SECTION 4 NUMERICAL MODELING

4.1 INTROQUCTION

The study of the circulation patterns inside a column reactor is of theoretical and practical significance, because of the wide use of column reactors in industry as chemical or bio-chemical reactors. The bubble column reactor offers several advantages over conventional fixed bed reactors: e.g., lower hydrogen to monoxide ratios can be tolerated and hot-spots are controlled in the bed so that catalyst deactivation is reduced. The gas may be introduced evenly through a distributor plate into the slurry, so the circulation patterns of the continuous liquid phase can be controlled.

Numerous mathematical models are available in the literature for calculation of relevant parameters such as the gas hold-up (i.e. volume fraction of the gas phase), the liquid velocity, and the size and strength of the liquid circulation cells. Freedman and Davidson (1969), Rietema and Ottengraf (1970) and Hills (1974) have reported on approximate models based on pressure balance to calculate liquid circulation velocity. Whalley and Davidson (1974) have shown that their model based on the energy balance predicted liquid circulation velocities which are in better agreement with experiments than those obtained from the models based on pressure balance. Joshi and Sharma (1979) have adapted the energy balance method and reported good agreement between their calculations and experiments for the values of the liquid velocity and void fraction. Clark, et al. (1987, 1989) have reviewed the so called "drift flux models" and presented their improved version. These models are mainly empirical relations which relate the superficial gas and liquid velocities to the average void fraction. Clark et al. suggested an approximate model to predict the empirical constant in one of these models, and found that it varied significantly as a function of Froude number and Galileo number. Their conclusion was that "a direct drift-flux approach is not suitable unless

the void distribution is known and that buoyancy effects are insignificant." A further restriction in these models is that the size and the location of recirculation zone must be assumed apriori. For example, in the model proposed by Clark et al. (1989) two-zones are identified, namely a central zone where only axial flow is assumed, and a lower zone where only radial flow is assumed. Such assumptions, which are inherant to most approximate models, neglect possibility of multiple circulation cells. To eliminate such restrictive assumptions, it is necessary to develop more rigorous computational fluid flow analysis with which the circulation and the void fraction distribution can be predicted apriori. However such comprehensive numerical simulations of gas/liquid two-phase systems are not given much attention in the literature. This is not surprising in view of the fact that the mathematical formulation for multi-phase flows is still in a stage of development. There is no definite form of the governing equations which is generally accepted (for a review, see Stewart and Wendroff, 1984). Other difficulties such as handling of interaction terms (interface conditions), the boundary and initial conditions, and interphase instabilities, make comprehensive numerical modeling a challenging research area, and it calls for more attention from the computational fluid dynamicists.

Here, it is reported on the results of a study where the flow and the circulation patterns inside an isothermal column reactor model has been simulated numerically using a finite volume approach. As a first step, only the equations of motion and continuity for the continuous phase, and the conservation of mass equation for the discrete phase have been solved. The gas velocity field is prescribed empirically. Only the laminar, bubbly flow regime is considered. This is done to avoid the complexities of a turbulence closure model at higher superficial gas velocities. These results constitute the

first stage of an ongoing research where the numerical solution of the continuum equations of motion for both phases are aimed at. In such a procedure, the only empiricism should come through the prescription of interfacial momentum exchange terms.

4.2 MATHEMATICAL MODEL

Consider an unsteady, gas-liquid flow inside a vertically situated circular reactor which is assumed to be isothermal and non-reacting. The gas-liquid flow is assumed to be in the bubbly flow regime which is characterized by a suspension of discrete air bubbles in a continuous liquid such as water. The mathematical model is based upon the conservation of mass and momentum for the liquid and gas phases including appropriate interface momentumn exchange terms. Invoking continuum assumptions and performing a space or time averaging over a macroscopic control volume, (see e.g., Anderson and Jackson, 1967; Homsy, 1983; Drew, 1983), these equations can be written in vector form analogous to the well known Navier-Stokes equations. Let the subcripts "1" and "2" or "ℓ" and "g" denote phase-1 (liquid) and phase-2 (gas), respectively; α be the void fraction (i.e. volume concentration of gas), $\rho_1=(1-\alpha)\rho_\ell$, $\rho_2=\alpha\rho_g$ be the macroscopic densities, ρ_ℓ and ρ_g being the microscopic liquid and gas densities, respectively; $\underline{u}_1$ be the liquid velocity vector (u_1, v_1, w_1) and $\underline{u}_2$ the gas velocity vector (u_2,v_2,w_2) in the axial x-, radial r-, and tangential, θ- directions of cylindrical coordinates, respectively. The continuity equation representing the conservation of mass for the liquid phase is

$$\frac{D\rho_1}{Dt} + \rho_1(\underline{\nabla}.\underline{u}_1) = \frac{\partial\rho_1}{\partial t} + \underline{\nabla}.(\rho_1\underline{u}_1) = 0 \qquad (4.1)$$

where D( )/Dt is the substantial derivative and $\underline{\nabla}.$ is the divergence operator. The term $\underline{\nabla}.\underline{u}_1$ is zero for an incompressible flow. There are no source/sink

terms in Eq.4.1 because there is no phase change due to chemical or thermal reactions. For numerical treatment Eq.4.1 is rewritten in the conservative form as

$$\frac{\partial \rho_1}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r}\left(\rho_1 r v_1\right) + \frac{1}{r}\frac{\partial}{\partial \theta}\left(\rho_1 w_1\right) + \frac{\partial}{\partial x}\left(\rho_1 u_1\right) = 0 \qquad (4.2)$$

The momentum equations for liquid phase, in vector form (see for example Celik, 1986), are

$$\rho_1 \frac{D\underline{u}_1}{Dt} = -(1-\alpha)\nabla P - \nabla\cdot\underline{\underline{\tau}} + F_{12}(\underline{u}_2 - \underline{u}_1) + \rho_1 \underline{g} + \underline{f}_c - w_1 \underline{e}_x \times \underline{u}_1/r \qquad (4.3)$$

In Eqs.(4.3), $\underline{\underline{\tau}}$ is the stress tensor, g is the acceleration of gravity, P is the pressure, F_{12} is the momentum exchange function between phase-1 and phase-2, $\underline{e}_x$ is the unit vector in x- direction, $\times$ denotes a vector cross product and $\underline{f}_c$ is the additional stress vector (0, $-\tau_{\theta\theta}/r$, $\tau_{r\theta}/r$) in x -, r -, and θ - directions, respectively. The components of the symmetric stress tensor $\underline{\underline{\tau}}$ for Newtonian fluids in cylindrical coordinates are:

$$\begin{aligned}
\tau_{xx} &= 2\mu\frac{\partial u}{\partial x} - \frac{2}{3}\mu\,\nabla\cdot\underline{u} \\
\tau_{rr} &= 2\mu\frac{\partial v}{\partial r} - \frac{2}{3}\mu\,\nabla\cdot\underline{u} \\
\tau_{\theta\theta} &= 2\mu\left(\frac{1}{r}\frac{\partial w}{\partial \theta} + \frac{v}{r}\right) - \frac{2}{3}\mu\,\nabla\cdot\underline{u} \\
\tau_{rx} &= \tau_{xr} = \mu\left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial r}\right) \\
\tau_{r\theta} &= \tau_{\theta r} = \mu\left(\frac{\partial w}{\partial r} + \frac{1}{r}\frac{\partial v}{\partial \theta} - \frac{w}{r}\right) \\
\tau_{x\theta} &= \tau_{\theta x} = \mu\left(\frac{1}{r}\frac{\partial u}{\partial \theta} + \frac{\partial w}{\partial x}\right)
\end{aligned} \qquad (4.4)$$

where μ is the liquid viscosity. The dilatation term $\nabla\cdot\underline{u}$ will be neglected in the momentum equations, since the effect of this term is minimal even for a wide range of compressible fluid flows provided that the Mach number is less than 0.30. It should be noted, however, that $\nabla\cdot\underline{u}$ will be kept in the equation of continuity and the resulting equations would be valid for many compressible fluid flow problems unless this term becomes very large under unusual circumstances, i.e. Mach numbers much larger than 0.3. In two-phase flows the

The term $F_{12}(\underline{u}_2-\underline{u}_1)$ in Eq.(4.3) represents the momentum exchange for liquid-phase equations, likewise, $F_{21}(\underline{u}_2-\underline{u}_1)$ is the momentum exchange term for gas-phase equations, hence $F_{12}=-F_{21}$. If the dilatation term $\nabla\cdot\underline{u}_1$ is neglected, the three components of Eq.4.3 in x-, r-, θ- directions, respectively, can be written in conservative form as follows

x - Momentum

$$\frac{\partial\rho_1 u_1}{\partial t}+\frac{\partial}{\partial x}(\rho_1u_1u_1)+\frac{1}{r}\frac{\partial}{\partial r}(r\rho_1u_1v_1)+\frac{1}{r}\frac{\partial}{\partial\theta}(\rho_1u_1w_1)$$
$$=\frac{\partial}{\partial x}(\tau_{xx})+\frac{1}{r}\frac{\partial}{\partial r}(r\tau_{rx})+\frac{1}{r}\frac{\partial}{\partial\theta}(\tau_{\theta x})-(1-\alpha)\frac{\partial p}{\partial x}+\rho_1g_x+F_{12}(u_2-u_1) \quad (4.5)$$

r - Momentum

$$\frac{\partial\rho_1 v_1}{\partial t}+\frac{\partial}{\partial x}(\rho_1u_1v_1)+\frac{1}{r}\frac{\partial}{\partial r}(r\rho_1v_1v_1)+\frac{1}{r}\frac{\partial}{\partial\theta}(\rho_1v_1w_1)-\rho_1\frac{w_1^2}{r}$$
$$=\frac{\partial}{\partial x}(\tau_{xr})+\frac{1}{r}\frac{\partial}{\partial r}(r\tau_{rr})+\frac{1}{r}\frac{\partial}{\partial\theta}(\tau_{\theta r})-\frac{\tau_{\theta\theta}}{r}-(1-\alpha)\frac{\partial p}{\partial r}+\rho_1g_r+F_{12}(v_2-v_1) \quad (4.6)$$

θ - Momentum

$$\frac{\partial\rho_1 w_1}{\partial t}+\frac{\partial}{\partial x}(\rho_1u_1w_1)+\frac{1}{r}\frac{\partial}{\partial r}(r\rho_1v_1w_1)+\frac{1}{r}\frac{\partial}{\partial\theta}(\rho_1w_1w_1)+\frac{\rho_1v_1w_1}{r}$$

$$= \frac{\partial}{\partial x}(\tau_{xx}) + \frac{1}{r}\frac{\partial}{\partial r}(r\tau_{rr}) + \frac{1}{r}\frac{\partial}{\partial\theta}(\tau_{\theta\theta}) + \frac{\tau_{rr}}{r} - (1-\alpha)\frac{1}{r}\frac{\partial P}{\partial\theta} + \rho_1 g_\theta + F_{12}(w_2 - w_1) \quad (4.7)$$

For the axisymmetric, non-swirling (i.e. $w = 0$) flow case with the typical geometry shown in Fig.4.1, Eqs.4.5-4.7 are greatly simplified. The final form of the liquid phase equations which will be solved numerically are:

Continuity

$$\frac{\partial}{\partial x}(\rho_1 u_1) + \frac{1}{r}\frac{\partial}{\partial r}(\rho_1 r v_1) = 0 \quad (4.8)$$

x - Momentum

$$\frac{\partial}{\partial x}(\rho_1 u_1 u_1) + \frac{1}{r}\frac{\partial}{\partial r}(r\rho_1 u_1 v_1) = -(1-\alpha)\frac{\partial P}{\partial x} - \rho_1 g + F_{12}(u_2 - u_1)$$

$$+ \frac{\partial}{\partial x}\left(\mu_\ell \frac{\partial u_1}{\partial x}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\mu_\ell \frac{\partial u_1}{\partial r}\right) + \frac{\partial}{\partial x}\left(\mu_\ell \frac{\partial u_1}{\partial x}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\mu_\ell \frac{\partial v_1}{\partial x}\right) \quad (4.9)$$

r - Momentum

$$\frac{\partial}{\partial x}(\rho_1 u_1 v_1) + \frac{1}{r}\frac{\partial}{\partial r}(r\rho_1 v_1 v_1) = -(1-\alpha)\frac{\partial P}{\partial r} + F_{12}(v_2 - v_1)$$

$$+ \frac{\partial}{\partial x}\left(\mu_\ell \frac{\partial v_1}{\partial x}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\mu_\ell \frac{\partial v_1}{\partial r}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\mu_\ell \frac{\partial v_1}{\partial r}\right) + \frac{\partial}{\partial x}\left(\mu_\ell \frac{\partial u_1}{\partial r}\right) - \mu_\ell \frac{2v_1}{r^2} \quad (4.10)$$

The equations for the gas phase can be obtained from Eqs. (4.8) to (4.10) by interchanging the subscripts "1" to "2", as well as "ℓ" and "g".

The global assumptions involved in deriving Eqs. (4.8) to (4.10) are: isothermal steady, axisymmetric, incompressible flow without swirl and without

chemical reactions.

It should be noted that the way the pressure gradient terms should be handled in Eqs.(4.8 - 4.10) is a controversial issue. There is considerable debate in the literature (see for example Stewart and Wendroff, 1984) whether $\nabla[(1-\alpha)P]$ or $(1-\alpha)\nabla P$ should be used in these equations. Both forms satisfy the condition that when the corresponding momentum equations for the two phases are added, the resulting pressure gradient term must be ∇P. The equal pressure model (Stewart and Wendroff, 1984) is adopted, i.e. $P_1=P_2=P$; this pressure is distributed as $(1-\alpha)P$ and αP between the liquid and gas phases, respectively. In this regard, the pressure gradient terms are being treated as part of the interfacial momentum exchange. The surface tension effects can be included in the interfacial momentum exchange function F_{12}; for different surface tension, σ, the drag force and hence the terminal velocity of a bubble are different. It should be noted, however, if we include a pressure difference $\Delta p=P_1-P_2=4\sigma/d_b$ due to surface tension, this does not alter the form of the above equations. This is because the bubble diameter d_b and the surface tension, σ, are fixed for a given flow regime and hence $P_2=P_1+4\sigma/d_b = P+4\sigma/d_b$ and $\nabla P_2=\nabla P$ again. In this regard, the pressure gradient terms are being treated as part of the interfacial momentum exchange. The surface tension effects are neglected in the present study.

The momentum exchange function F_{12} will be prescribed empirically in the functional form

$$F_{12} = F_{12}(\alpha, Re_b) \qquad (4.11)$$

where Re_b is the bubble Reynolds number which is defined as $Re_b=\rho_1|\underline{u}_2-\underline{u}_1|d_b/\mu_1$, with d_b being the bubble diameter. The explicit form of Eq.4.11 is discussed in the next subsection.

Once $F_{12} = F_{12}(\alpha, Re_b)$ is prescribed, Eqs.(4.8) through (4.10) written for

both phases constitute a closed set of 6 differential equations for the 6 unknowns, namely α, P, u_1, v_1, u_2 and v_2. For the present numerical simulations these equations are reduced to 4 equations and 4 unknowns by assuming a slip velocity relation of the form

$$\underline{u}_S = \underline{u}_2 - \underline{u}_1 = f(\alpha, Re_b) \qquad (4.12)$$

This explicit form of Eq.4.12 is discussed in the following sections.

Interfacial Momentum Exchange

The momentum transfer between two phases takes place via several mechanisms, the most important of which being the viscous drag force resulting from the shear stress at the interface and the form drag due to the pressure distribution on the surface of individual bubbles. Other possible mechanisms for momentum transfer include added mass effect, magnus effect (due to rotation), pressure gradient, and shear rate effects of the surrounding fluid (see for example Hinze, 1972). For brevity these forces will not be considered in the present analysis. Instead, all these effects will be lumped into the drag function Eq. (4.11).

In the bubbly flow regime, the total drag force can be related to that of a single bubble. Hirt (1982) used the following relation for water droplets in steam (for our problem, ρ_g in the original expression is replaced by ρ_ℓ).

$$F_{12} = \frac{3}{4}\,\alpha^2(1-\alpha)\,\rho_\ell\,\frac{|\underline{u}_1 - \underline{u}_2|}{d_b}\,C_D \qquad (4.13)$$

Syamlal and O'Brien (1988) suggested the following empirical relation for dispersed solid particles in a continous liquid or gas phase

$$F_{12} = \frac{3}{4}\,\frac{\alpha^2(1-\alpha)\rho_\ell|\underline{u}_1 - \underline{u}_2|}{d_b}\,C_D^* \qquad (4.14)$$

where C_D^* is another empirical drag function given by

$$C_D^* = \frac{C_D\,(\,Re_b <= Re_b/V_r\,)}{V_r^2} \qquad (4.15)$$

In Eq. (4.15) $C_D = C_D(Re_b)$ is the drag coefficient for an isolated particle and V_r is the ratio of terminal velocity of a group of particles to that of an isolated particle. Neither of the equations (4.13) or (4.15) is strictly applicable to the bubbly flow regime. However, to a first approximation the simpler relation used by Hirt (1982) should be sufficient for our purposes, provided that C_D is replaced by an empirical relation for bubbles in water.

Such a C_D relation can be derived by curve fitting to the experimental data presented by Clift et al. (1978). For bubbles in pure liquid systems, the following function is suggested by us,

$$C_D = a\ Re_b^{-b} \qquad (4.16)$$

The coefficients a and b are given in Table 4.1 for different Reynolds number ranges. This particular form is adapted because it simplifies the calculation of slip velocities considerably.

Table 4.1 Coefficients for Eq.(4.16) for Air Bubbles in Pure Liquids

Re_b range	a	b
0 - 2	24	1.000
2 - 10	23.66	0.981
10 - 100	14.9	0.780
100 - 1000	6.9	0.416

Simplification for the Gas Phase

Instead of solving for the gas phase momentum equations, the gas velocities are determined from a slip velocity relation of the form of Eq.(4.12).

For small void ratios (i.e. dilute flow with a dispersed gas phase) the gas velocities can be calculated in the radial and axial-direction, respectively, as

$$v_s = 0 \quad \text{or} \quad v_\ell = v_g \tag{4.17}$$

$$u_g = u_s + u_\ell \tag{4.18}$$

where the slip velocity is given by

$$u_s = U_{b\infty}(1-\alpha) \tag{4.19}$$

$U_{b\infty}$ is the terminal velocity of an isolated bubble in an infinite liquid medium. The effect of void ratio, α, on the slip velocity as given in Eq.(4.19) is suggested by Wallis (1962). $U_{b\infty}$ can be calculated by equating the drag force to the difference of the buoyancy force and the weight of the bubble. With the drag relation, Eq.(4.16), this force balance results in

$$U_{b\infty} = \left[\frac{4}{3a} \frac{(\rho_\ell - \rho_g)}{\rho_\ell} g\, d_b \left(\frac{\rho_\ell d_b}{\mu_\ell} \right)^b \right]^{1/(2-b)} \tag{4.20}$$

For example with $b = 1$ and $a = 24$, (i.e., Stokes range) Eq.(4.20) reduces to

$$U_{b\infty} = \frac{1}{18} \frac{(\rho_\ell - \rho_g)}{\mu_\ell} g\, d_b^2 \tag{4.21}$$

If the water (or liquid) is not pure, the degree of contamination may have significant influence on $U_{b\infty}$. For such cases, the empirical data presented by Clift et al. (1978) can be used. Another alternative is to use the terminal velocity relations presented by Hewitt (1982, chapter 2) where the terminal velocity of bubbles in clean fluids is expressed as a function of Re_b and the Galileo number $G_a = g\rho_\ell/\rho_\ell\sigma^3$.

4.3 DESCRIPTION OF CASES STUDIED

The numerical study simulated, as closely as possible, the experiments performed by Rietema and Ottengraf (1970) where a laminar liquid circulation

and bubble street formation were investigated in a Quickfit glass column. The geometric configuration for the glass column is shown in Fig. 4.1. The experimental conditions for the numerically simulated case were: liquid (glycerol water solution) density ρ_ℓ =1153 kg/m^3, liquid viscosity μ_ℓ=0.35kg/m-s, air flow rate Q_a=11.4cm^3/s, gas hold-up ϵ_g=74 cm^3, bubble diameter d_b=0.54 cm and bubble street radius r_s=5.0 cm. The glass column had a diameter of 22 cm and a height of 122 cm. Initially the column was filled with the liquid solution up to a depth of 82 cm. If the gas hold-up of 74 cm^3 is added to the liquid volume, the total mixture volume requires a column height of approximately 82.2 cm. This value was used in the simulations. Air bubbles were formed by means of injection needles. According to experiments, vertical baffles were placed along the wall, so that a reasonably symmetrical bubble street could be created. The effect of the baffles is not considered in the present study. The liquid velocity profile from the experimental work (Rietema and Ottengraf, 1970) is shown in Fig. 4.2.

For the set of calculations where $\alpha(x,r)$ is obtained from the solution of Eq.(4.28), a step function $\alpha=\alpha_0$ for $r \leq r_{so}$; $\alpha_0=0$ for $r > r_{so}$ was assumed at the inlet (see Fig. 4.12b). α_0 was approximated as the area fraction of injection holes to the total area. A hole diameter of 0.5 d_b was assumed. r_{so}/R values were varied between 0.3 and 0.9 to study the influence of distribution at the inlet on the overall circulation patterns.

Profiles for α - distribution

As a further simplification in the present model, the void fraction is assumed to vary as $\alpha(x,r) = \alpha_c(x)\ \alpha(r)$, and the shape of the profiles $\alpha=\alpha(r)$ are prescribed empirically. Among various shapes investigated are cosine, linear and parabolic profiles.

The cosine profile is given by

$$\alpha(r) = \begin{cases} 0.5\,\alpha_c\,[1+\cos(\pi r/r_s)] & r \le r_s \\ 0 & r_s < r \le R \end{cases} \qquad (4.22)$$

where R is the column radius and r_s is the radius of the bubble street as observed from experiments (Rietema and Ottengraf, 1970). Eq.(4.22) represents a smooth function which satisfies the zero derivative conditions at r=0 and $r=r_s$. The linear profile is given by

$$\alpha(r) = \alpha_c\,(1-r/r_s) \qquad (4.23)$$

where
$$r/R = -\alpha_c(1-x/L) + 1 \quad \text{for } 3/4 < x/L \le 1$$
$$r_s/R = 0.45 \quad \text{for } 1/4 < x/L \le 3/4 \qquad (4.24)$$
$$r/R = -\alpha_c x/L + 1 \quad \text{for } 0 < x/L \le 1/4$$

The parabolic profile is given by

$$\alpha(r) = \alpha_c\,\left(1 - \frac{r^2}{r_s^2}\right) \qquad (4.25)$$

where
$$r/R = 1 - \left((L-x)/L\right)^{0.437} \quad \text{for } 3/4 < x/L \le 1$$
$$r_s/R = 0.45 \quad \text{for } 1/4 < x/L \le 3/4 \qquad (4.26)$$
$$r/R = 1 - (x/\_)^{0.437} \quad \text{for } 0 < x/L \le 1/4$$

Examples of these profiles are shown in Figures 4.5b, 4.6a and 4.7a, respectively.

The center line value α_c for the three cases is determined from continuity, i. e.

$$Q_g = 2\pi \int_0^{R} \alpha_c\, \alpha(r) u_g(x,r) r\,dr \qquad (4.27)$$

Equation for α-distribution

Calculations are also performed where $\alpha(x,r)$ is calculated from conservation of mass equation for the gas phase:

$$\frac{\partial}{\partial x}(\alpha u_2) + \frac{1}{r}\frac{\partial}{\partial r}(r \alpha u_2) = 0 \qquad (4.28)$$

The advantage of prescribing the α-profiles instead of determining them from Eq.(4.28) is that all the computational uncertainties in solving Eq.(4.28), such as numerical diffusion are eliminated. Further, the former makes it possible to investigate the influence of various α-profiles on the circulation patterns.

The boundary condition for $\alpha(0,r)$ at the inlet of the bubble column is determined by the constant gas volume flow rate Q_a given by Eq.(4.27), where $\alpha(0,r)$ is prescribed as a step function, such as

$$\alpha(0,r) = \alpha_c \qquad \text{for } 0 < r/R \leq r_{so}/R$$
$$\alpha(0,r) = 0 \qquad \text{for } r_{so}/R < r/R \leq 1 \qquad (4.29)$$

where r_{so} represents the location of the last row of holes on the distributor plate. The boundary condition for $\alpha(L,r)$ at free surface is also determined by Eq.(4.27) to satisfy the continuity.

4.4 NUMERICAL METHOD

The form of equations for the continuous liquid phase (Eqs.4.9 and 4.10) is amenable for using the finite volume technique (e.g. Patankar, 1980) which has been successfully used for solution of steady, incompressible, single phase, recirculating flow problems. This formulation takes into account density variation (say due to buoyancy effects) in space which is suitable for the present problem where the microscopic density is constant but the macroscrpic density varies according to $\rho_1=\rho_\ell(1-\alpha)$. The so called "SIMPLE" algorithm of Patankar (1980) is employed to calculate the pressure field iteratively. However, modifications have been made to account for the modified