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# Numerical simulation to determine the mass transfer coefficient in gas-liquid phase in an absorbed column

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## Abstract

The flow regime, gas-liquid specific interfacial area, coalescence of bubbles, individual mass transfer, and bubble distribution are important parameters for bubble columns design, and more important is the volumetric mass transfer coefficient $k_La$. Many studies in the literature are focusing on the enhancement of mass transfer coefficient with different method and different particle. In this paper a numerical simulation is used to predict mass transfer coefficient with respect to both time and space for both gas and liquid phase. The mass transfer coefficient $k_La$ in gas/liquid system was measured by the unsteady state dynamic method, where the nitrogen was introduced first into water until the dissolved oxygen concentration would zero; the latter was measured by means of an oxygen electrode. In special cases for both liquid and gas phases the mass transfer coefficient $k_La$ could determined with analytic method. The agreement between numerical simulations and analytical method is found to be perfect.

Keywords: Gas-liquid system, mass transfer coefficient, absorption, Numerical and analytical method

## 1. Introduction

The main Bubble columns are widely used as gas-liquid contactors in many applications such as: chemical, petrochemical, bio-reactions, coal liquefaction and waste water treatment. Due to their simple construction, low operating cost, high energy efficiency and good mass and heat transfer, bubble columns offer many advantages when used as gas-liquid contactors [19].most studies on gas-liquid phase were devoted to the experimental determination of the design parameters for gas-liquid phase, such as flow regime, individual mass transfer, gas-liquid specific interfacial area and more specifically, of the mass transfer coefficient $k_La$. Several authors have studied the hydrodynamic behavior and the design parameter of bubble

columns [8-15], so as the bubble size distribution [16-21], and the effect of different parameter on the mass transfer coefficient $k_La$ [1-4, 22, 23]. Nikakhtari and Hill [4] studied the effect of packed bed on mass transfer coefficient in an external loop airlift bioreactor; they found that a small quantity of nylon mesh packing increased the overall volumetric oxygen mass transfer coefficient by a factor of 3.73 compared to an unpacked riser, they used a mathematical model to predicted the value of mass transfer coefficient. Several authors [4-7], have improved mathematical models to estimate the value of mass transfer coefficient, the method to predict the value of mass transfer coefficient is very important because the results depended on the method which is used to calculate the value of mass transfer coefficient. In the present paper, a numerical simulation is used to predict the mass transfer coefficient $k_La$, for both liquid and gas phases, the value of the mass transfer coefficient would change until the experimental data were in agreement with the calculated data. The mass transfer coefficient $k_La$ in gas/liquid system was measured by the unsteady state dynamic method, the water was as liquid phase and the oxygen was as gas phase

## 2. Experimental Apparatus and Procedures

Mass transfer measurements are carried out using the apparatus shown in Figure1

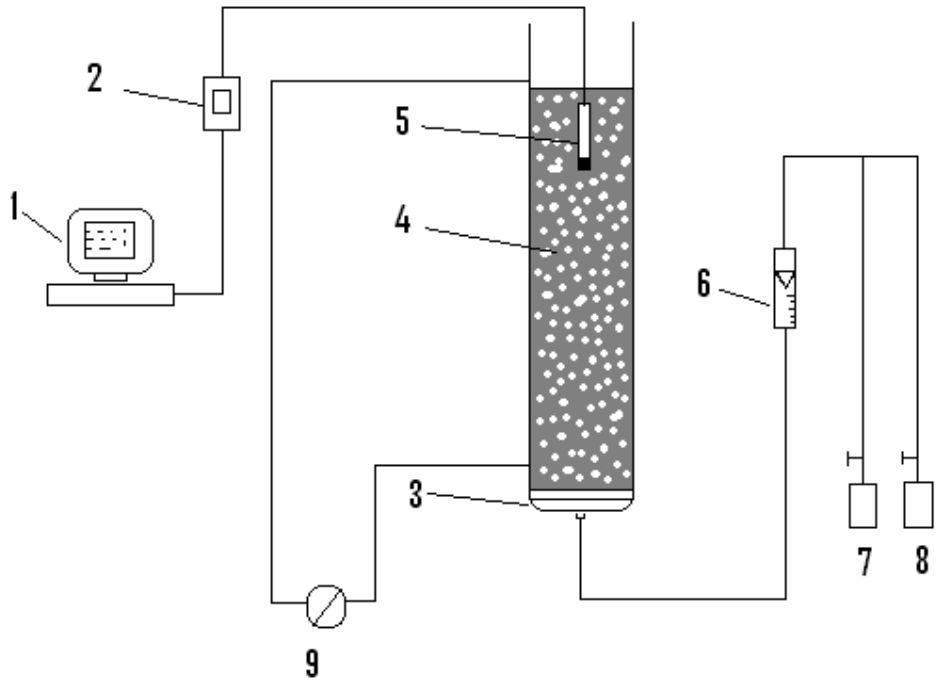


Figure 1 Schematic diagram for experimental set-up

1. PC 2. Data recorder 3. Sieve plate 4.bubble column 5.Oxygen electrode
6. Rota meter 7. Nitrogen 8. Air 9. pump

A cylindrical bubble column reactor made of glass with height 300 cm filled with 100 cm water (4) was used. The internal and external diameters of the cylindrical tube are 10 cm and 10.4 cm respectively. The liquid is recycled used a pump. The mass transfer coefficient $k_La$ in gas/liquid system is measured by the unsteady state dynamic method, where the nitrogen (7) is introduced first into water until the dissolved oxygen concentration would zero; the latter was measured by means of an oxygen electrode (5) in four different places. The air (8) is passed through sieve plate (3) into water at different flow rates measured with a rota meter (6); the data are registered with data recorder device (2) and saved in computer (1).

## 3. Model

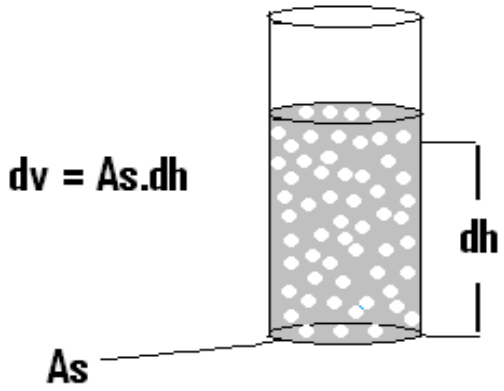


Figure 2 the control volume of oxygen in bubble column

In the bubble column, the gas and liquid phases are in contact with each other throughout the height of the A cylindrical bubble column reactor. The concentration of Oxygen being transferred varies in each phase as it flow through the reactor. In order to determine oxygen mass transfer between the air and liquid phases, it is necessary to cope with this variation, therefore; oxygen mass balance for a volume element that extended across the tube was performed. The flow distribution assumed uniformly therefore no radial gradients of concentration or velocity for the gas or liquid across the tube.

Transfer volume expressed as

$$\partial v_G = A_s \, \partial h \qquad (1)$$

$$\frac{\partial C_G}{\partial h} = -\frac{A_S(1-\varphi_G)}{V_G} \cdot (k \cdot C_G - C_L) \cdot k_L a \tag{2}$$

Since oxygen is transferred through the differential element by both diffusion and bulk flow, and is accumulated in the water, the conservation equation for oxygen in water is

$$\frac{\partial C_L}{\partial t} = -\frac{V_G}{A_S(1-\varphi_G)} \cdot \frac{\partial C_G}{\partial h} \tag{3}$$

Substitution of Equation (2) into Equation (3) gives

$$\frac{\partial C_L}{\partial t} = \quad (k \cdot C_G - C_L) \cdot k_L a \tag{4}$$

Where

$$k = \frac{C_L^*}{C_G^*} \tag{5}$$

So as:

$$k = \frac{V_M \cdot \rho W \cdot p_{Ges}}{MW \cdot He} \tag{6}$$

**4. Numerical method**

The equations (2) and (4) would solve used a numerical solution as following:

*Liquid phase:*

$$C_{L\ k,i+1} = C_{L\ i,k} + k_L a\,(k \cdot C_{G\ i,k} - C_{L\ i,k}) \cdot \Delta t \tag{7}$$

$\Delta t = 0.1$ (s) $t \leq 20$ (s)

$\Delta t = 0.5$ (s) $t > 20$ (s)

*Gas phase:*

$$C_{G\,k+1,i} = C_{G\,i\,k} - \frac{k_L a\,(1-\varphi_G)}{W_{SG}} \cdot \left(k \cdot C_{G\,i,k} - C_{L\,i,k}\right) \cdot \Delta h \qquad (8)$$

$\Delta h = 0.01$ (m)

Excel worksheet was used to estimate the value of the mass transfer coefficient $k_La$ for the Equations (7) and (8).

## 5. Analytical method

For more exact an analytical method could be comparison to the numerical results as following:

*Liquid phase:*

For the First distance where the Liquid stay on the plate and the Gas would pass into the liquid phase, for the first distance h = 0, getting:

$$C_G = C^*_G = \text{konstant.} \qquad (9)$$

Because, in the first distance there is no change in the gas phase with (h = 0)

From equation (5) getting the following equation:

$$C^*_L = k \cdot C^*_G \qquad (10)$$

Substitution of equation (9) and the equation (10) into equation (4) gives

$$\frac{\partial C_L}{\partial t} = \left(k \cdot C^*_G - C_L\right) \cdot k_L a = \left(C^*_L - C_L\right) \cdot k_L a \qquad (11)$$

From the equation (11) getting the following equation:

$$\frac{C_L}{C_L^*} = \left[1 - \exp\left(-t \cdot k_L a\right)\right] \tag{12}$$

Equation (12) is the final form, which predict the mass transfer coefficient with the analytical method in the Liquid phase

*Gas phase:*

In the first inlet of the Gas into the Liquid, the gas bubble would contact the Liquid phase through the column height (Δh)

$$C_L = 0 = \text{konstant.} \tag{13}$$

Substitution of equation (13) into the equation (2)
Gives the equation (14) as following:

$$\frac{\partial C_G}{\partial h} = -\frac{A_S\left(1-\varphi_G\right)}{V_G} \cdot k_L a \cdot k \cdot C_G \tag{14}$$

Substitution of equation (9) into the equation (14) gives:

$$\frac{C_G}{C_G^*} = \exp\left(\frac{-A_S\left(1-\varphi_G\right)\cdot k_L a \cdot k \cdot h}{V_G}\right) \tag{15}$$

The superficial gas velocity could calculate as following:

$$\frac{V_G}{A_S} = W_{SG} \tag{16}$$

Substitution of equation (16) into the equation (15)
Gives the equation (17) as following:

$$\frac{C_G}{C_G^*} = \exp\left(\frac{-k \cdot k_L a\left(1-\varphi_G\right)\cdot h}{W_{sG}}\right) \tag{17}$$

Equation (17) is the final form, which predict the mass transfer coefficient with the analytical method in the Gas phase

## 6. Results and Discussion

Figure (3) shows the comparison between the numerical calculated results and the experimental data in different height of the liquid. As shown the agreement between numerical calculated results and experimental data is found to be perfect.
The oxygen concentration was measured with oxygen electrode in four different distances (0.5 m, 1 m, 1.5m, and 2m). Using the numerical simulation of the mass transfer coefficient $k_La$ value in equation (7) could find the medial value for the mass transfer coefficient $k_La$.

The comparison between the numerical simulation results and the analytical results is shown in the figures (4 and 5) figure 4 shows the results for the Gas phase and the figure 5 shows the results for the Liquid phase, as shown there is a best agreement between numerical and analytical results. In figure 4 are the results of the numerical simulation using equation (7) and the results of analytical method using equation (12).

As shown the agreement between numerical calculated results and the analytical results is found to be perfect.

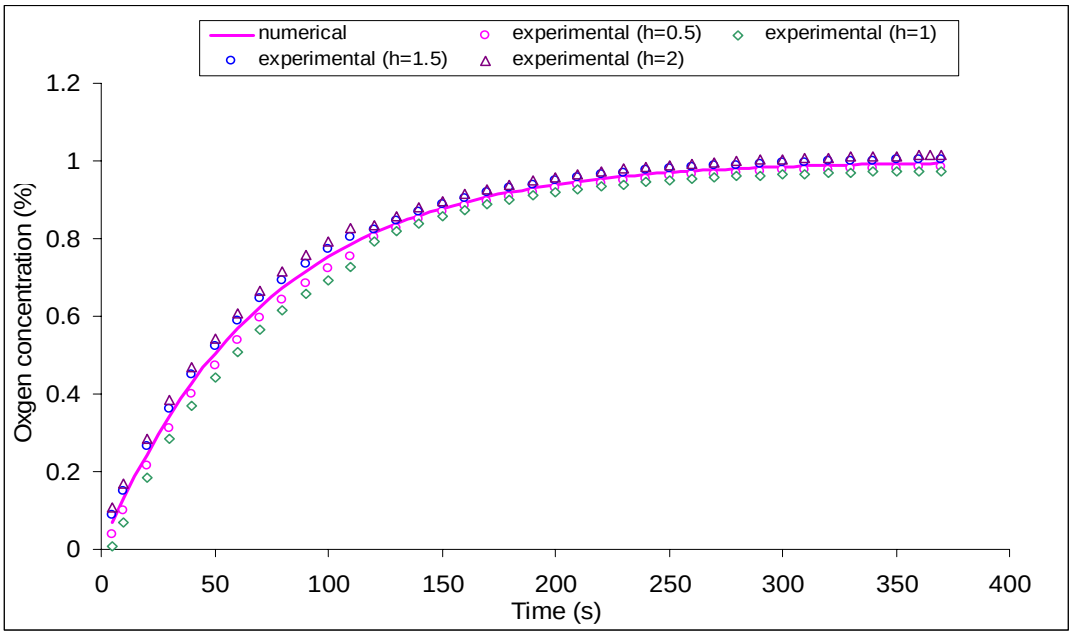


Figure 3 Experimental data compared to calculated data in Liquid phase at Gas velocity = 0.01 m/s

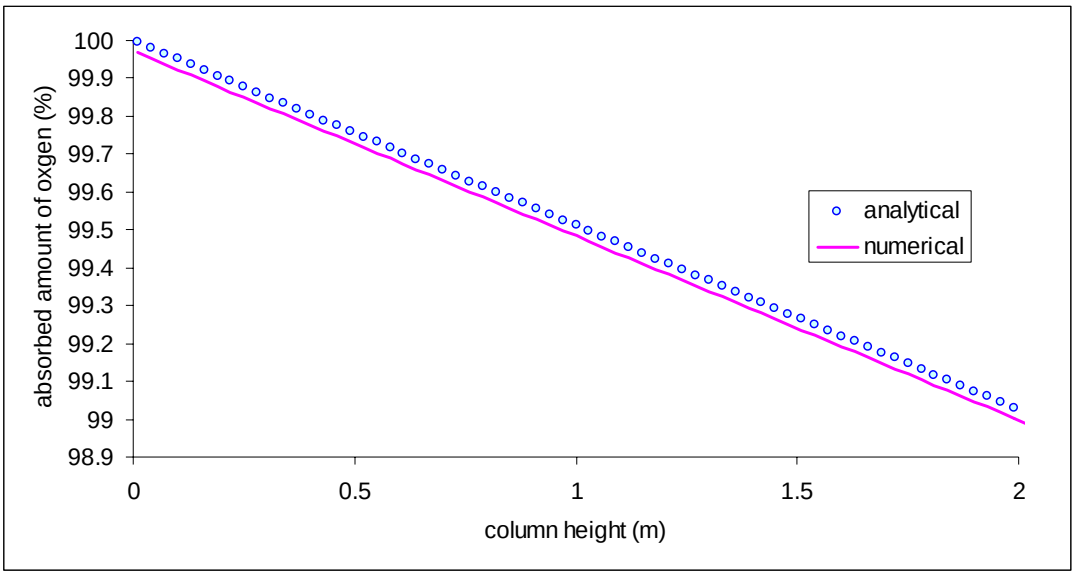


Figure 4 Comparison between numerical simulation and analytical method in the Gas phase

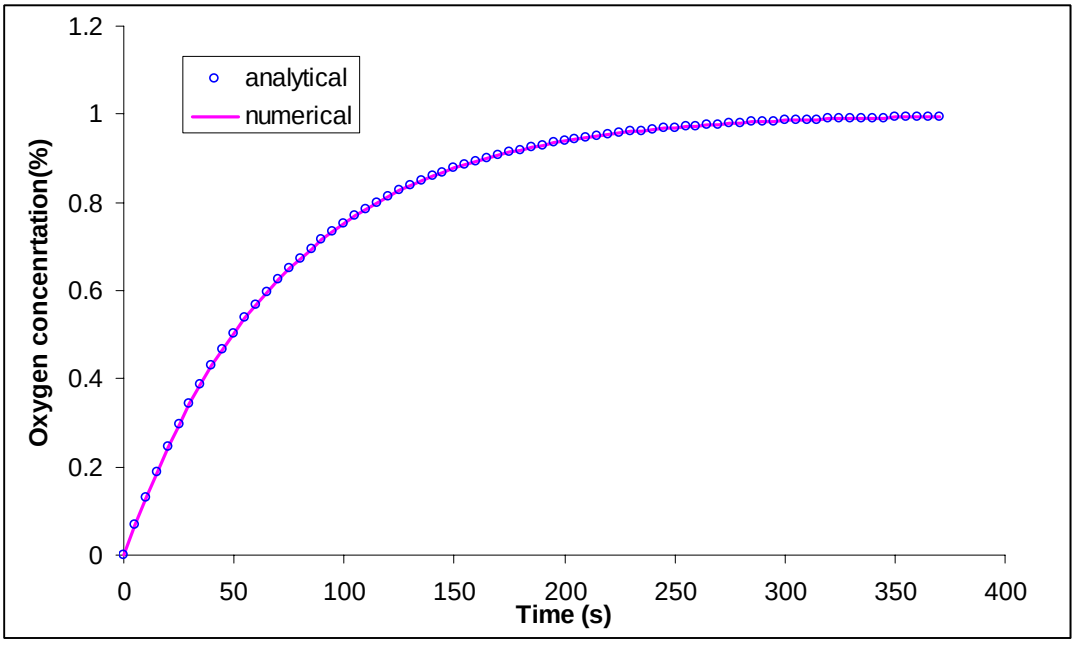


Figure 5 Comparison between numerical simulation and analytical method in the Liquid phase

## 7. Conclusion

a numerical simulation is used to predict the mass transfer coefficient with respect to both time and space for both gas and liquid phase. Experimentally the gas concentration in liquid phase was measured in four different Positions by the unsteady state dynamic method. The equation (7) was used to estimate the value of the mass transfer coefficient for the liquid phase and the equation (8) was used to estimate the value of the mass transfer coefficient for the gas phase. The following parameters were used; superficial gas velocity was (0.01 m/s - 0.06 m/s), $\Delta h = 0.01$ m, $\Delta t = 0.1$ s for $t \leq 20$ and $\Delta t = 0.5$ for $t > 20$. In the Liquid phase the equation (7) was the best fit for the experimental data. For both the Liquid and gas phases the comparison between numerical method and analytical method is found in agreement

## 8. Acknowledgements

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## 9. Nomenclature

| | |
|---|---|
| $A_S$ | cross section area ($m^2$) |
| $C_L$ | oxygen concentration in water ($kmol/m^3$) |
| $C_G$ | oxygen concentration in atmospheric air ($kmol/m^3$) |
| d | diameter (mm) |
| h | height of the column (cm) |
| He | Henry coefficient bar / (kmol $O_2$/kmol $H_2O$) |
| $k_La$ | mass transfer coefficient (1/s) |
| $M_W$ | molar mass of water (kg / kmol) |
| $P_G$ | gas pressure (Pa) |
| t | time (s) |
| $W_SG$ | superficial gas velocity (m/s) |
| V | volume of the column ($m^3$) |
| $V_G$ | gas flow rate ($m^3/s$) |
| $V_M$ | molar volume of the gas in normal condition ($m^3/kmol$) |
| $\varphi_G$ | gas ratio (%) |
| $\rho_W$ | water density ($kg/m^3$) |

**References**

[1] Sohbi, B., Edreder, E., (2006) *17th International Congress of Chemical and Process Engineering 27 - 31 August 2006, Prague - Czech Republic, Conference proceeding.*

[2] Zhao, W.R., Shi, H.X., Wang, D.H., (2004). *Journal of Zhejiang University SCIENCE,* 5(6):714-720

[3] Vazquez, G., Cancela, M.A., Riverol, C., Alvarez, E., Navaza, J.M., (2000). *Chem. Eng. J.,* 78:13-19.

[4] Nikakhtari, H., Hill, G.A., (2005). *Ind.Eng. Chem. Res*. 44: 1067-1072.

[5] Dhanasekharan, K.M., Sanyal, J., Jain, A., Haidari, A., (2005). *Chemical Engineering Science* **60**, 1, 213-218.

[6] Olmos, E., Gentric, C., Vial, Ch., Wild, G., Midoux, N., (2001). *Chemical Engineering Science* **56**, 6359-6365.

[7] Shimizu, K., Takada, S., Minekawa, K., Kawase, Y., (2000). *Chemical Engineering Journal* **78**, 21–28.

[8] Shah, Y.T., Kelkar, B.G., Godbole, S.P., Deckwer, W-D., (1982). *A.I.Ch.E. News paper* 28, 353 –379.

[9] Mouza, A.A., Dalakoglou, G.K., Paras, S.V., (2005). *Chemical Engineering Science* 60, 1465-1475.

[10] Kaidi, F., Rihani, R., Ben Amira, E., Naceur, M.W., Bensmaili, A., (2006). *17th International Congress of Chemical and Process Engineering 27 - 31 August 2006, Prague - Czech Republic, Conference proceeding.*

[11] Lefebvre, S., Guy, C., (1999). *Chemical Engineering Science* 54: 4895-4902.

[12] Hebrard, G., Bastoul, D., Roustan, M., (1996). *Transactions of the Institution of Chemical Engineers* **74**, 406–414.

[13] Loimer, T., Machu, G., Schaflinger, U., (2004). *Chemical Engineering Science* **59**, 809–818.

[14] Colella, D., Vinci, D., Bagatin, R., Masi, M., Bakr, E., A., (1999). *Chemical Engineering Science* **54**, 4767-4777.

[15] Camarasa, E, Vial, C, Poncin, S., Wild, G, Midoux, N, Bouillard, J, (1999). *Chemical Engineering and Processing* 38,

[16] Lehr, F., Millies, M., Mewes, D., (2002). *A.I.Ch.E. Journal* **48**, 11, 2426-2443.

[17] Lage, P., L., C., Esposito, R., O., (1999). *Powder Technology* **101**, 142-150.

[18] Miyahara, T., Tanaka, A., (1997*). Journal of Chemical Engineering of Japan* **30**, 2, 353-355.

[19] Kazakis, N.A. , Mouza A.A., Paras S.V., (2006). *17th International Congress of Chemical and Process Engineering 27 - 31 August 2006, Prague - Czech Republic, Conference proceeding.*

[20] Polli, M., Stanislao, M., Bagatin, R., Bakr, E., A., Masi, M.,(2002*). Chemical Engineering Science* **57**, 97–205.

[21] Parthasarathy, R., Ahmed, N., (1996). *Journal of Chemical Engineering of Japan* **29**, 6, 1030-1034.

[22] Dumont, E., Delmas, H., (2003). *Chemical Engineering and Processing*, 42, 419-438.

[23] Galaction, A.-I., Cascaval, D., Oniscu, C., Turnea, M., (2004). *Bioprocess and Biosystems Engineering*, 26, 231-238.