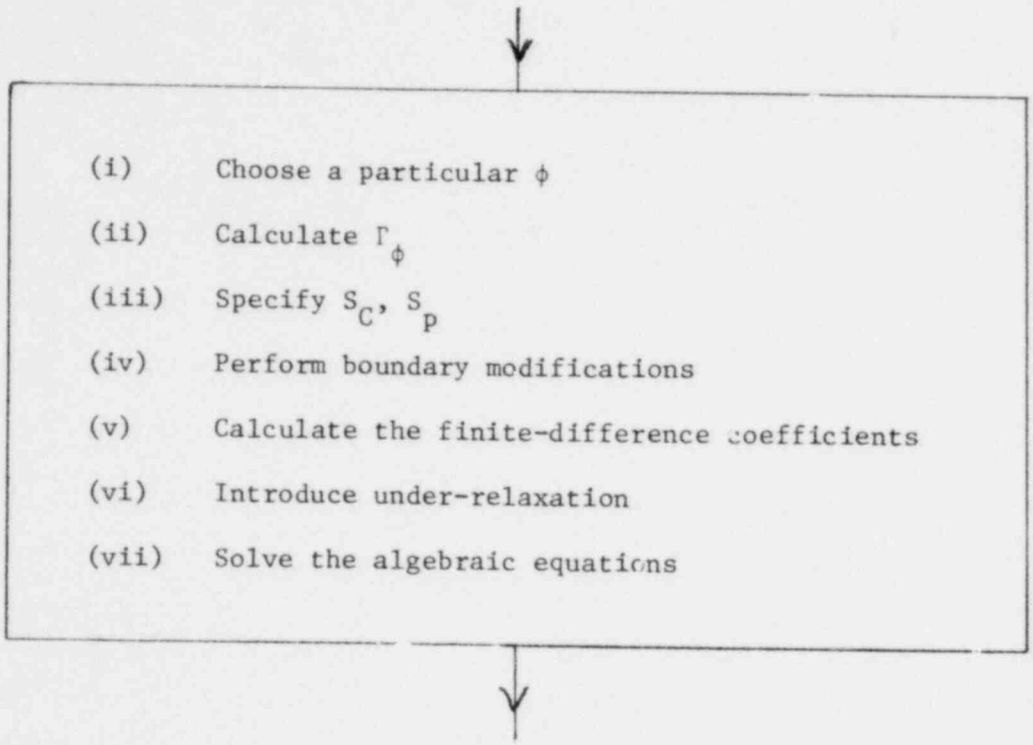

Fig. 12.3 General ϕ Equation Sequence

Separate operations in this sequence can best be performed in separate subroutines. In particular, subroutines for the calculation of Γ_ϕ, S_C and S_p, for boundary modifications, and for the equation-solving algorithm are especially convenient.

13. CONCLUDING REMARKS

This report has described a general numerical method for the solution of three-dimensional, single-phase/two-phase, steady/unsteady flow problems with heat transfer. The method is based on the control-volume approach, which is easy to interpret in physical terms and which ensures overall conservation. Calculation practices and iteration sequences, which have been found to be accurate and efficient for single-phase have been extended to two-phase flows. The structure of the computer program has been outlined by way of flow charts. A systematic implementation of this information, with careful and step-by-step testing, is expected to lead to an efficient and reliable computer program.

14. ACKNOWLEDGEMENTS

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APPENDIX A

Formulations for Cylindrical Co-ordinates

Governing Equations

Continuity Equation : Phase 1

$$\frac{\partial}{\partial t}(\rho_1\alpha_1) + \nabla\cdot(\rho_1\alpha_1\bar{v}_1) = \Omega_1 \qquad [A.1]$$

Continuity equation for Phase 2 is similar. Combined continuity equation:

$$\frac{\partial}{\partial t}(\rho_1\alpha_1 + \rho_2\alpha_2) + \nabla\cdot(\rho_1\alpha_1\bar{v}_1 + \rho_2\alpha_2\bar{v}_2) = 0 \qquad [A.2]$$

Here, $\bar{v}$ is the velocity vector, ρ is the density, Ω is the source, and α (to avoid confusion with co-ordinate θ) is the void fraction.

Momentum Equation : Phase 1

r-direction:

$$\frac{\partial}{\partial t}(\rho_1\alpha_1 v_{r1}) + \nabla\cdot(\rho_1\alpha_1\bar{v}_i v_{r1}) - \frac{\rho_1\alpha_1 v_{\theta 1}^2}{r} = -\alpha_1\frac{\partial p}{\partial r}$$

$$+ \nabla\cdot(\alpha_1\Gamma_{v1}\nabla v_{r1}) + V_{r1} + \rho_1\alpha_1 g_r + \Omega_{m1r} + K_r(v_{r2} - v_{r1}) \qquad [A.3]$$

θ-direction:

$$\frac{\partial}{\partial t}(\rho_1\alpha_1 v_{\theta 1}) + \nabla\cdot(\rho_1\alpha_1\bar{v}_1 v_{\theta 1}) + \frac{\rho_1\alpha_1 v_{r1} v_{\theta 1}}{r} = -\frac{1}{r}\alpha_1\frac{\partial p}{\partial\theta}$$

$$+ \nabla\cdot(\alpha_1\Gamma_{v1}\nabla v_{\theta 1}) + V_{\theta 1} + \rho_1\alpha_1 g_\theta + \Omega_{m1\theta} + K_\theta(v_{\theta 2} - v_{\theta 1}) \qquad [A.4]$$

z-direction:

$$\frac{\partial}{\partial t}(\rho_1\alpha_1 v_{z1}) + \nabla\cdot(\rho_1\alpha_1\bar{v}_1 v_{z1}) = -\alpha_1\frac{\partial p}{\partial z} + \nabla\cdot(\alpha_1\Gamma_{v1}\nabla v_{z1})$$

$$+ V_{z1} + \rho_1\alpha_1 g_z + \Omega_{m1z} + K_z(v_{z2} - v_{z1}) \qquad [A.5]$$

Here, v_r, v_θ, and v_z are velocities in r, θ, and z direction, respectively. The viscous contribution to the momentum equation is divided into two parts: the term

$$\nabla \cdot (\alpha_1 \Gamma_{v1} \nabla) \bar{v}_1 \quad ,$$

and the term $\bar{V}_1$ which contains the remaining contribution. The momentum equations for Phase 2 are similar.

Energy Equation : Phase 1:

$$\frac{\partial}{\partial t} (\rho_1 \alpha_1 h_1) + \nabla \cdot (\rho_1 \alpha_1 h_1 \bar{v}) = \nabla \cdot (\Gamma_{h1} \alpha_1 \nabla h_1) + \alpha_1 \frac{\partial p}{\partial t}$$

$$+ \Omega_{h1} + R (T_2 - T_1) + \Phi_1 + Q_1 \quad . \qquad [A.6]$$

Similarity

We can see that all conservation equations in cylindrical co-ordinates have also the same general form.

$$\frac{\partial}{\partial t} (\rho \alpha \phi) + \nabla \cdot (\bar{J}_\phi) = S_\phi \quad , \qquad [A.7]$$

where

$$\bar{J}_\phi = (\rho \alpha \bar{v} \phi - \Gamma \alpha \nabla \phi) \; . \qquad [A.8]$$

We can, therefore, apply all formulations for Cartesian co-ordinates to cylindrical co-ordinates with simple transformations shown in Table A.1. The source terms for both systems and for Phase 1 are presented in Table A.2. The viscous contributions in source terms in two co-ordinate systems are also different. These are presented in Table A.3.

Table A.1 Transformations Between Cartesian and Cylindrical Co-ordinate Systems

Cartesian Co-ordinates	Cylindrical Co-ordinates
x	r
y	θ
z	z
Δx	Δr
Δy	$r\Delta\theta$
Δz	Δz
u	v_r
v	v_θ
w	v_z

Table A.2 Source Terms in the Cartesian and Cylindrical Co-ordinate Systems

	Cartesian Co-ordinates	Cylindrical Co-ordinates
Continuity	Ω_1	Ω_1
Momentum		
(i)	$(\rho_1\alpha_1 g_x + V_{1x} + \Omega_{m1x} + K_x u_2 - K_x u_1)$	$(\rho_1\alpha_1 g_r + V_{1r} + \Omega_{m1r} + \frac{\rho_1\alpha_1 v_{\theta 1}^2}{r}$ * $+ K_r v_{r2} - K_r v_{r1})$
(ii)	$(\rho_1\alpha_1 g_y + V_{1y} + \Omega_{m1y} + K_y v_2 - K_y v_1)$	$(\rho_1\alpha_1 g_\theta + V_{1\theta} + \Omega_{m1\theta} - \frac{\rho_1\alpha_1 v_{r1} v_{\theta 1}}{r}$ ** $+ K_\theta v_{\theta 2} - K_\theta v_{\theta 1})$
(iii)	$(\rho_1\alpha_1 g_z + V_{1z} + \Omega_{m1z} + K_z w_2 - K_z w_1)$	$(\rho_1\alpha_1 g_z + V_{1z} + \Omega_{m1z} + v_z v_{z2} - K_z v_{z1})$
Energy	$\left(\alpha_1 \frac{\partial p}{\partial t} + \Omega_{h1} + \Phi_1 + Q_1 + RT_2 - {}^{p}T_1\right)$	$\left(\alpha_1 \frac{\partial p}{\partial t} + \Omega_{h1} + \Phi_1 + Q_1 + RT_2 - RT_1\right)$

* Centrifugal force term.

** Coriolis force term.

Table A.3 Viscous Contributions in the Source Terms for Cartesian and Cylindrical Systems

	Cartesian	Cylindrical
1.	$V_x = \frac{\partial}{\partial x}\left(\mu\alpha \frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu\alpha \frac{\partial v}{\partial x}\right) + \frac{\partial}{\partial z}\left(\mu\alpha \frac{\partial w}{\partial x}\right) - \frac{2}{3}\frac{\partial}{\partial x}(\mu\alpha\nabla\cdot\bar{v})$	$V_r = \frac{1}{r}\frac{\partial}{\partial r}\left(\mu\alpha r \frac{\partial v_r}{\partial r}\right) - \frac{2}{3}\frac{\partial}{\partial r}(\mu\alpha\nabla\cdot\bar{v}) + \frac{1}{r}\frac{\partial}{\partial\theta}\left(\mu\alpha r \frac{\partial}{\partial r}\left(\frac{v_\theta}{r}\right)\right) + \frac{\partial}{\partial z}\left(\mu\alpha \frac{\partial v_z}{\partial r}\right) - \frac{2\mu\alpha}{r^2}\frac{\partial v_\theta}{\partial\theta} - \frac{2\mu\alpha v_r}{r^2}$
2.	$V_y = \frac{\partial}{\partial x}\left(\mu\alpha \frac{\partial u}{\partial y}\right) + \frac{\partial}{\partial y}\left(\mu\alpha \frac{\partial v}{\partial y}\right) + \frac{\partial}{\partial z}\left(\mu\alpha \frac{\partial w}{\partial y}\right) - \frac{2}{3}\frac{\partial}{\partial y}(\mu\alpha\nabla\cdot\bar{v})$	$V_\theta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(\mu\alpha r \frac{\partial v_\theta}{\partial\theta}\right) - \frac{v_\theta}{r^2}\frac{\partial}{\partial r}(\mu\alpha r) + \frac{1}{r}\frac{\partial}{\partial\theta}\left[\frac{\mu\alpha}{r}\frac{\partial v_\theta}{\partial\theta} + \frac{2\mu\alpha v_r}{r} - \frac{2}{3}\mu\alpha\nabla\cdot\bar{v}\right] + \frac{\partial}{\partial z}\left(\frac{\mu\alpha}{r}\frac{\partial v_z}{\partial\theta}\right)$
3.	$V_z = \frac{\partial}{\partial x}\left(\mu\alpha \frac{\partial u}{\partial z}\right) + \frac{\partial}{\partial y}\left(\mu\alpha \frac{\partial v}{\partial z}\right) + \frac{\partial}{\partial z}\left(\mu\alpha \frac{\partial w}{\partial z}\right) - \frac{2}{3}\frac{\partial}{\partial z}(\mu\alpha\nabla\cdot\bar{v})$	$V_z = \frac{1}{r}\frac{\partial}{\partial r}\left(\mu\alpha r \frac{\partial v_r}{\partial z}\right) + \frac{1}{r}\frac{\partial}{\partial\theta}\left(\mu\alpha \frac{\partial v_\theta}{\partial z}\right) + \frac{\partial}{\partial z}\left(\mu\alpha \frac{\partial v_z}{\partial z} - \frac{2}{3}\mu\alpha\nabla\cdot\bar{v}\right)$

APPENDIX B

Formulations for Spherical Co-ordinate Systems

Governing Equations

Continuity Equation : Phase 1

$$\frac{\partial}{\partial t}(\rho_1\alpha_1) + \nabla\cdot(\rho_1\alpha_1\bar{v}_1) = \Omega_1 \quad . \qquad [B.1]$$

Momentum Equation : Phase 1

r-direction:

$$\frac{\partial}{\partial t}(\rho_1\alpha_1 v_{r1}) + \nabla\cdot(\rho_1\alpha_1\bar{v}_1 v_{r1}) - \frac{\rho_1\alpha_1}{r}\left(v_{\theta 1}^2 + v_{\phi 1}^2\right) = -\alpha_1\frac{\partial p}{\partial r}$$

$$+ \nabla\cdot(\alpha_1\Gamma_{v1}\nabla v_{r1}) + V_{r1} + \rho_1\alpha_1 g_r + \Omega_{m1r} + K_r\,(v_{r2} - v_{r1}) \,. \qquad [B.2]$$

θ-direction:

$$\frac{\partial}{\partial t}(\rho_1\alpha_1 v_{\theta 1}) + \nabla\cdot(\rho_1\alpha_1\bar{v}_1 v_{\theta 1}) + \frac{\rho_1\alpha_1}{r}\left(v_{r1}v_{\theta 1} - v_{\phi 1}^2\cot\theta\right) = -\frac{\alpha_1}{r}\frac{\partial p}{\partial \theta}$$

$$+ \nabla\cdot(\alpha_1\Gamma_{v1}\nabla v_{\theta 1}) + V_{\theta 1} + \rho_1\alpha_1 g_\theta + \Omega_{m1\theta} + K_\theta\,(v_{\theta 2} - v_{\theta 1}) \,. \qquad [B.3]$$

φ-direction:

$$\frac{\partial}{\partial t}(\rho_1\alpha_1 v_{\phi 1}) + \nabla\cdot(\rho_1\alpha_1\bar{v}_1 v_{\phi 1}) + \frac{\rho_1\alpha_1}{r}\left[v_{\phi 1}v_{r1} + v_{\theta 1}v_{\phi 1}\cot\theta\right] =$$

$$-\frac{\alpha_1}{r\sin\theta}\frac{\partial p}{\partial \phi} + \nabla\cdot(\alpha_1\Gamma_{v1}\nabla v_{\phi 1}) + V_{\phi 1} + \rho_1\alpha_1 g_\phi + \Omega_{m1\phi}$$

$$+ K_\phi\,(v_{\phi 2} - v_{\phi 1}) \,. \qquad [B.4]$$

Here, the viscous contribution to the momentum equation is divided into two parts: the term

$$\nabla\cdot(\alpha_1\Gamma_{v1}\nabla)\bar{v} \quad ,$$

and the term $\bar{V}_1$ which contains the remaining contribution. The momentum equations for Phase 2 are similar.

Energy Equation : Phase 1:

$$\frac{\partial}{\partial t}(\rho_1\alpha_1 h_1) + \nabla\cdot(\rho_1\alpha_1 h_1\bar{v}) = \nabla\cdot(\Gamma_{h1}\alpha_1\nabla h_1) + \alpha_1\frac{\partial p}{\partial t} + \Omega_{h1}$$

$$+ R\,(T_2 - T_1) + \Phi_1 + Q_1 \qquad [B.5]$$

We can see the same similarities as shown in Appendix A. We can follow the same procedure and show that all Cartesian formulations can be applied to spherical geometries with the transformations given in Table B.1. The source terms and the viscous contributions for spherical co-ordinates are presented in Tables B.2 and B.3, respectively.

Table B.1 Transformations Between Cartesian and Spherical Co-ordinate Systems

Cartesian Co-ordinates	Spherical Co-ordinates
x	r
y	θ
z	ϕ
Δx	Δr
Δy	$r\Delta\theta$
Δz	$r\sin\theta\Delta\phi$
u	v_r
v	v_θ
w	v_ϕ

Table B.2 Source Terms in the Cartesian and Spherical Co-ordinate Systems

Cartesian Co-ordinates

Continuity

$$\Omega_1$$

Momentum

x-direction

$$(\rho_1\alpha_1 g_x + V_{1x} + \Omega_{mlx} + K_x u_2 - K_x u_1)$$

y-direction

$$(\rho_1\alpha_1 g_y + V_{1y} + \Omega_{mly} + K_y v_2 - K_y v_1)$$

z-direction

$$(\rho_1\alpha_1 g_z + V_{1z} + \Omega_{mlz} + K_z w_2 - K_z w_1)$$

Energy

$$\left(\alpha_1 \frac{\partial p}{\partial t} + \Omega_{h1} + \Phi_1 + Q_1 + RT_2 - RT_1\right)$$

Spherical Co-ordinates

Continuity

$$\Omega_1$$

Momentum

r-direction

$$\left(\rho_1\alpha_1 g_r + V_{r1} + \Omega_{mlr} + \frac{\rho_1\alpha_1 \left(v_{\theta 1}^2 + v_{\phi 1}^2\right)}{r} + K_r v_{r2} - K_r v_{r1}\right)$$

θ-direction

$$\left(\rho_1\alpha_1 g_\theta + V_{\theta 1} + \Omega_{ml\theta} - \frac{\rho_1\alpha_1 v_{r1} v_{\theta 1}}{r} + \frac{\rho_1\alpha_1 v_{\phi 1}^2 \cot\theta}{r} + K_\theta v_{\theta 2} - K_\theta v_{\theta 1}\right)$$

ϕ-direction

$$\left(\rho_1\alpha_1 g_\phi + V_{\phi 1} + \Omega_{ml\phi} - \frac{\rho_1\alpha_1 v_{\phi 1} v_{r1}}{r} - \frac{\rho_1\alpha_1 v_{\theta 1} v_{\phi 1} \cot\theta}{r} + K_\phi v_{\phi 2} - K_\phi v_{\phi 1}\right)$$

Energy

$$\left(\alpha_1 \frac{\partial p}{\partial t} + \Omega_{h1} + \Phi_1 + Q_1 + RT_2 - RT_1\right)$$

Table B.3 Viscous Contributions in the Source Terms for Cartesian and Spherical Systems

Cartesian

x-direction

$$V_x = \frac{\partial}{\partial x}\left(\mu\alpha \frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu\alpha \frac{\partial v}{\partial x}\right) + \frac{\partial}{\partial z}\left(\mu\alpha \frac{\partial w}{\partial x}\right) - \frac{2}{3}\frac{\partial}{\partial x}(\mu\alpha\nabla\cdot\bar{v})$$

y-direction

$$V_y = \frac{\partial}{\partial x}\left(\mu\alpha \frac{\partial u}{\partial y}\right) + \frac{\partial}{\partial y}\left(\mu\alpha \frac{\partial v}{\partial y}\right) + \frac{\partial}{\partial z}\left(\mu\alpha \frac{\partial w}{\partial y}\right) - \frac{2}{3}\frac{\partial}{\partial y}(\mu\alpha\nabla\cdot\bar{v})$$

z-direction

$$V_z = \frac{\partial}{\partial x}\left(\mu\alpha \frac{\partial u}{\partial z}\right) + \frac{\partial}{\partial y}\left(\mu\alpha \frac{\partial v}{\partial z}\right) + \frac{\partial}{\partial z}\left(\mu\alpha \frac{\partial w}{\partial z}\right) - \frac{2}{3}\frac{\partial}{\partial z}(\mu\alpha\nabla\cdot\bar{v})$$

Spherical

r-direction

$$V_r = -\mu\alpha\left[\frac{2v_r}{r^2} + \frac{2}{r^2}\frac{\partial v_\theta}{\partial\theta} + \frac{2v_\theta\cot\theta}{r^2} + \frac{2}{r^2\sin\theta}\frac{\partial v_\phi}{\partial\phi}\right] + \frac{\partial}{\partial r}(1/3\mu\alpha\nabla\cdot\bar{v}) - \left(\frac{\partial v_r}{\partial r}\cdot\nabla\mu\alpha\right)$$

θ-direction

$$V_\theta = \frac{\mu\alpha}{r}\left[\frac{2}{r}\frac{\partial v_r}{\partial\theta} - \frac{v_\theta}{r\sin^2\theta} - \frac{2\cos\theta}{r\sin^2\theta}\frac{\partial v_\phi}{\partial\phi}\right] + \frac{1}{r}\frac{\partial}{\partial\theta}(1/3\mu\alpha\nabla\cdot\bar{v}) - \left(\frac{1}{r}\frac{\partial v_\theta}{\partial\theta}\cdot\nabla\mu\alpha\right)$$

ϕ-direction

$$V_\phi = \frac{\mu\alpha}{r\sin\theta}\left[-\frac{v_\phi}{r\sin\theta} + \frac{2}{r\sin\theta}\frac{\partial v_r}{\partial\phi} + \frac{2\cos\theta}{r\sin\theta}\frac{\partial v_\theta}{\partial\phi}\right] + \frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}(1/3\mu\alpha\nabla\cdot\bar{v}) - \frac{1}{r\sin\theta}\left(\frac{\partial v_\phi}{\partial\phi}\cdot\nabla\mu\alpha\right)$$

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