7.5. Effects of Gas Distributors

One of the major topic in studies of bubble column reactors for engineering application is the effect of the different type of gas spargers on the characteristics of the flow field and in turn on the mass/heat transfer properties. Numerical simulation may provide useful information in this regard. We have made a group of simulations of a 15-cm wide column. Each simulation uses a different gas distributor, which are: one, three, and nine injectors and a uniform distributor. The injectors are set symmetric about the center-line of the column. By uniform distributor we mean that the gas velocity at the inlet, i.e. at the bottom of the column, is uniformly set to a constant value. Among these four cases, the one with the uniform distributor is considered as the closest to realty. In most bubble column reactors, the gas is introduced into the column through many tiny holes on a perforated plate. The size of these holes is usually of the order of 0.1 mm or even smaller, and the holes are distributed uniformly on the plate. A perforated plate, whose open area is of the order of 0.1%, would have hundreds holes. Obviously it is impossible to resolve the holes in a numerical simulation. Thus an uniform distribution of gas velocity and volume fraction at the bottom would be a reasonable boundary condition for simulations.

In the cases simulated, while the gas is injected in different ways into the column, the superficial velocity is kept the same for all the runs. Figure 7.8 shows the flow pattern for these four cases. One notes that the overall gas holdup for each case is the same. This indicates that the overall gas holdup is not affected by the gas distributors and depends on the gas superficial velocity U_{sup} only. Some differences are observed in the large structures in each case. The wave length of the meandering structure in the columns with three and nine injectors are smaller than those with one and uniform distributors. The mean liquid velocity and gas holdup profiles for the middle section of the column are shown in Figure 7.9. One can see that the differences between all the cases are quite small. It is thus confirmed that changes in gas distributors induce only limited effects on the mean properties and flow structures.

7.6. Quantitative Comparison With Experiments

To further verify our numerical results, we conducted quantitative comparisons of the mean velocity, turbulence intensities and shear stress profiles with the experimental data provided by Mudde *et al*. (1997). Figure 7.10 shows the vertical and horizontal mean velocity profiles of a 11-cm wide column at 1 cm/s gas superficial velocity. The compared profiles are for the middle section of the column where the mean flow is usually assumed one dimensional. The numerical prediction of the mean horizontal velocity, $\bar{u}$, is essentially zero as expected. The experimental data, however, is non-zero and exhibits an inward flow. As pointed out by Mudde *et al*. (1997), this is attributed to a systematic error due to the difficulty in tracking the particles in the fast-moving bubble stream and other biased measurements. The comparison of the mean vertical velocity profile is quite good except in the near-wall region. One reason for this discrepancy is that the boundary layer is too thin to be resolved in our current simulations.

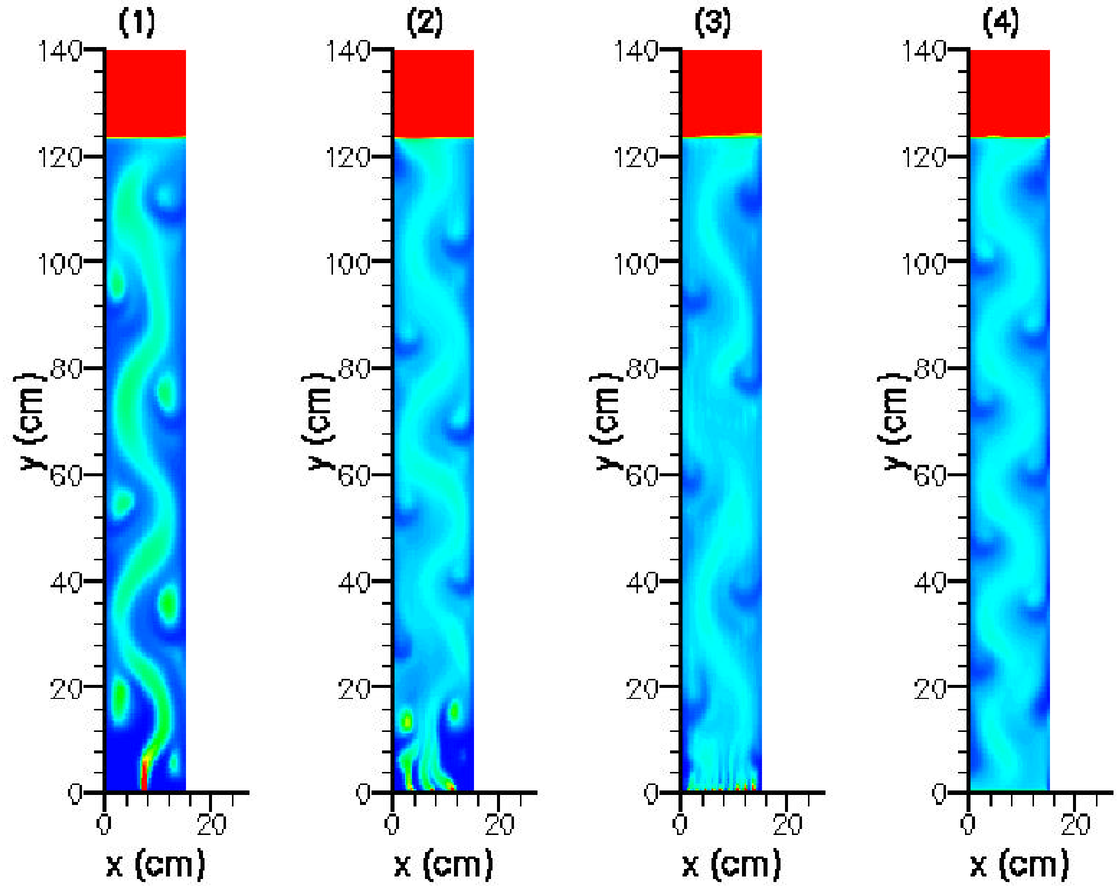

Figure 7.8: The Instantaneous Gas Holdup Contour of 15-cm Wide Column at U_{sup}=1 cm/s with: (1) 1-jet; (2) 3-jet; (3) 9-jet; (4) Uniform Gas Distributor

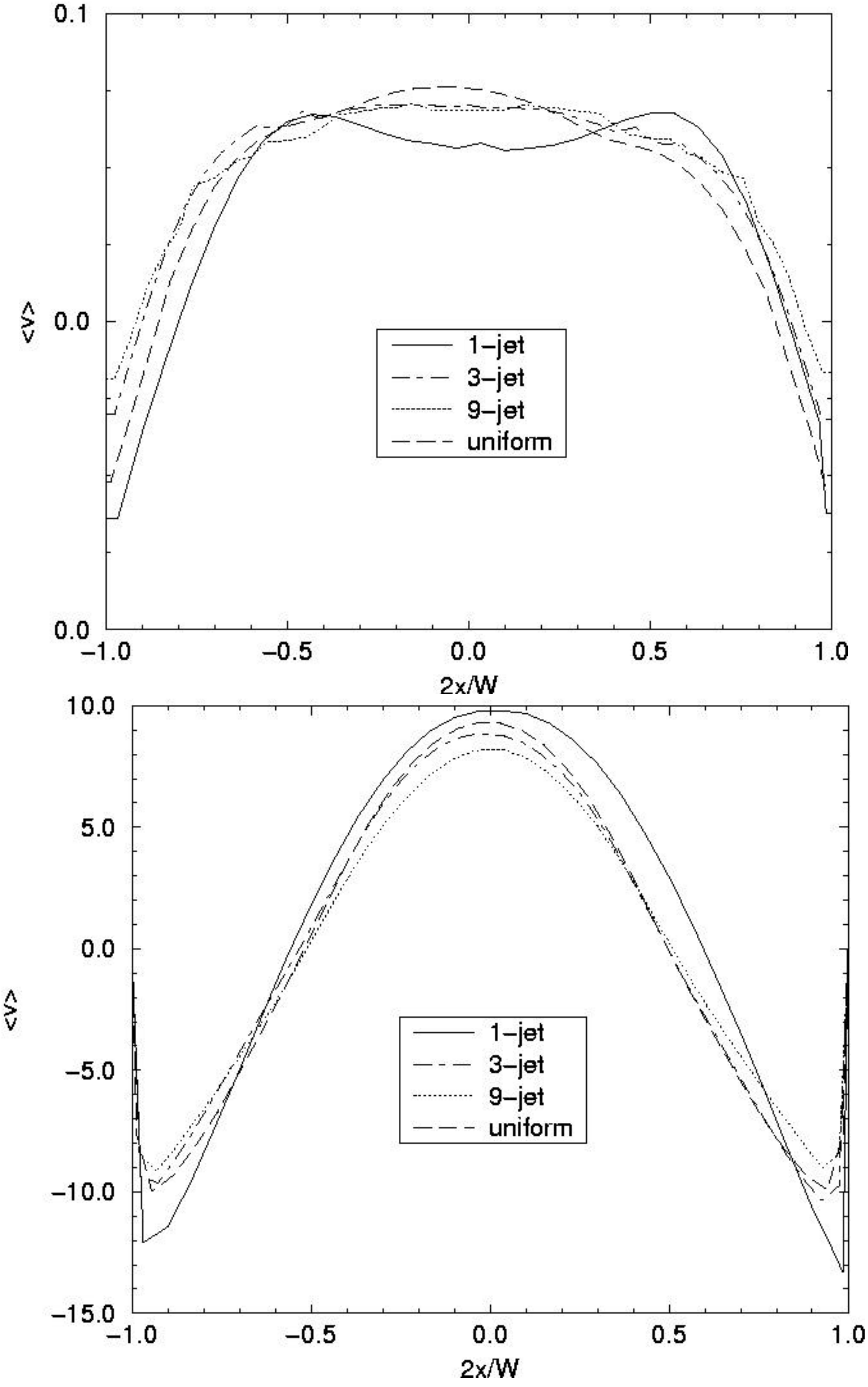

Figure 7.9: Time Averaged Profiles Gas Holdup and the Vertical Velocity of the Liquid Phase at the Middle Section of 15-cm Wide Column at U_{sup}= 1 (cm/s), With Different Gas Distributors

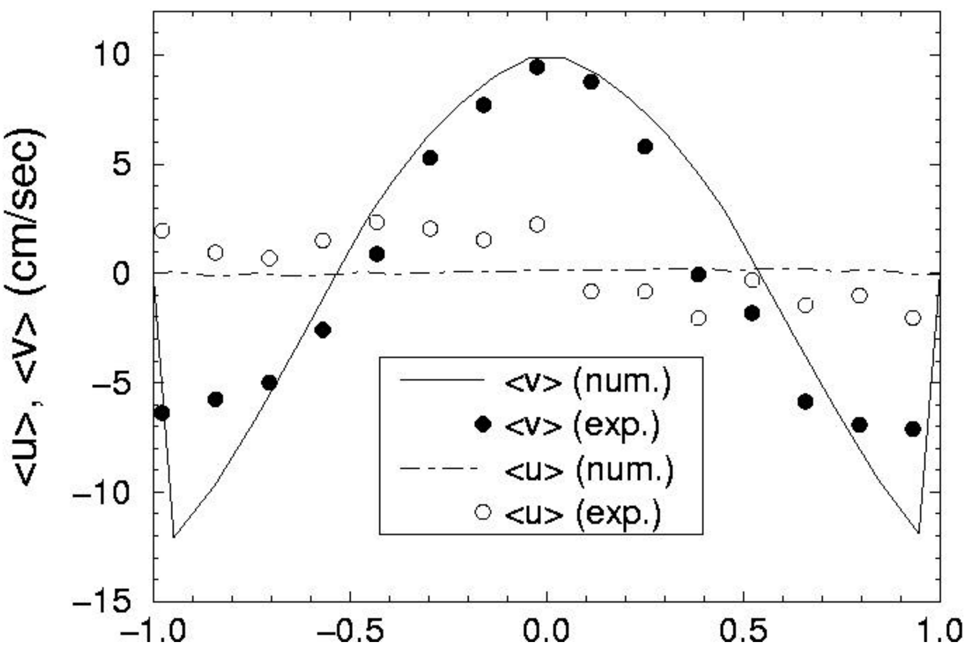

Figure 7.10: Time-Averaged Velocity Profiles for the Middle Section of 11-cm Wide Column at U_{sup}=1 (cm/s)

For a 15-cm wide column, the comparisons of the mean vertical liquid velocity are made for the middle, lower and upper sections, as shown in figure 7.11. Again the numerical values match the data quite well particularly in the lower section. The case of a 32-cm wide column is also compared with the experimental data as shown in Figure 7.12. Since the window of PIV measurement covers only half of the column, the data is provided for the left half of the column. Notice that the gas superficial velocity for this case is relatively high, i.e. U_{sup} =1.9 cm/s. Still the comparison is very satisfactory.

The numerical prediction of turbulence intensities, $\overline{u'u'}$ and $\overline{v'v'}$, and Reynolds shear stress, $\overline{u'v'}$, of 15-cm column under U_{sup} =1.0 (cm/s) are compared with data in Figure 7.13. The $\overline{u'u'}$ reaches a peak at the central portion of the column since u attain its highest magnitude in the center due to the nature of the meandering motion of the central plume. The peaks of $\overline{v'v'}$ at the near-wall vortical region are consistent with the fact that the flow dynamically changes from upward to downward in such areas. Although the general trend of the numerical values match the data, there are significant differences in the values. It is clear that the simulation under predicts the turbulence related properties. This simply means that our simulations are not able to resolve all the scales of turbulence. However, the good comparisons of mean velocity profile indicate that the effects of turbulence, here mainly the bubble-induced turbulence, are properly modeled and included in the calculation.

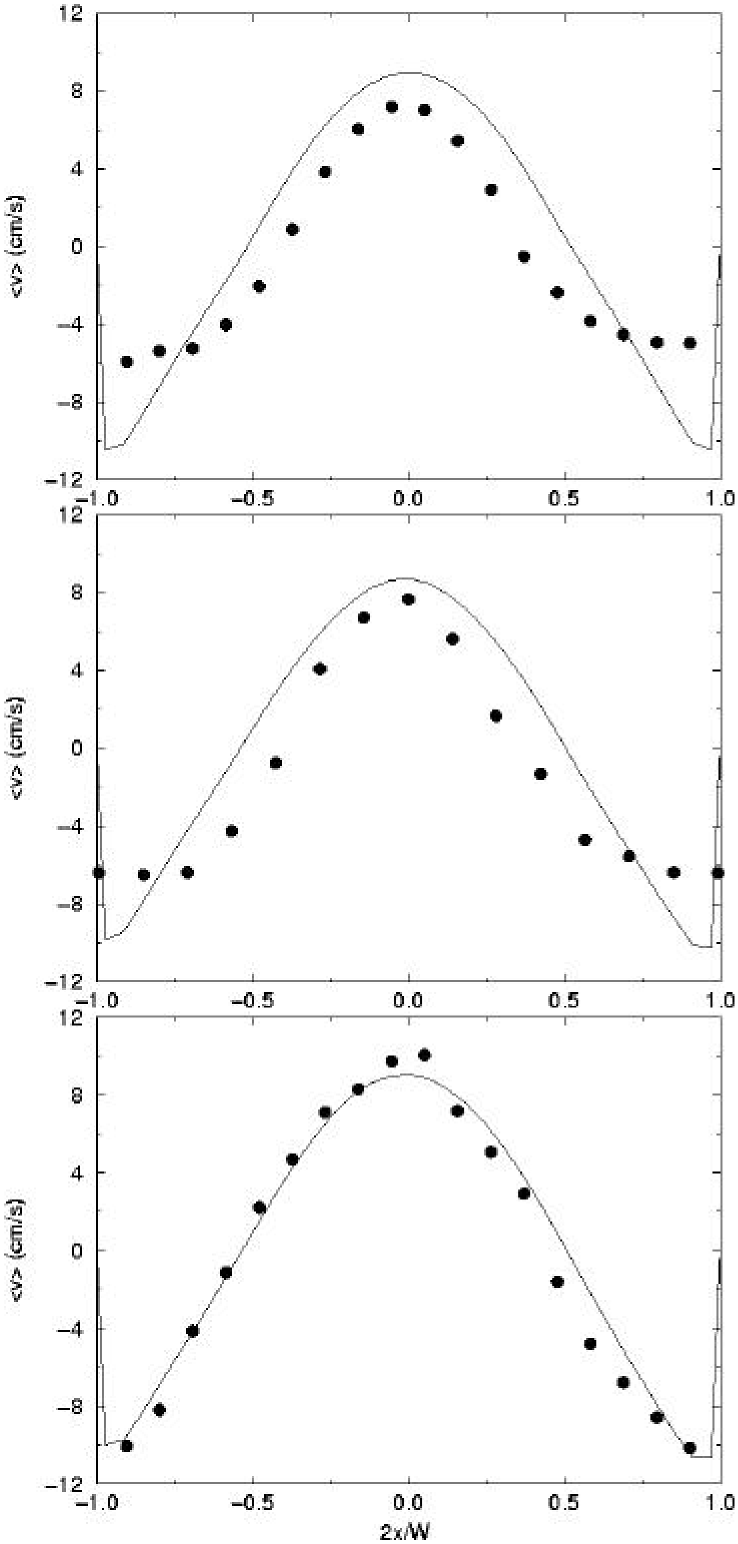

Figure 7.11: Time-Averaged Velocity Profiles for 15-cm Wide Column at U_{sup}=1 cm/s. Top: Upper Section; Middle: Middle Section; Bottom: Lower Section. — and • are the Numerical Prediction and Experimental Data, Respectively

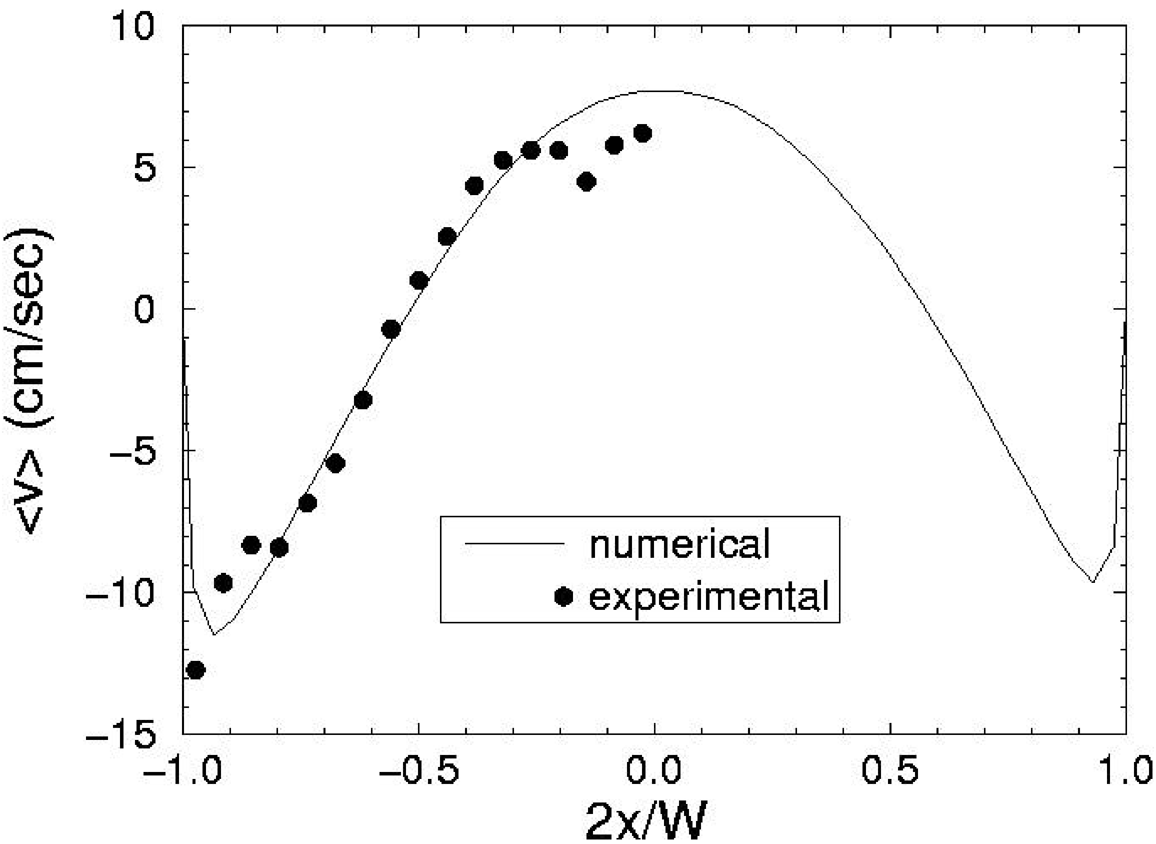

Figure 7.12: Time-Averaged Velocity Profile for the Middle Section of a 32-cm wide Column at U_{sup}=1.9 cm/s

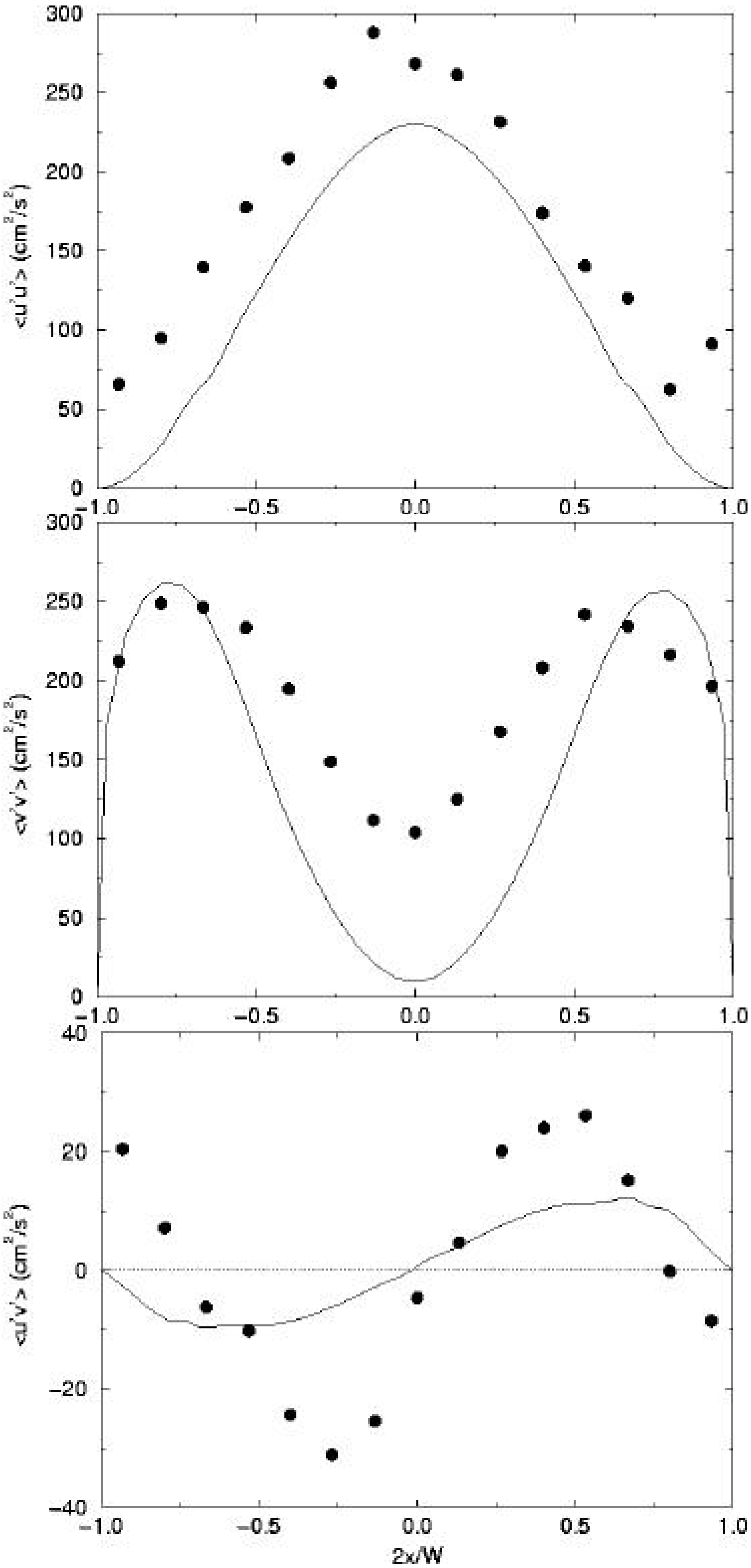

Figure 7.13: Turbulence Intensities and Reynolds Shear Stress in the Middle Section of 15-cm Wide Column Operated at U_{sup}=1 cm/s. — is the Numerical Values; • is the Experimental Data by Mudde *et al.* (1997)

7.7. Conclusions

The numerical simulation of gas-liquid flow in two-dimensional bubble columns using Eulerian/Eulerian two-fluid model is able to capture the characteristics of large structures. Quantitative comparisons with the experimental data reveal that, by applying simple models of inter-phase momentum transfer and bubble-induced turbulent viscosity in the liquid phase, the two-fluid simulations provide satisfactory results for the mean flow quantities at least for the case of dispersed bubbly flow, i.e. low gas superficial velocities. To extend the work to higher gas velocity and three-dimensional column, more sophisticated models for the forces on bubbles and turbulence may be needed.

Table 7.1: Column Size and Flow Conditions

Column width (cm)	U_{sup} (cm/s)	Static liquid height (cm)	Number of gas injectors	Aspect ratio
11.2	1.0	110	2	9.8
15.2	1.0	110	3	7.2
32.0	1.2	110	6	3.4
32.0	1.9	110	6	3.4

7.8. Notation

u_c	liquid velocity field
u_d	gas velocity field
ε_c	liquid volume fraction
ε_d	gas volume fraction
U_{sup}	superficial gas velocity
d_p	bubble diameter
τ	surface tension
ρ_c	liquid mass density
ρ_d	gas mass density
μ_c	liquid viscosity
Eo	Eotvos number $\equiv d_p^2 \rho_c g / \tau$
Re	bubble Reynolds number $\equiv d \lvert u_c - u_d \rvert \rho_c / \mu_c$

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8. SUMMARY AND CONCLUSIONS

It is appropriate to summarize here the various tasks originally set for this study, the accomplishments achieved and the conclusions reached. Overall, all of the objectives set for this cooperative Industry-University grant have been achieved or exceeded.

The original goals set for this study, the related accomplishments and conclusions are listed below, grouped by individual tasks.

Task 1. Develop a computerized mathematical procedure (based on physics of radiation and Monte Carlo calculations) for calibration of the Computer Automated Radioactive Particle Tracking Technique (CARPT) that will eliminate the currently lengthy in-situ calibration and allow the technique to be used in the field on high pressure units. Specifically, plan the use of CARPT on a high pressure bubble column.

- Monte Carlo based procedure for calibration of detectors and for determination of radioactive particle position during CARPT runs has been developed and fully implemented. Details are described in Chapter 5 of this report.
- CARPT runs have been executed as planned at elevated pressure (Chapter 4 of this report). This necessitated the construction of a specialized facility at WU and of a novel particle positioning device for calibration purposes.
- •• As a result of the availability of the Monte Carlo procedure, future CARPT runs at elevated pressures will be much easier to implement and will be more accurate.
- •• The basic liquid recirculation flow pattern is apparently unaffected by pressure. In the time averaged sense a single liquid recirculation cell is observed, with the liquid rising in the middle of the column and falling by the walls. The magnitude of liquid velocities is diminished at elevated pressure.

Task 2. Improve the accuracy of the CARPT technique and compare the velocities obtained by CARPT in certain regions of the column to those determined by the Heat Transfer Probe and Particle Image Velocimetry (PIV).

- The accuracy of the CARPT technique, especially for evaluation of instantaneous velocities, was greatly improved by implementation of a wavelet based filter (Chapter III of the First Annual Technical Report) and by the Monte Carlo technique (Chapter 5 in this report).
- A thorough comparison of PIV and CARPT data in a 4" diameter column at superficial gas velocity and low holdup, where PIV results can be deemed very accurate, validated fully CARPT measurements (Chapter 4 of the Second Annual Technical Report).

- Comparison of CARPT data with Laser Doppler Anemometry (LDA) and Hot Film Anemometry (HFA) indicate good agreement (Chapter 6 of Second Annual Technical Report).

•• Extensive comparison of various techniques revealed that at low superficial gas velocities all of them can provide good results. At such conditions of low gas holdup PIV, LDA and HFA have the capabilities of revealing fine structures of the flow and dynamic behavior at high frequencies, which are the features which CARPT lacks. However, CARPT always provides an accurate description of the mean flow quantities and of the dynamic features of the large flow structures. This information is obtainable by CARPT at very high superficial gas velocities when, due to very high gas holdup, all other techniques fail. The heat transfer probe (HP) which also can be used at high superficial gas velocities underestimates the mean velocities such conditions.

Task 3. Develop local probes for accessing velocities, holdups and heat transfer coefficients in bubble column reactors.

- A special heat transfer probe was developed (OSU) and tested (ER&E) to measure the instantaneous heat transfer coefficient due to gas bubbles injected in liquid and liquid-solid systems (Chapter IV of the First Annual Technical Report).

- A light transmittance probe was developed (OSU) and tested to quantify the bubble characteristics and frequencies of bubble passage (Chapter 7 of the Second Technical Report).

- A high framing, high resolution, high capacity PIV system was developed for the purposes of this study at OSU (Chapter 5 of the Second Annual Technical Report).

- A computer tomography system (CT) was implemented to obtain gas holdup profiles at different gas superficial velocities (Chapter 3 of Second Annual Technical Report, Chapter 3 of this report).

•• Reliable time averaged density profiles can be obtained by gamma ray based in bubble columns.

•• Local heat transfer coefficients can be assessed effectively with the developed probe.

•• PIV and optical probes are valuable research tools for quantification of bubbly flows.

Task 4. Collect velocity and voidage profile data in gas-liquid and gas-liquid-solid systems at different solids loadings and at close to atmospheric pressure.

- The collected velocity and holdup profiles were used for validation of the various techniques such as in CARPT-PIV comparisons (Chapter 5 of Second Annual Technical Report), for comparison of CFD predictions and models (Chapter 6 of Second Technical Report and Chapter 7 of this report) and for augmentation of the data base for evaluation of important fluid dynamic parameters (Chapter 6 of this report).

•• A very useful correlation has been developed at OSU for prediction of bubble rise velocity. The validity of this correlation in high pressure, high temperature systems was validated (Chapter 6 of this report).

Task 5. Use state-of-the-art hydrodynamic models and codes to predict velocity and holdup fields under conditions studied experimentally. Search for most suitable constitutive forms (e.g., lift, drag, turbulence closure models, etc.) to reach agreement between calculated and experimentally observed values. Try to assess the effect of elevated operating pressure on various constitutive forms.

- A fundamentally based computational method was developed at OSU based on the volume averaged method, the dispersed particle method, and the volume of fluid to simulate the transient behavior of a rising bubble in gas-liquid-solid (Chapter 6 of this report).

- The Euler-Euler two-fluid model, in the framework of the Los Alamos CFDLIB code, was adopted for simulation of flow fields in the whole bubble column. Mixing length and bubble induced turbulence closures were tried (Chapter 9 of Second Annual Technical Report and Chapter 7 of this report).

- As an interim measure an engineering phenomenological model was developed for both liquid and gas flow and mixing based on the collected data base on this and related studies. This model captures the essence of the observed recirculation and mixing phenomena (Chapter 8 of the Second Annual Technical Report).

•• The fundamental model at OSU predicts well the bubble shape, trajectory and rise velocity in slurries.

•• The Euler-Euler model predicts well the time averaged quantities and dynamic features of large structures in bubbly flows (2D columns).

Task 6. Collect the data in a high pressure 6" diameter bubble column and compare to model predictions. Also collect high pressure PIV data in slurry systems at Ohio State University. Refine the models if needed.

- Instead of collecting high pressure data at the Florham Park Exxon Research and Engineering facility, an equivalent experimental set-up was developed, with additional funding from ER&E, at Washington University. This change in plans was necessitated by the safety and radioactive material licensing issues which prevented the work to be conducted at Exxon facilities. The fact that a high pressure 6" bubble column facility had to be designed and constructed at WU necessitated the 9 month (no-cost to DOE) extension of this research. High pressure data for gas holdup and velocity were conducted in the 6" column at WU (Chapter 3 and 4 of this report).

- High pressure data in smaller diameter columns was also collected via PIV and other techniques at OSU and used for development of correlations for various fluid dynamic parameters (Chapter 6 of this report).

- An improved understanding emerged about the behavior of high pressure bubble columns and slurry bubble columns. High pressure delays the transition to churn turbulent flow, flattens the observed gas holdup profiles at high gas superficial velocity and reduces the magnitude of liquid recirculation.

All of the above accomplishments bring us closer to our goal of improved quantitative understanding of fluid dynamics in bubble columns. The progress in this University-Industry joint project was greatly helped and assisted by the complementary companion DOE subcontract via Air Products to both Washington University and Ohio State University. The contract DE FC 95 22 PC 9 5051 is gratefully acknowledged.