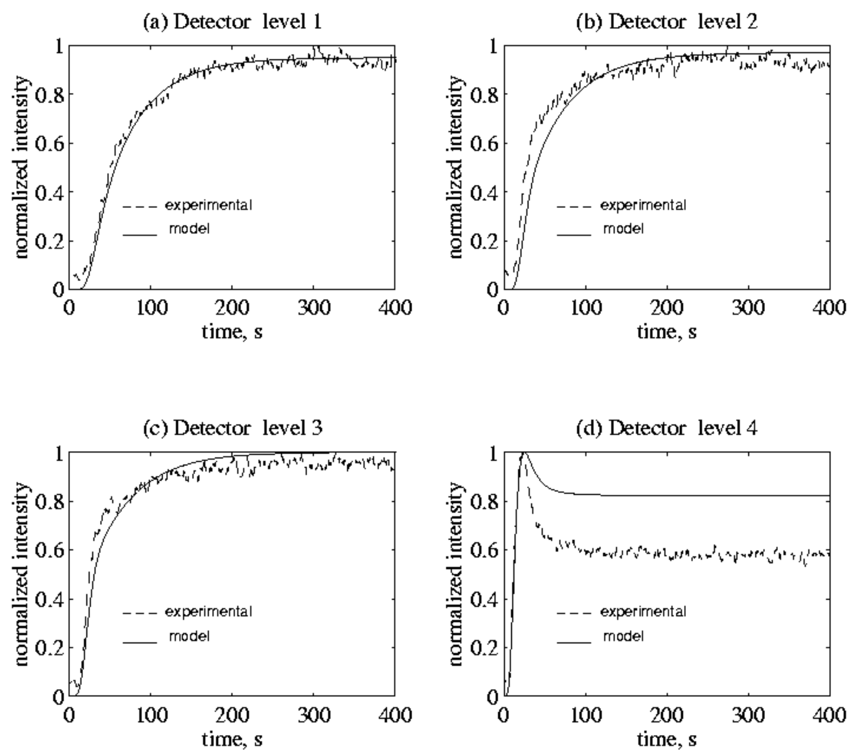

Figure 2.16 Comparison of Model Prediction with Experimental Detector Responses for Wall Injection at Level N1, Run 14.6

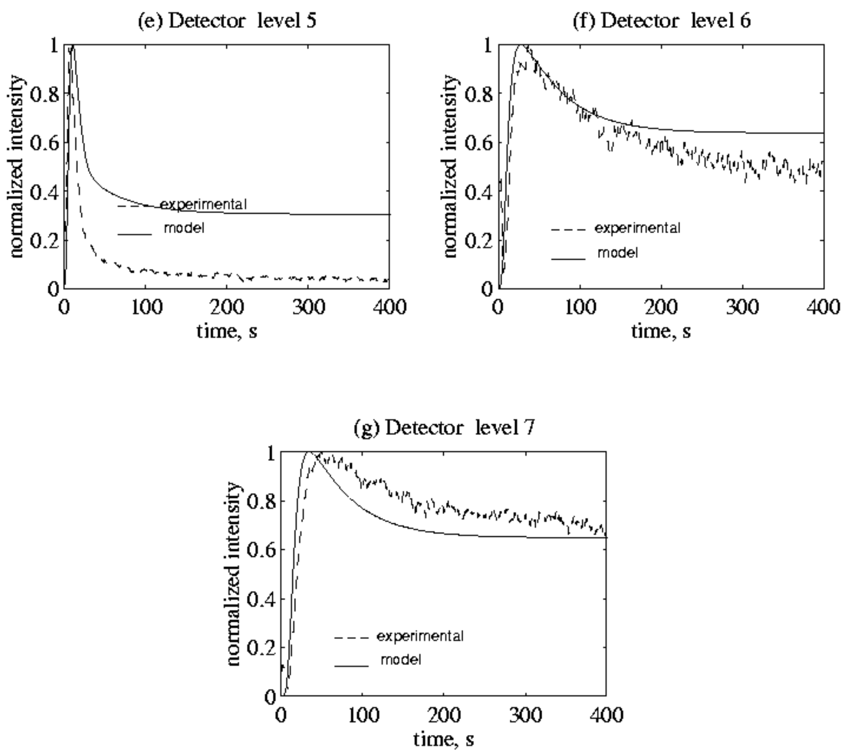

Figure 2.17 Comparison of Model Prediction with Experimental Detector Responses for Wall Injection at Level N1, Run 14.6

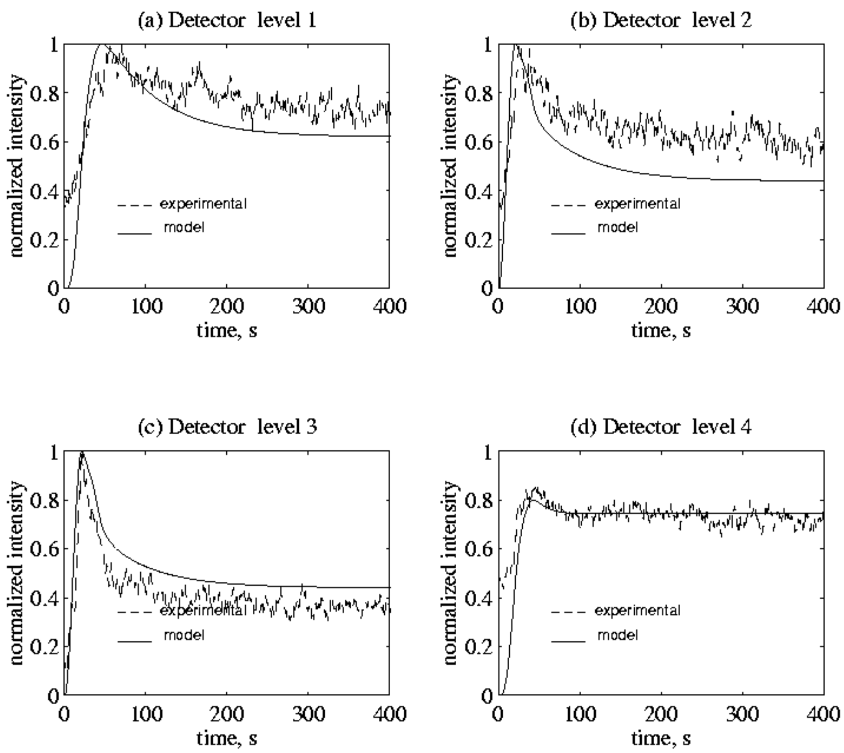

Figure 2.18 Comparison of Model Prediction with Experimental Detector Responses for Center Injection at Level N2, Run 14.6

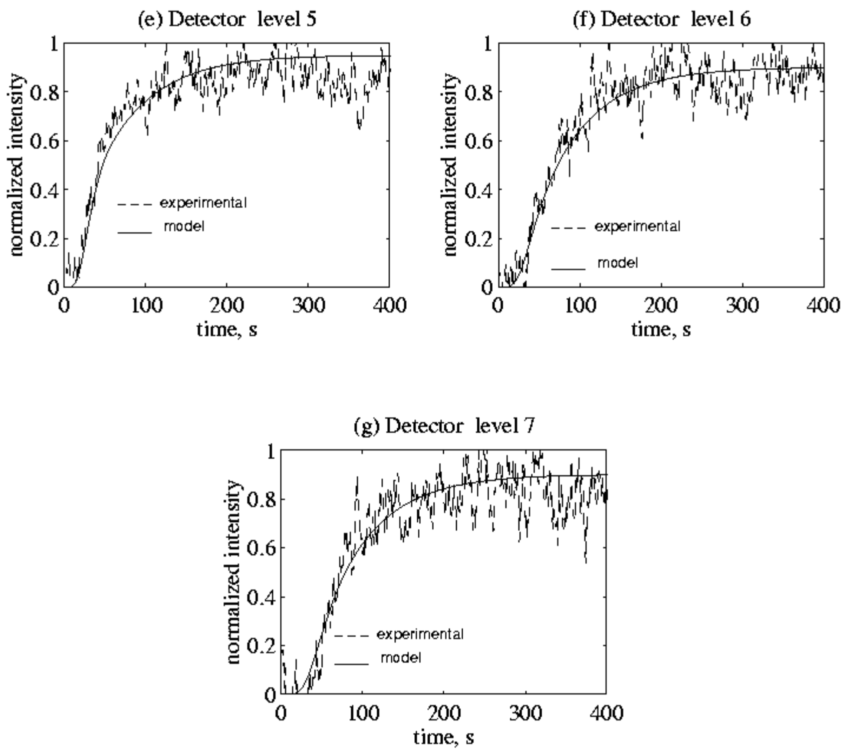

Figure 2.19 Comparison of Model Prediction with Experimental Detector Responses for Center Injection at Level N2, Run 14.6

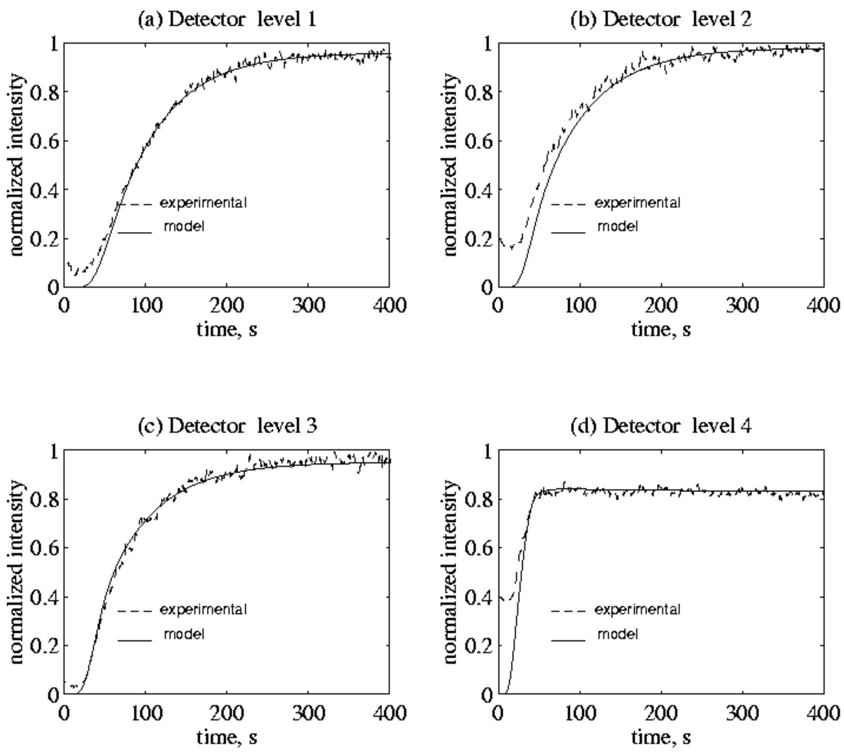

Figure 2.20 Comparison of Model Prediction with Experimental Detector Responses for Center Injection at Level N1, Run 14.6

Table 2.3 List of Estimated Average Fluid Dynamic Parameters for the LaPorte AFDU during Methanol Synthesis

Run No.	U_{g0} cm/s	$\bar{\varepsilon}_g$	U_{ge} cm/s	$\bar{u}_{rec}$ cm/s	$\overline{D}_{zz}$ cm^2/s	$\overline{D}_{rr}$ cm^2/s
14.6	25.0	0.39	47.4	47.6	965.2	114.1
14.7	14.0	0.33	33.1	41.2	854.0	100.7
14.8	36.0	0.38	44.7	46.5	946.0	111.3

It should be noted that while Runs 14.6 and 14.7 were at a higher pressure of 52 atm, Run 14.8, which was carried out at a higher superficial gas velocity of 36 cm/s, was at a lower pressure of 36 atm. The effect of pressure is evident in the gas holdup measurements, which indicate a lower holdup for Run 14.8 in comparison with Run 14.6, although it was operated at a higher superficial gas velocity.

The results of the model predictions for the various injections of Runs 14.7 and 14.8 are shown elsewhere (Degaleesan, 1997). It is clear from these figures that the model is, in general, able to correctly predict the mixing patterns within the reactor shown by the detector responses. By using a single set of input parameters (Table 2.3) for a given experimental condition, the model is able to capture the mixing patterns for the various injection locations, as measured by detectors at all levels. This substantiates using the proposed convective-diffusion model to describe liquid mixing based on liquid recirculation and turbulence, and suggests that the preliminary scaleup rules developed result in a good estimate of the input fluid dynamic model parameters. Such comparisons indirectly justify the proposed methodology of characterization of churn-turbulent bubble columns by using the gas holdup in the reactor as a means of accounting for the effects of pressure, solids and other system parameters.

The approach used for evaluation of the model parameters stresses the importance of measurement and prediction of the gas holdup and its radial distribution in the column. Several correlations exist in the literature that account for the effects of pressure and liquid properties on overall gas holdup. However, there is no good agreement between the correlations, even at atmospheric pressure. Table 2.4 shows the correlations used to estimate the transition holdup and transition gas velocity based on the bimodal bubble size distribution in churn-turbulent flow. Measurements of large bubble holdup and rise velocities, using dynamic gas disengagement (DGD) under different process conditions, have resulted in correlations listed in Table 2.5.

A combination of the correlations of Wilkinson et al. (1992) for the transition holdup and velocity (1T. in Table 2.4), along with that of Krishna and Ellenberger (1996) for the dilute phase holdup (2L. in Table 2.5), seems to yield the best estimates for the global gas holdup compared to experimental data in the AFDU during methanol synthesis (Table 2.1). The slurry phase properties existing under experimental conditions in the AFDU are considered, instead of the liquid (except for the surface tension, σ, since no data were available for the slurry), resulting in gas holdups reported in Table 2.6. The estimated values of the overall gas holdup show

Table 2.4 Correlations for Estimating the Transition Holdup and Transition Gas Velocity based on the Bimodal Bubble Size Distribution in Churn-Turbulent Flow (SI units)

No.	Reference	
1T.	Wilkinson et al. (1992)	$\varepsilon_{trans} = 0.5\exp(-193\rho_g^{-0.61}\mu_l^{0.5}\sigma^{0.11})$ $\frac{V_{small}\mu_l}{\sigma} = 2.25\left(\frac{\mu_l^4 g}{\rho_l\sigma^3}\right)^{0.273}\left(\frac{\rho_l}{\rho_g}\right)^{0.03}$ $U_{trans} = \varepsilon_{trans}V_{small}$
2T.	Reilly et al. (1994)	$\varepsilon_{trans} = 4.457\sqrt{\frac{\rho_g^{0.96}}{\rho_l}}\sigma^{0.12}$ $V_{small} = \frac{1}{2.84}\frac{1}{\rho_g^{0.04}}\sigma^{0.12}$ $U_{trans} = \varepsilon_{trans}V_{small}(1-\varepsilon_{trans})$

Table 2.5 Correlations for Estimating the Large Bubble Holdup and Overall Holdup based on the Bimodal Bubble Size Distribution in Churn-Turbulent Flow (SI units)

No.	Ref.		
1L.	Wilkinson et al. (1992)	$\frac{V_{lb}\mu_l}{\sigma} = \frac{V_{small}\mu_l}{\sigma} +$ $2.4\left[\frac{(U_g - U_{trans})\mu_l}{\sigma}\right]^{0.757}\left(\frac{\mu_l^4 g}{\rho_l\sigma^3}\right)^{0.077}\left(\frac{\rho_l}{\rho_g}\right)^{0.077}$ $\varepsilon_{lb} = \frac{(U_g - U_{trans})}{V_{lb}}$	$\bar{\varepsilon}_g = \varepsilon_{trans} + \varepsilon_{lb}$
2L.	Krishna et al. (1996)	$\varepsilon_{lb} = \frac{0.268}{D_c^{0.18}}(U_g - U_{trans})^{0.58}$	$\bar{\varepsilon}_g = \varepsilon_{lb} +$ $\varepsilon_{trans}(1-\varepsilon_{lb})$

reasonable agreement with the measured average holdup, especially at the two higher gas velocities. However, the estimated transition gas velocity from bubbly flow to churn-turbulent flow seems low when compared with experimental results for atmospheric air-water systems. This is partly due to the high values of the holdup of the small bubbles. The high holdup of small bubbles (transition holdup), which is the same for Runs 14.6 and 14.7, results in a higher value of the gas holdup for Run 14.7 (U_g = 14.0 cm/s), compared with experimental measurements.

The correlations of Wilkinson et al. (1992) yield much higher values for the large bubble holdup (1L. in Table 2.5). This may be caused by the fact that his correlation does not take into consideration the effect of column diameter on large bubble holdup (which is supposed to decrease with increase in column diameter). Reilly's correlation (2T. in Table 2.4), which resulted in moderate estimates of the transition gas velocity and holdup under atmospheric conditions, greatly overpredicts the transition holdup for the current high-pressure data. For example, for Run 14.6, the transition holdup calculated from Reilly's correlation gives ε_{trans} = 0.58, which is much higher than the overall gas holdup measured in the reactor, ~ 0.4. This points to the disparity in the available correlations, which perform well only under a certain range of operating and process conditions.

Table 2.6 Estimation of Global Gas Holdup in the Reactor Using Correlations from the Literature

Run No.	U_{g0} cm/s	Press. MPa	Wilkinson (1992)		Krishna et al. 1996		Measured
			ε_{trans}	U_{trans} (m/s)	ε_{lb}	$\bar{\varepsilon}_g$	$\bar{\varepsilon}_g$
14.6	25.0	5.2	0.28	0.056	0.120	0.40	0.39
14.7	14.0	5.2	0.28	0.056	0.073	0.35	0.33
14.8	36.0	3.6	0.24	0.049	0.160	0.40	0.38

Correlations such as those presented above are useful in estimating the global gas holdup. There is still no way (empirical or theoretical) to predict the holdup profiles in the reactor. For such situations, global holdup measurements from DP and NDG prove to be helpful in calculating the gas holdup profile, as discussed earlier.

2.5 Summary

The two-dimensional axisymmetric convection-diffusion model provides a good representation of internal liquid mixing in bubble columns. The instantaneous flow in bubble columns is highly turbulent and transient in nature, and the time-averaged velocity profile does not exist in the column at any instant in time; however, by properly accounting for the churn-turbulent flow via the turbulent eddy diffusivities, the model is able to statistically capture the large-scale transient flow patterns in the column, thereby yielding the characteristic overshoots seen by the detectors at various axial locations. This represents the meso-scale and macro-scale mixing in the column, which is of importance for modeling bubble column reactors. Results also imply that CARPT measurements for the turbulent eddy diffusivities can provide suitable closure for the $\langle \vec{u}' C' \rangle^x$ terms appearing in the original balance equations. Such model predictions for liquid mixing in bubble columns are the first of their kind, and are truly “predictions,” involving no fitting parameters. The developed model, along with experimental input for the model parameters, therefore allows us to study the influence of fluid dynamics on liquid mixing in bubble columns.

The developed scaleup strategy reported in the 12th and 13th quarterly reports (Degaleesan, 1997) for evaluating the model parameters in the AFDU slurry bubble column reactor during methanol synthesis, results in fairly good predictions of the characteristic mixing times within the column as measured by the radiation detectors at various axial locations. This indirectly substantiates the proposed methodology of using the gas holdup in churn-turbulent flows, at sufficiently high gas velocities, to characterize the systems of interest.

2.6 References

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