CHAPTER 3

THEORETICAL BACKGROUND

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3-1- Evaluation of gas hold-up (ε_G)

In a slurry Bubble reactor there are three phases; a gas phase, a liquid phase, and a solid phase. Each of them occupies a certain volume, and it is very important to define these volumes to manage the conversion in this reactor.

Suppose that the volume fraction of the solid phase is ε_s, of the gas is ε_G, and of the liquid is ε_L. It is clear that

$$\varepsilon_G + \varepsilon_s + \varepsilon_L = 1. \qquad (3\text{-}1)$$

To calculate ε_G or gas holdup, simple fluid mechanics can be applied using static head balance as follows:
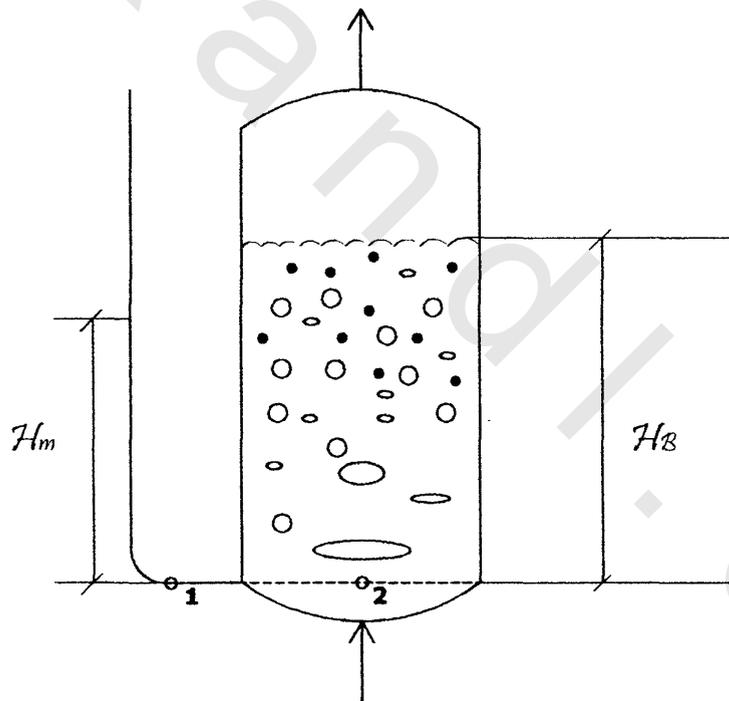

Figure (3-1): Slurry Bubble Column

For the above figure point (1) and point (2) are in the same level

So the pressure at point (1) in the water manometer = the pressure at point (2) inside the slurry bubble column

ρ_w density of water

H_m the height of water in the manometer

ρ_{av} average density in the slurry bubble column

H_B the height of the slurry in the column

$$g\,H_m\,\rho_w = g\,H_B\,\rho_{av} \qquad\qquad (3\text{-}2)$$

$$\rho_{av} \qquad\qquad = (H_m\,\rho_w)\,/\,H_B \qquad\qquad (3\text{-}3)$$

$$\varepsilon_s\,\rho_s + \varepsilon_G\,\rho_g + \varepsilon_L\,\rho_L = (H_m\,\rho_w)/H_B \qquad\qquad (3\text{-}4)$$

ρ_g is very small w.r.t ρ_L and ρ_s and the product of $\varepsilon_G\,\rho_g$ is even smaller and can be neglected

Substituting for E_L from equation *(3-1)*

$$\varepsilon_s\,\rho_s + (\,1 - \varepsilon_s - \varepsilon_G\,)\,\rho_L = (H_m\,\rho_w)/H_B \qquad\qquad (3\text{-}5)$$

Rearranging equation (3-5) the gas hold-up can be evaluated using equation *(3-6)*

$$\varepsilon_G = \varepsilon_s\,[(\rho_s/\rho_L) - 1] + 1 - [(H_m\,\rho_w)\,/\,(H_B\,\rho_L)] \qquad\qquad (3\text{-}6)$$

If the liquid phase in the bubble column is water then

$$\varepsilon_G = \varepsilon_s\,[(\rho_s/\rho_w) - 1] + 1 - (H_m/\,H_B) \qquad\qquad (3\text{-}7)$$

Then knowing the weight of solids charged to the bubble column and its density, its volume can be calculated.

Measuring the expanded bed height, the solid volume fraction can be calculated as volume of (solid phase / volume of expanded bed).

Measuring the water column in the manometer (H_m), the gas hold-up (ε_G) can be calculated from equation *(3-7)*

3-2- Evaluation of the Axial Dispersion Coefficient

The back mixing characteristics of the various phases in multi phase reactors can be evaluated from the Residence Time Distribution RTD of a tracer injected at one or more locations in the system and its concentration is detected as a function of time at one or more down stream positions. In this work an instantaneous probe (electrode) to sense any change in concentration was used. Various types of tracers, such as salt solution, dye, or heat can be used, the selection of the proper tracer for a given system is extremely important, so that the RTD is characteristic of the flowing phase.

3-2-1-The basic requirements for a satisfactory tracer

1- The tracer should be miscible in and has physical properties similar to the fluid phase of interest. It should not be transferable to other phase or phases in the system.

2- The tracer should be accurately detectable in small concentrations, so that only a small quantity needs to be injected into the system thus minimizing disturbances in the established flow patterns.

Also, a concentration range which yields a linear response on the detection equipment is advantageous.

3- Normally the tracer should be non-reacting so that the analysis is kept simple.

4- The tracer detection device should cause the least possible amount of disturbance in the flow patterns, in our case there are sand particles in the liquid phase, so the detection device must be suitable to prevent any solids deposition on the used probe.

5- Good sensitivity and quick response time in the detection and recording equipment are needed

3-2-2-Calculations of Axial Dispersion Coefficient

The one dimensional dispersion model, the axially-dispersed plug flow model equation *(3-8)* has been widely accepted to account for mixing in tubular reactors, referring to figure *(3-2)*:
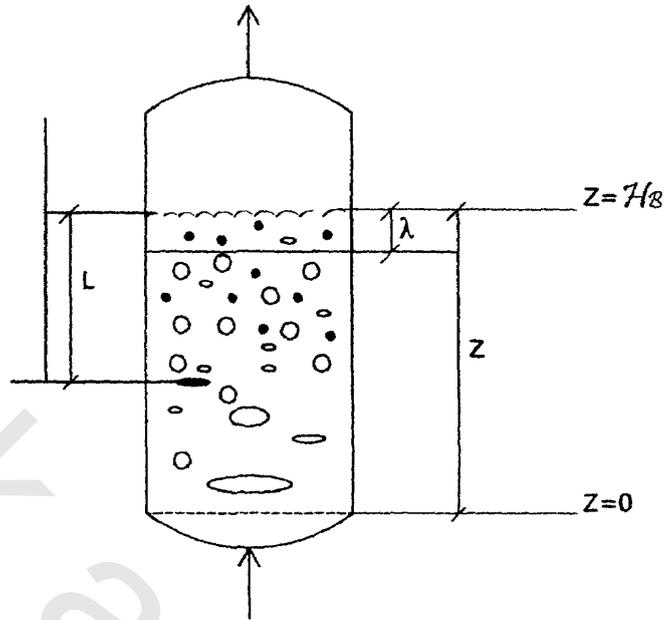

Figure (3-2): Slurry Bubble Column

$$\partial C/\partial t = D_{ax,L}\,[\partial^2 C/\partial Z^2] + V_L[\partial C/\partial t] \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (3\text{-}8)$$

Under liquid non-flow conditions equation (3-8) reduces to

$$\partial C/\partial t = D_{ax,L}\,[\partial^2 C/\partial Z^2] \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (3\text{-}9)$$

With the boundary conditions:

$$\partial C/\partial Z = 0 \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (3\text{-}10)$$

At the bottom of the column $Z = 0$ and at the top of bubble layer $Z = H_B$

And the initial conditions at $t = 0$

$$C\,(Z,\,0) = C_0 \quad for \quad 0 \le Z \le \lambda \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (3\text{-}11)$$

$$C\,(z,\,0) = 0 \quad for \quad Z \ge \lambda \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (3\text{-}12)$$

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At the bottom of the column $Z = 0$ and at the top of bubble layer $Z = H_B$

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$$C(z, 0) = 0 \quad for \quad Z \geq \lambda \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (3-12)$$

Where λ is the height filled with tracer (volume of tracer pulse divided by column cross-sectional area)

The solution of differential equation [Ohki and Inoue (1970)]is:

$$\frac{C}{C_E} = 1 + \frac{2H_B}{\pi\lambda} \sum_{n=1}^{\infty} \left[\frac{1}{n} \sin\frac{n\pi}{H_B}\lambda . \cos\frac{n\pi}{H_B}.L.\exp\left\{ -\left(\frac{n\pi}{H_B}\right)^2 D_{ax,L}t \right\} \right] \ldots\ldots\ldots\ldots\ldots (3-13)$$

Where $C_E H_B = C_0 \lambda$

When $n\lambda <<< H_B$ Eq. (3-13) gives approximate form as

$$\frac{C}{C_E} = 1 + 2\sum_{n=1}^{\infty} \left[\left(\cos\frac{n\pi}{H_B}.L \right) * \exp\left\{ -n^2\left(\frac{\pi}{H_B}\right)^2 D_{ax,L}t \right\} \right] \ldots\ldots\ldots\ldots\ldots (3-14)$$

$$\frac{C}{C_E} = 1 + 2 \sum_{n=1}^{\infty} \left(\cos\frac{n\pi}{H_B}.L \right) * \exp -n^2\theta$$

Where $\theta = \left\{ \left(\frac{\pi}{H_B}\right)^2 D_{ax,L}t \right\} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (3-15)$

In practice, six terms are sufficient to evaluate $D_{ax,L}$ with an error less than 1% . $D_{ax,l}$ can be evaluated from equation *(3-14)* by successive iteration , by assuming a value for $D_{ax,l}$ and solving for C/C_E until the evaluated C/C_E agrees with the experimentally obtained value within a special tolerance limit. Ohki and Inuoue (1970) proposed a graphical technique to calculate $D_{ax,l}$. they plotted C/C_E as a function of $D_{ax,l} (\pi/H_B)^2 t$ with L/H_B as a parameter, Fig.(3-3) is constructed on this basis, with n=6
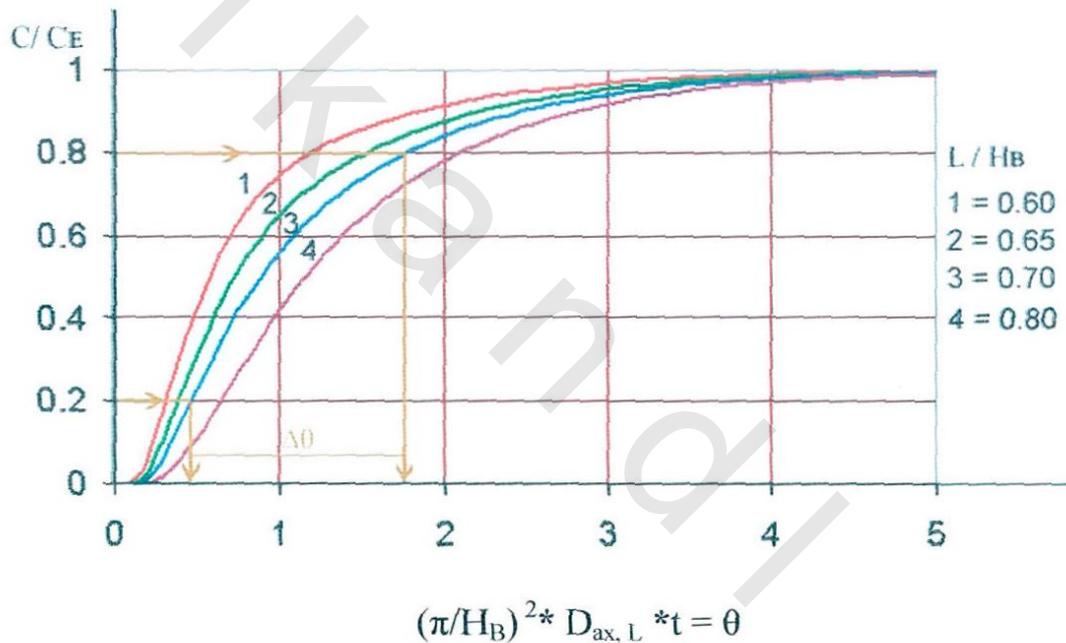

$$(\pi/H_B)^2 * D_{ax,L} * t = \theta$$

Figure (3-3): Tracer Response Curves Derived from the Diffusion

Model

From the recorded curves as shown in Fig. (3-4) the time interval Δt required to change the relative concentration of the liquid from 0.2 to 0.8 can be measured.
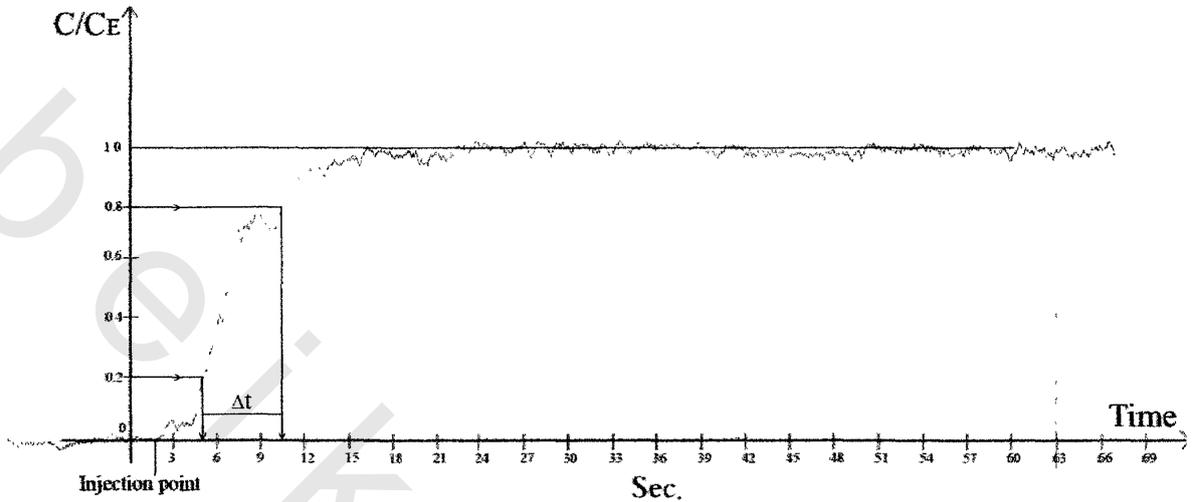

Figure (3-4): Tracer Response in 20 Cm Column from X-Y Recorder

$$\Delta t = [\, t_{C/C_E = 0.8} - t_{C/C_E = 0.2} \,] \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (3\text{-}16)$$

This time interval is theoretically related to the dispersion coefficient

From Eq. *(3-15)*

$$\theta = [\pi/H_B]^2 D_{ax,L} t \longrightarrow \Delta\theta = [\pi/H_B]^2 D_{ax,L}\, \Delta t \dots\dots\dots\dots\dots (3\text{-}17)$$

Where $\Delta\theta$ is obtained from Fig. *(3- 3)*. The dispersion coefficient is calculated from equation *(3-18)*

$$D_{ax,L} = (H_B/\pi)^2 * \Delta\theta/\Delta t \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (3\text{-}18)$$