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

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

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

$$\begin{aligned} \alpha(0,r) &= \alpha_c && \text{for } 0 < r/R \leq r_{so}/R \\ \alpha(0,r) &= 0 && \text{for } r_{so}/R < r/R \leq 1 \end{aligned} \tag{4.29}$$

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 gravity term, pressure gradients $(1-\alpha)\partial P/\partial x$ and $(1-\alpha)\partial P/\partial r$, and additional momentum source terms, namely $F_{12}(u_2-u_1)$ and $F_{12}(v_2-v_1)$. These modifications have been incorporated in a readily available computer code, TEACH (Gosman and Ideriah, 1976; Durst and Loy, 1984) and the modified version has been used for the present calculations.

The "hybrid" difference scheme is used for discretization of the equations. This scheme has the property that it switches from central to upwind differencing for high Pecklet numbers ($Pe=\rho_1 \Delta x u_l/\mu_l$) for the convective terms; for the diffusive terms, the central differencing is employed at all times. For the present application the maximum Pe had an order of magnitude of 1.0. That is, the flow was mainly dominated by viscous forces, and the central differencing is used for most of the flow region. This is an important feature of the method especially for calculating the void fraction distribution from Eq.(4.28) which has no physical diffusion. Since the central differencing is a second order accurate scheme, it minimizes the truncation errors and hence the numerical diffusion.

Boundary Conditions

No slip condition was enforced for the liquid velocities at the walls and at the air inlet (distributor plate); at the centerline (r=0) symmetry conditions were imposed. The free surface was assumed to be undisturbed at which the axial-velocity, u_l, was set equal zero (i.e. no liquid flux through the surface). The radial velocity, v_l, at the free surface was calculated from the condition $\partial v_l/\partial x=0$; this is a somewhat arbitrary condition used as a first approximation since no other information is available on v_l.

Boundary conditions are needed for α when it is calculated from Eq.(4.28). Since there is no mass flux through the walls $\partial\alpha/\partial r=0$ was used at the side walls; the same condition applies at the centerline due to symmetry. At the inlet, a uniform distribution $\alpha=\alpha_0$ was assumed, and α_0 was estimated from the number of holes on the distributor plate, i.e., $\alpha_0=\Sigma A_j/A$, $j=1,2,\ldots,N$, A_j is the area of an individual hole, A is the total cross-sectional area of the inlet, and N is the number of the holes. Then from Eq.(4.27) the gas velocity is calculated for a given air flow rate, Q_a.

The α values at the free surface are not needed for the calculations, $\alpha=1$ was imposed at the grid points just outside the free surface. The present method uses a staggered grid arrangement in which the velocities are staggered and the scalar quantities are stored at centers of main grid cells. The gas velocity at the free surface is calculated from Eq.(4.27) to satisfy continuity once α was determined there.

Convergence and Grid Independence

To ensure properly converged numerical solutions, not only the total residues of difference equations were checked, but also the net liquid circulation, Q_{net} and the maximum relative change in the axial velocity, $\Delta u_{max}/u_{max}$. The net liquid volume circulated should be zero for the present problem. This is normalized by the recirculated liquid volume, Q_{cir}, given by

$$Q_{cir} = 2\pi \int_0^{r_o}(1-\alpha)\ u_\ell\ r\ dr = -2\pi \int_{r_o}^{R}(1-\alpha)\ u_\ell\ r\ dr \qquad (4.30)$$

where r_o is the zero cross point for u_ℓ. After about 300 iterations, both $\Delta u_{max}/u_{max}$ and Q_{net}/Q_{cir} values were less than 10^{-5} which are shown in Fig.4.3 and Fig.4.4, respectively. Calculations were continued another 200 iterations to ensure complete convergence.

Two uniform grid distributions were used, namely a coarse grid of 23x12 (Δx=4cm, Δr=1cm), and a fine grid of 42x23 (Δx=2cm and Δr=0.5cm). The difference in liquid velocity from the coarse grid and fine grid solutions was less than 1%. The fine grid solutions are presented in this paper unless stated otherwise.

4.5 RESULT AND DISCUSSION

Results with Prescribed α - Profiles

The results of the calculations using a cosine profile for the shape of $\alpha(r)$ distribution are depicted in Figs. 4.5a through 4.5d. The predicted streamlines plotted in Fig. 4.5a show the commonly observed circulation pattern with a downward flow near the wall and an upward flow near the center of the reactor. The stream function is calculated from

$$\psi = 2\pi \int_0^R (1-\alpha)\, \rho_\ell\, u_\ell\, r\, dr \qquad (4.31)$$

The total volume of the circulated liquid can be read off from Fig. 4.5a as $Q_{cir} \cong 0.16 m^3/s$. The center of the circulation zone is predicted to be close to the free surface. As it will be discussed later, the circulation pattern is a direct result of the void-fraction distribution. The corresponding α diatribution is shown in Fig. 4.5b. Though the shape of the α-distribution is assumed, its magnitude is calculated as part of the solution. Fig. 4.5b shows that α decreases with the axial distance. This occurs as a result of the increase in the gas velocity towards the free surface; to satisfy continuity Eq.(4.27) as the mean value of u_g increases, that of α should decrease. The predicted liquid velocity profiles are shown in Fig. 4.5c. The predicted value of centerline velocity, $u_{\ell c} \cong 22$ cm/s, at $x/L=0.5$ is considerably higher than the measured value of $u_{\ell c} \cong 10.5$ cm. The boundary of the reverse flow where $u_\ell=0$ is predicted as $r/R=0.50$ which is in good agreement with experiments. The agreement is also good for the maximum reverse flow velocities which are seen to be 3-4 and 3-5 cm/s for experiments and predictions, respectively. Of course, these quantities do change with axial distance and with the prescribed bubble-street radius, r_s.

The influence of different void fraction-profile shapes on the results were also investigated where the gas flow rate and the bubble-street diameter were fixed. Fig. 4.6b shows the resulting of liquid velocity distribution with prescribed linear α distribution and Fig. 4.7b shows the resulting of liquid velocity distribution with prescribed parabolic α distribution. The linear and parabolic α-profiles does not influence the results very much. The reverse flow boundary and the maximum reverse flow velocities are affected the least. The centerline liquid velocity is somewhat higher for the parabolic profile compared to the others. These results show that it is the magnitute of the α-distribution and the bubble-street diameter which primarily affect the flow pattern in a column reactor.

Results with Varing Street Diameters

Comparisons of the results were made by varying the bubble street radii as r_{so}/R=0.27, 0.45, and 0.65. The results for r_s/R=0.27 and 0.65 are shown in Fig. 4.8 and Fig. 4.9. These figures show that a decrease in r_{so} causes an increase in α values, thus an increase in the liquid velocity and vise versa. This also affects the boundary of the reverse flow zone. For example, for r_s/R=0.65, the predicted centerline velocity is about 18cm/s and for r_{so}/R=0.27 it is about 26 cm/s at the mid-height of the column. Consequantly, the uncertainties in measuring the region where α=0 (i.e. no air bubbles) will result in differences between the experiments and predictions.

Results with Predicted α - Distribution

Further results of the predictions are depicted in Figs. 10-13 where

α-distribution was calculated from Eq.(4.28) directly. The Subroutine CALCAL is modified for the purpose of α calculation. The inlet boundary condition was a step function as described by Eq.(4.29), where $\alpha=\alpha_0$ for $r/R < r_{so}/R$ and $\alpha=0$ otherwise. r_{so}/R is the value of the cut-off point for the α - step function at $x=0$. r_{so}/R is chosen as 0.45, 0.6, 0.7 and 0.9 for the investigating the nfluence of air distribution at the distributor plate. Fig. 4.10, Fig. 4.11, Fig. 4.12 and Fig. 4.13 show the results of r_{so}/R=0.45, 0.6, 0.7 and 0.9 respectively. Fig. 4.10a, Fig. 4.11a, Fig. 4.12a and Fig. 4.13a are the profiles of α distributions for the four cases at different section along the column. The resulting recirculation patterns shown in Fig. 4.10b, Fig. 4.11b, Fig. 4.12b and Fig. 4.13b are quite different. The center of the recirculation zone moved towards the bottom of the reactor as the value of r_{so}/R increases. By compariing the results from the predicted α-distribution shown in Fig. 4.10a with the results from prescribed cosine α distribution as shown in Fig. 4.5a. It can be seen that with the same street diameters, the overall magnitude of α is lower in Fig. 4.10a than that in Fig. 4.5a, and it does not vary much in the axial direction (see also Fig. 4.10c). On the other hand, the centerline-gas velocity first increases and then decreases with the axial distance (Fig. 4.10f) remaining fairly flat near the mid-height of the column. Fig. 4.10a also shows that narrow bubble street prescribed at the inlet is dispersed radially inward and outward as a result of convective gas velocities in this direction. The contour plots of α-distribution for r_{so}/R=0.45, 0.6, 0.7 and 0.9 shown in Figs. 4.10e, 4.11e, 4.12e, and 4.13e indicate that first, the bubbles are convected towards the center of the tube near inlet then outwards towards the wall near the free surface, where the radial gas velocity (=liquid velocity) is inward and outward, respectively. This is in conformity with the usual experimental observations (e.g. Freedman and Davidson, 1969). In this case there is a much closer agreement between the measured and predicted velocity profile at $x/L=0.5$ as shown in Fig. 4.10c. The location of the measurements is reported (Rietema and Ottengraf, 1970) to be near the mid-height of the column. The magnitude of the predicted u_ℓ values decreases because the overall α values are lower and hence less drag force is impacted on the liquid by the gas flow.

The values of the cut-off point r_{so}/R for the α-step function at $x=0$ were chosen arbitrarily. This brings the question of what exactly this value should be? Strictly speaking, this should be the location of the last row of injection holes on the distributor plate, but this information was not available from the experiments considered here. A further increase of this parameter to $r_{so}/R=0.7$ resulted in much closer agreement between the measured and predicted liquid velocities (Fig. 4.12c), but the center of the recirculation zone moved further down towards the inlet (Fig. 4.12a). The results show that, increasing the value of r_{so}/R, decreases the liquid velocity at the centerline. As shown in Fig. 4.13c, liquid velocity has a small value when the air flow is distributed over 90% of the inlet area. For the same case, Fig. 4.13b shows very little variation in α distribution in the axial direction from that prescribed at the inlet. The results depicted in Figures 4.14a and 4.14b show that the circulation is negligibly small when α is uniformly distributed over the whole cross-section of the inlet area.