PREDICTION OF MASS TRANSFER COEFFICIENT IN BUBBLE COLUMN USING ARTIFICIAL NEURAL NETWORK

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ABSTRACT

The volumetric mass transfer coefficient $k_L.a$ was calculated using two gases (air and CO_2) in water and NaOH solution. The experiments were carried out using 0.1 m column diameter. Empirical and Artificial Neural Network (ANN) correlation were developed to predicted mass transfer coefficient in form of dimensionless groups (Sh, Re,Bo and We). The use of Back Propagation Neural Network (BPNN) gave better results than other correlations found in literature and than the empirical one found in this study.

الخلاصة

تمت دراسة معامل الانتقال الحجمي في عمود فقاعي ذو قطر 0.1 متر يحتوي على موزع للغاز ذو 79 فتحة بقطر 2 مليمتر لكل فتحة باستخدام الهواء و ثاني اوكسيد الكاربون للطور الغازي و الماء ومحلول هيدروكسيد الصوديوم للطور السائل.

تم تطوير معادلة عامة وإستخدام الشبكة الذكية المصطنعة (ANN) لحساب معامل انتقال الكتلة الحجمي من خلال استخدام مجاميع عديمة الوحدات (We,Sh,Re,Bo). إستخدام الشبكة الذكية من نوع التوالد العكسي (BPNN) اعطى نتائج متميزة احسن من تلك الموجودة في الادبيات.

KEYWORDS

Bubble column, Mass transfer coefficient, Artificial neural network.

INTRODUCTION

One of the most important applications of the gas-liquid reaction is the bubble column reactor. Bubble columns are widely used in industry for carrying out a variety of chemical reactions such as hydrogenations, oxidations and the Fischer–Tropsch synthesis. Mass transfer is one of the key parameters determining the design and scale up of bubble column reactors used in a wide spectrum of industrial process(Kantarci,et al;2005).

Mass transfer coefficients depend strongly on the fluid dynamics and are mostly quantified through correlation in which the gas holdup plays an important role. Gas holdup is a dimensionless key parameter for design purposes that characterizes transport phenomena of bubble column systems. It is basically defined as the volume fraction of gas phase occupied by the gas bubbles. Gas holdup for the two phase bubble column reactor can be estimated using the following relation (Pandit and Doshi, 2005; Vandu and Krishna R., 2004):

$$\varepsilon_G = \frac{H_D - H_C}{H_D} \qquad (1)$$

Anther factor that effecting mass transfer is the superficial gas velocity, which is the average velocity of the gas that is sparged into the column, and it is simply expressed as the volumetric flow rate divided by the cross-sectional area of the column (Lakota et. al. 2002, Bouaifi et. al. 2001). The volumetric gas to liquid (GL) mass transfer coefficient (k_L.a) in bubble column reactor is mainly determined by (i) the GL interfacial area (a) determined by the bubble diameter (d_b) and the gas holdup ε_G and (ii) the liquid side mass transfer coefficient (k_L) is determined by the slip velocity between bubble and liquid phase (U_b) and the bubble diameter. Gas-liquid interfacial area (a) is determined by the gas holdup and the bubble diameter (equation 2).The gas-liquid interfacial area (a) is calculated too from video imaging (Mouza et. al., 2004, Krishna and van Baten 2003).

$$a = \frac{6\,\varepsilon_G}{d_b} \qquad (2)$$

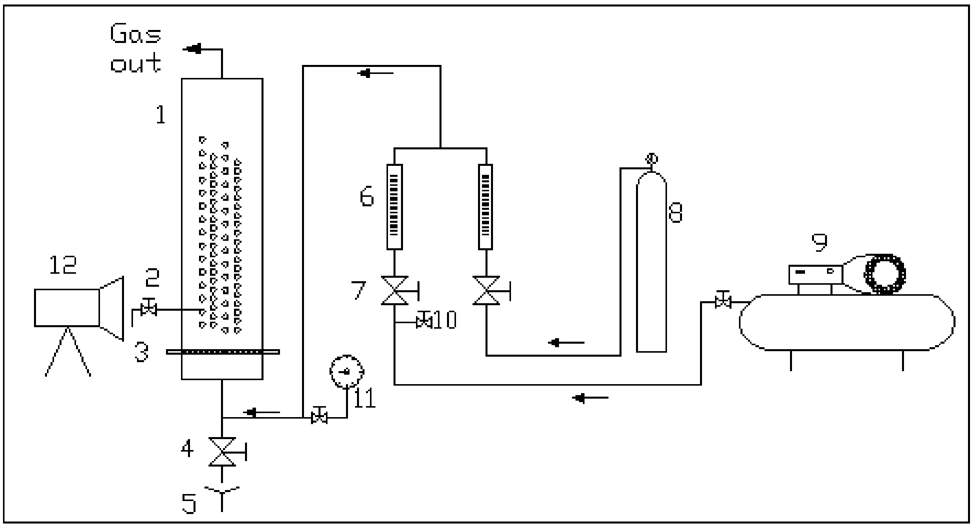
ARTIFICIAL NEURAL NETWORK MODEL

Artificial Neural Network (ANN) models have been recently given an increasing attention in chemical engineering applications, including parameters prediction, modeling, process optimization, process simulation and process control. Back Propagation Neural Network (BPNN) and radial biasis function are employed, whereas for problems involving data clustering, adaptive resonance theory, network for binary signals and Kohonen self-organizing map are used (Shaikh A., Al-Dahhan M. 2003). A back propagation network with a single hidden layer of processing elements can model any continuous function to any degree of accuracy. , since back propagation is based on a relatively simple form of optimization known as gradient descent, mathematically astute observers soon proposed modifications using more powerful techniques such as conjugate gradient and Newton's methods. Back propagation is still the most widely used variant. Its two primary virtues are that it is simple and easy to understand, and it works for a wide range of problems. (Bao, 2005; Young 2001). The basic back propagation algorithm consists of three steps. The input pattern is presented to the input layer of the network. These inputs are propagated through the network until they reach the output units. This forward pass produces the actual or predicted output pattern. Because back propagation is a supervised learning algorithm, the desired outputs are given as part of the training vector. The actual network outputs are subtracted from the desired outputs and an error signal is produced. This error signal is then the basis for the back propagation step, whereby the errors are passed back through the neural network by computing the contribution of each hidden processing unit and deriving the corresponding adjustment needed to produce the correct output. The connection weights are then adjusted and the neural network has just "learned" from an experience (Rzempoluck E. J. 1998).

Adding a single layer of hidden units turns the linear neural network into a nonlinear one, capable of performing multivariate logistic regression, but with some distinct advantages over the traditional statistical technique (Wu R. C. 1997, You X. Y. and Yang Z. S. 2003).

EXPERIMENTAL WORK

The schematic of the bubble column reactor setup is illustrated in Fig1. The column is constructed from QVF Pyrex glass. The inside diameter of bubble column reactor is (0.1 m) and its height is (1.5 m).



1- QVF bubble column
2- Sampling valve
3- Gas distributor
4- Drain valve
5- Drain
6- Rotameters
7- Regulating valves
8- CO_2 cylinder
9- Air compressor
10- Vent valve.
11- Pressure Gauge
12- Photo camera

Fig. 1, Typical experimental set-up for 0.1 m diameter column

The perforated plate used in the bubble column is constructed from aluminum of (2 mm) thickness with perforated holes of 2 mm diameter on a triangular pitch of 11 mm. The total holes were 79 holes as shown in Fig.2.

EXPERIMENTAL PROCEDURE

(i) Using a stationary liquid phase of 2500 ml tap water containing 0.7 gm sodium sulfate and 0.0025 gm cobalt for oxygen scavenging from the water, air was introduced into the bubble column and at varying flow rates of 0.886,2,3,5 and 7 m^3/hr. Samples of water from the column were taken every 30 seconds and were tested for dissolved oxygen using Winkler titration.

(ii) Same as above except that the gas was 50-50 air and carbon monoxide and the liquid was sodium hydroxide solution. And the liquid samples were analyzed for sodium carbonate content using standard method.

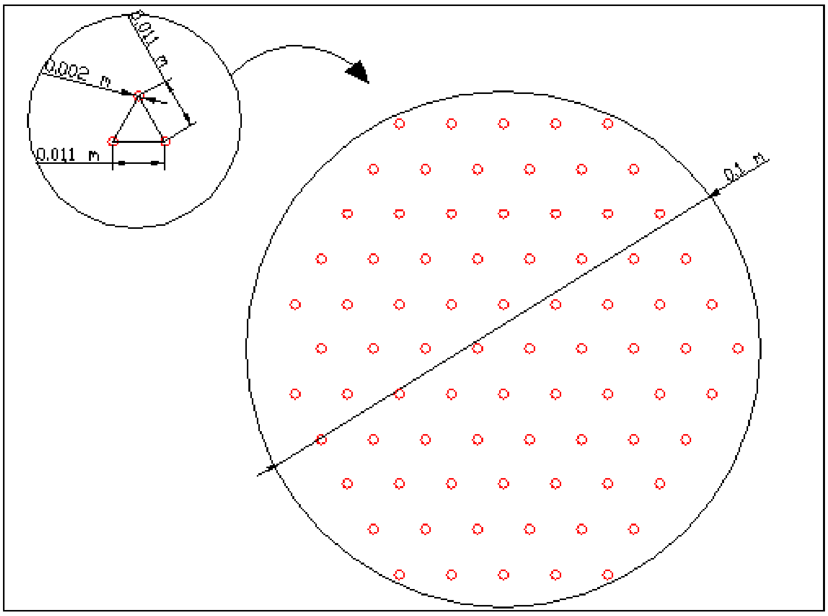


Fig.2, Gas Distributor.

RESULTS AND DISCUSSION

For air-water system, Fig.3, shows the relation between the ratio C/C^* and time for different gas velocities. It's obvious that increasing air velocity decreases the time needed for saturation.

For carbon dioxide- sodium hydroxide system, Fig.4, illustrates the variation of CO_2 concentration profile with time. It can be seen that increasing normality causes an increase in CO_2 absorption due to increasing the reaction rate

CALCULATION OF GAS HOLDUP

Gas holdup was determined using visual measurements. For each run, the gas flow rate was adjusted with sufficient time given for steady state to be reached in the column after which the increase in dispersion height was recorded; Fig. 5, shows the change of gas holdup with superficial gas velocity.

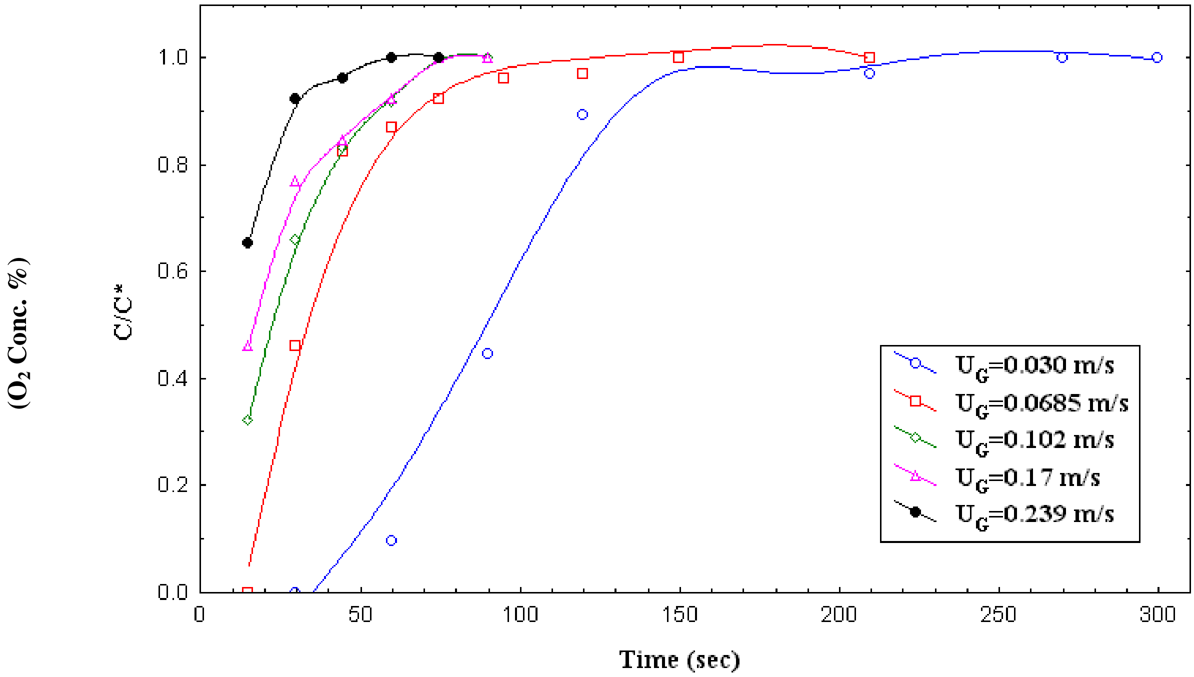


Fig. 3, Transient approach to steady state in bubble column reactor (For air- water system.

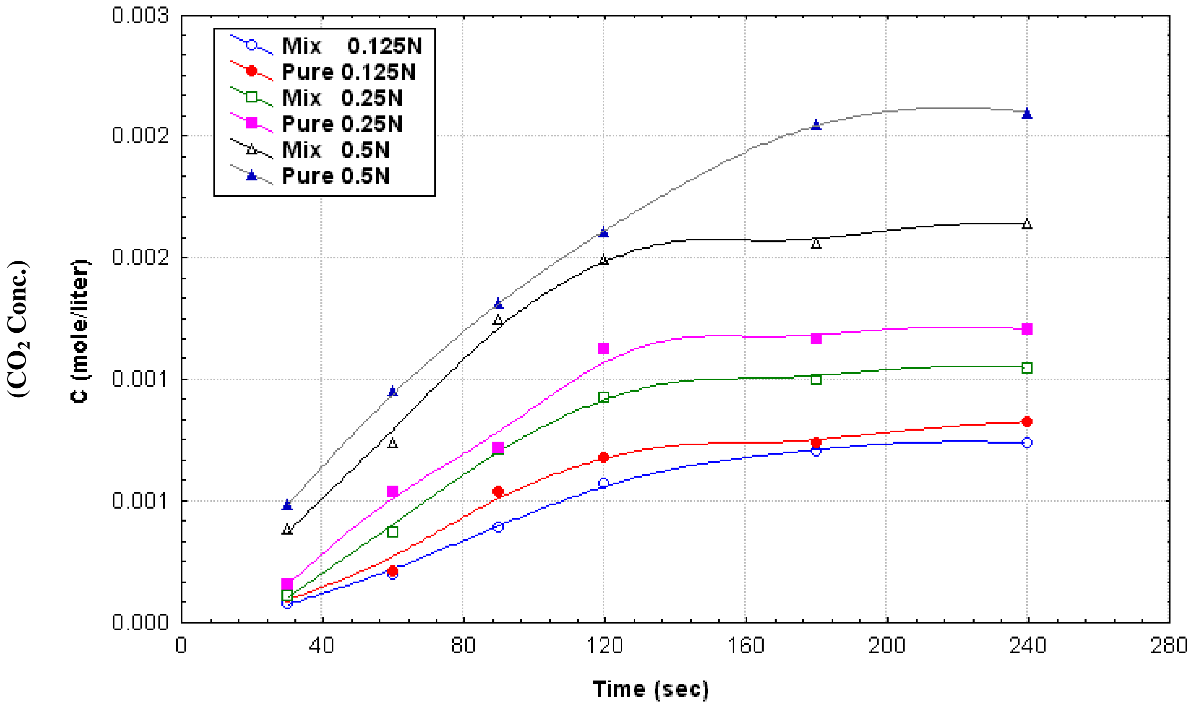


Fig.4, CO_2 absorption in NaOH solution. (Mix: mean Air-CO_2 gas mixtures).

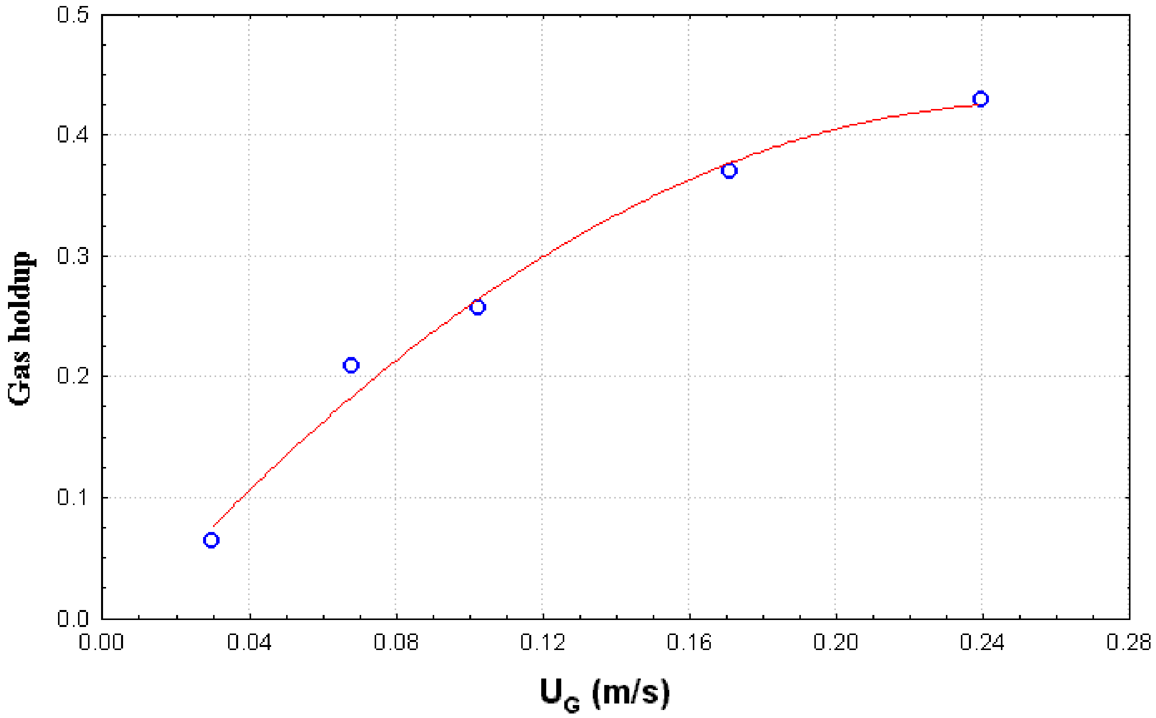


Fig. 5, Gas holdup ε_G as a function of superficial gas velocity (Air-water).

Calculation of Bubble Diameter

With the aid of the Bhavaraju et al. (1978) correlation that shows below, the bubble size diameter was calculated.

$$\frac{d_b}{d_o} = 3.23\left(\frac{4\rho_L Q}{\pi\mu_L d_o}\right)^{-0.1}\left(\frac{Q^2}{d_o^5 g}\right)^{0.21} \qquad (3)$$

Fig. 6 shows the bubble distribution in the bubble column reactor with the superficial gas velocity.

Calculation of Mass Transfer Coefficient

For calculating volumetric mass transfer coefficient; an equation developed by Vandu and Krishna (2003) based on two film theory was used:

$$\frac{C_L}{C_L^*} = 1 - \exp\left(-\frac{k_L.a}{1-\varepsilon_G}t\right) \qquad (4)$$

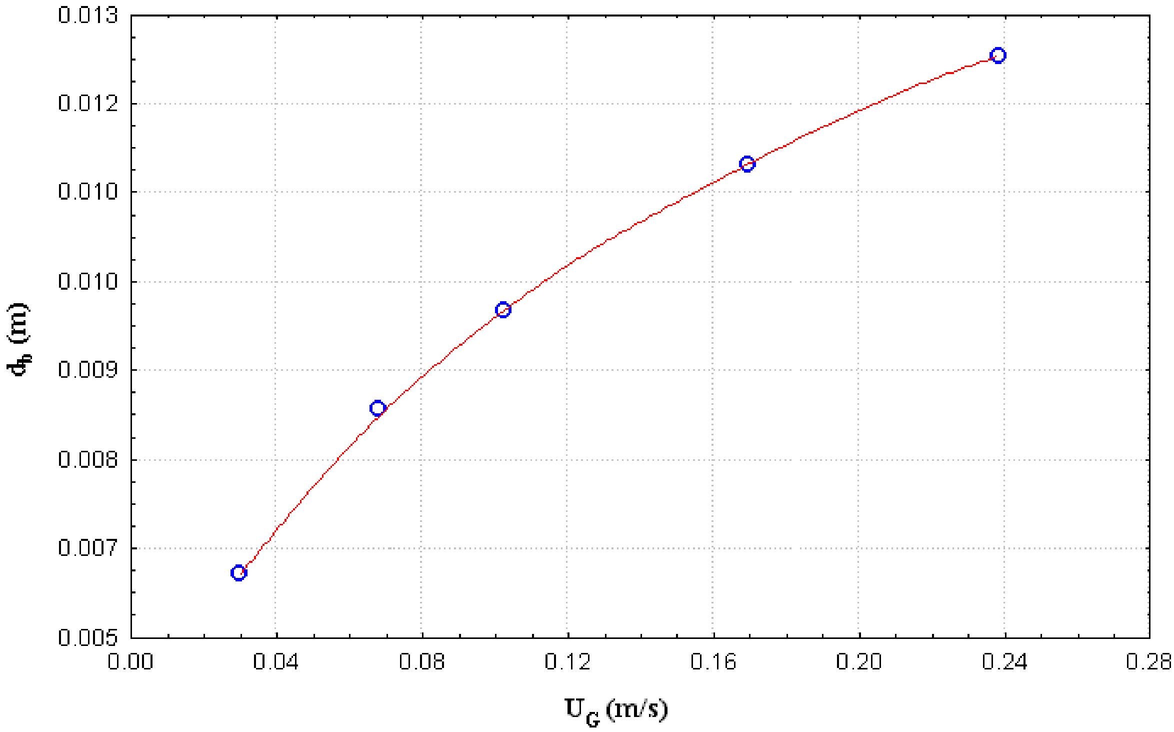


Fig. 6, Bubble size vs. superficial gas velocity (Air-water).

The only unknown constant in equation (4) is k_L.a; which can be determined by a regression of equation (4) to the actual concentration data. With the aid of STATISTCA for Window Release 5, (1995), equation (4) can be solved to find k_L.a. Fig. 7, shows the volumetric mass transfer coefficient k_L.a in relation to superficial gas velocity. Increasing the superficial gas velocity leads to increasing in k_L.a. With the aid of equation (2), interfacial area and mass transfer coefficient k_L were calculated. Fig. 8, and 9 show k_L and (a) as a function to superficial gas velocity. Comparison between the two figures shows no significant variation of k_L with gas superficial gas velocity but (a) increases significantly with increasing U_G. Similar findings were reported by Behkish, (2004); Kantarci et. al.,(2005); and Ruthiya, (2005).

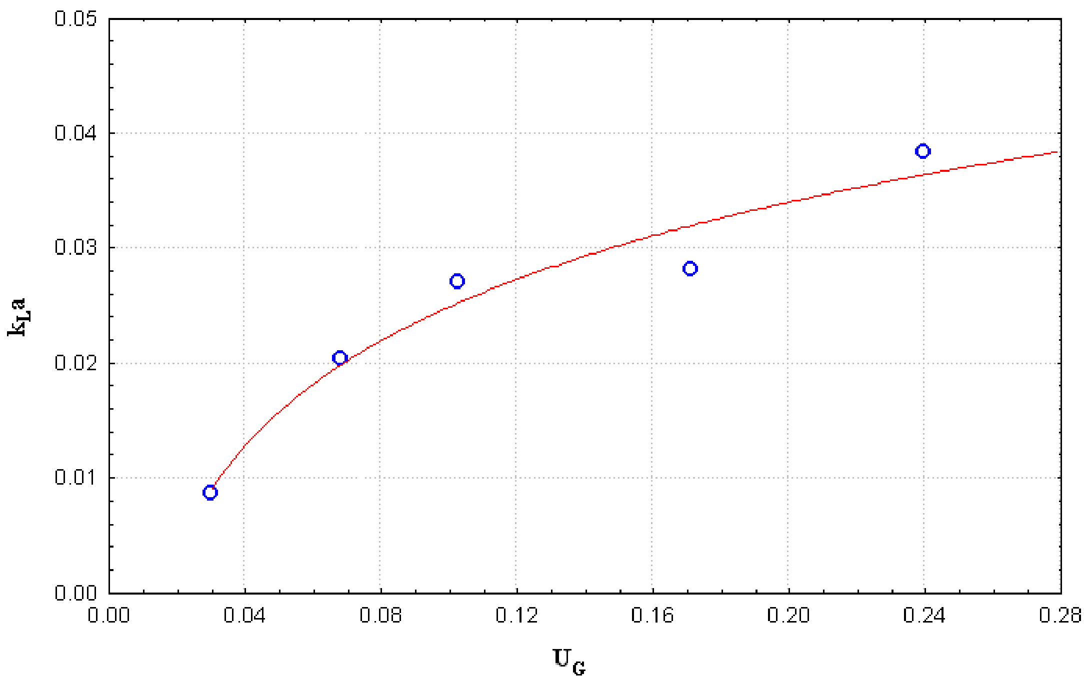


Fig. 7, $k_L.a$ (s^{-1}) vs. superficial gas velocity U_G (m/s) (Air-water).

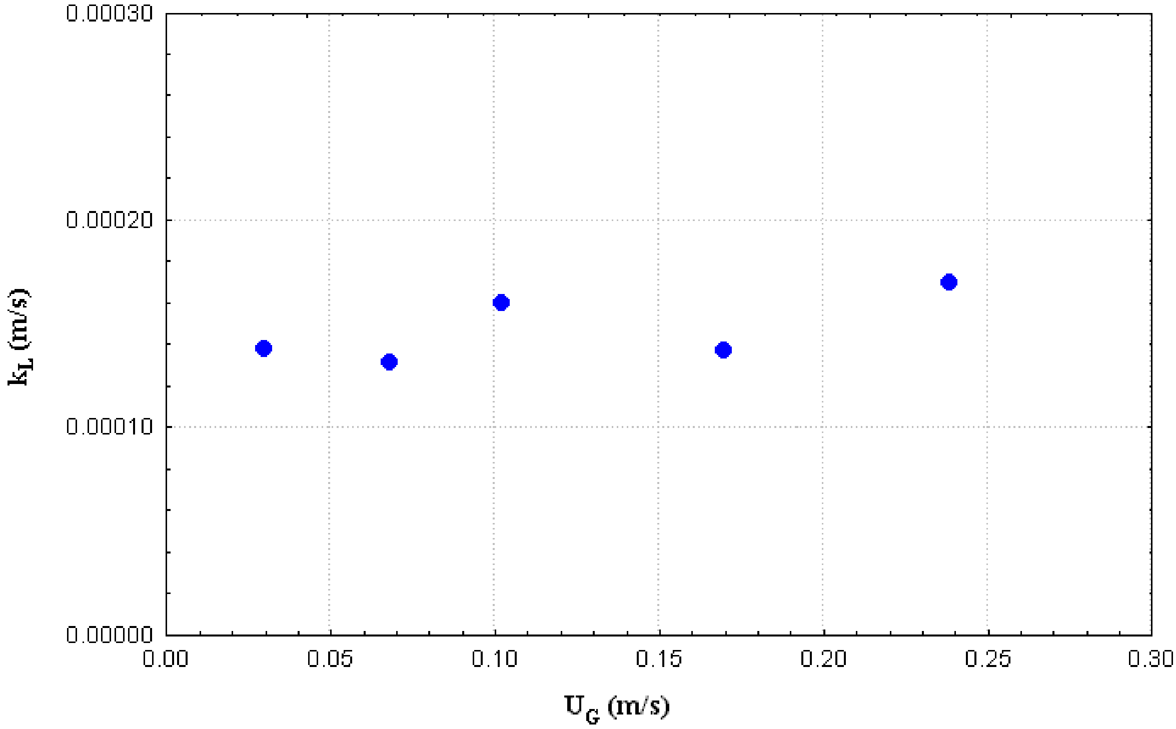


Fig. 8, Variation of k_L with superficial gas velocity (Air-water).

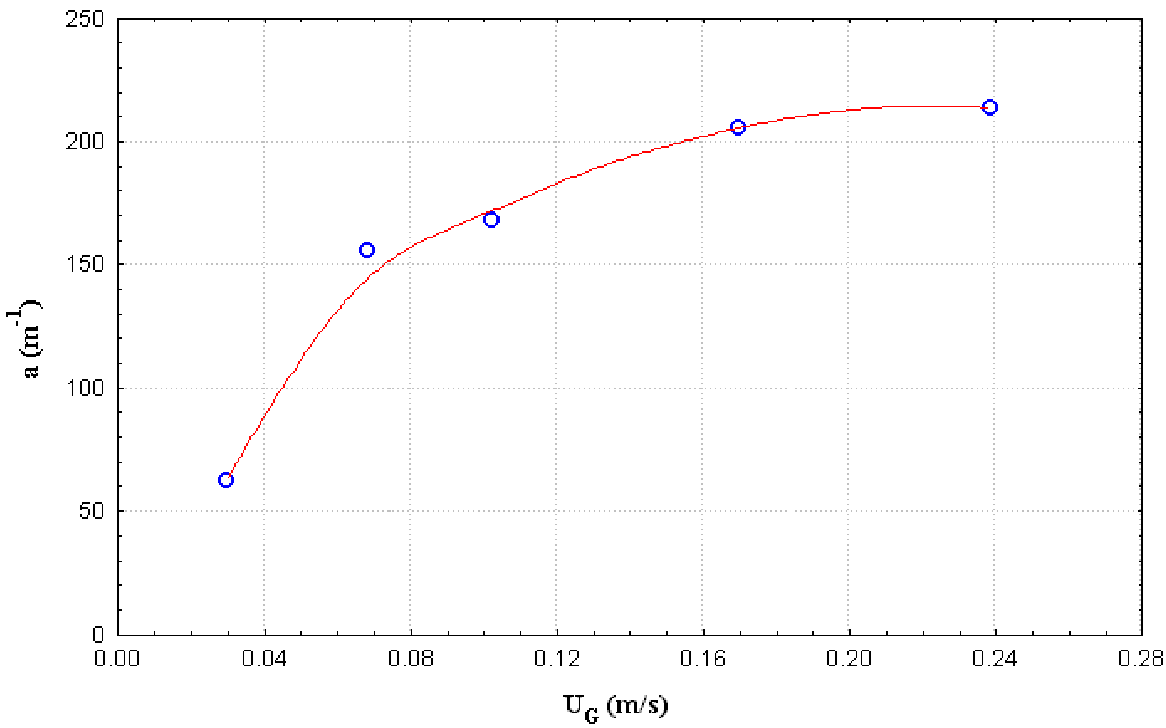


Fig. 9, Variation of interfacial area with superficial gas velocity (Air-water).

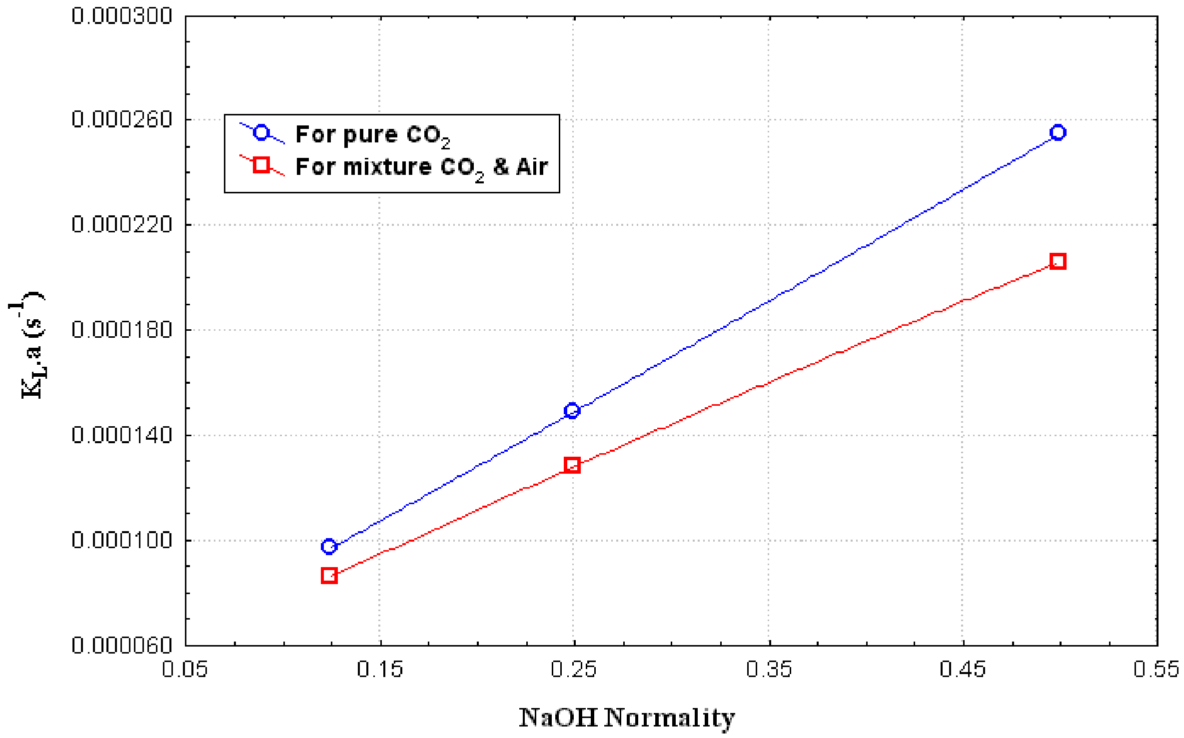


Fig.10, k_L.a as a function of NaOH normality (CO_2- NaOH).

For CO_2- NaOH system, Fig. 10, shows the volumetric mass transfer coefficient calculated using equation (4) and STATISTCA for Window Release 5, (1995).

CORRELATION OF MASS TRANSFER COEFFICIENT

Two approaches were used to correlate the experimental mass transfer data obtained in this search. The first method was to develop empirical correlations, and the second was to use ANN correlation. A literature search as listed in Table (1) for bubble column reactor was conducted to obtain mass transfer data.

Table 1, Literature search for air-water system and 0.1 m column diameter

No.	Authors	Operating Condition	No. of points
1	(Krishna and Van Baten, 2003).	d_o=0.5 mm N_o=1200	7
2	(Vandu, 2004)	d_o=0.5 mm N_o=199	21

EMPIRICAL CORRELATION

The k_L values obtained in this study for oxygen dissolved in water in bubble column reactor along with the literature data given in the references listed in Table (1) were correlated using dimensionless groups; the correlation was calculated using STATISTCA for Window Release 5, (1995):

$$Sh = 1.63\,Re^{0.88}\,Bo^{-0.04}\,We^{0.268} \quad (5)$$

It should be noted that all dimensionless groups in equation (5) are based on the physical properties of fluid which listed in Table (2), also Table (3) showes The limits of dimensionless groups.

Table 2, physical properties of air-water system (Ruthiya, 2005)

Fluid	Density Kg/m^3	Viscosity Pa.s	Surface Tension N/m	Diffusivity m^2/s
Water	998	$1*10^{-3}$	$72*10^{-3}$	$2.11*10^{-9}$
Air	1.3	$1.7*10^{-3}$	$72*10^{-3}$	$1*10^{-5}$

Table 3, The limits of Dimensionless groups.

No.	Variable	Minimum	Maximum
1	Bo	0.247	19.3
2	We	0.0003	49.93
3	Re	110	2887.4
4	Sh	87.94	3121.9

ARTIFICIAL NEURAL NETWORK CORRELATION

Using the Simulent version 3.05 (1997) computer software, ANN correlation were developed to predicte the mass transfer coefficient in bubble column using k_L values obtained in this study for oxygen dissolved in water in bubble column reactor along with the literature data given in the references listed in Table 1. Fig.11, shows the architecture of the BPNN with three inputs, one hidden layer with four nodes and one output. Table 4 shows the weighting parameters produced by training the net.

Table 4, Weighted parameters for trained BPNN.

	w_{ij}				
	1	2	3	4	5
1	-45.716	23.269	-69.555	11.38	
2	8.695	1.8127	2.7085	-1.71227	
3	19.0316	-5.265	15.374	1.0333	
4	8.257	2.096	3.393	-1.097	
	w_{jk}				
1	-0.7308	-5.0748	1.67166	6.8745	1.312057

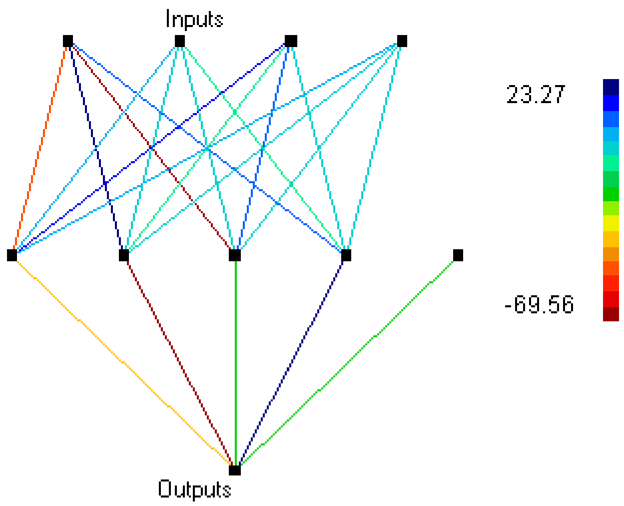


Fig. 11, ANN architecture

Comparison of the ANN Correlation with the Published Correlations

The literature correlations listed in Table 5 along with equation (5) were used to predict the mass transfer through Sherwood number. Fig.12, shows the comparison between the experimental and predicate Sherwood number of different correlations. Table 6 shows the comparison between the AARE and σ for the different correlations. It is obvious that ANN correlation is a better choice to correlate the experimental data through its lower values of AARE and σ (12.79% and 10%).

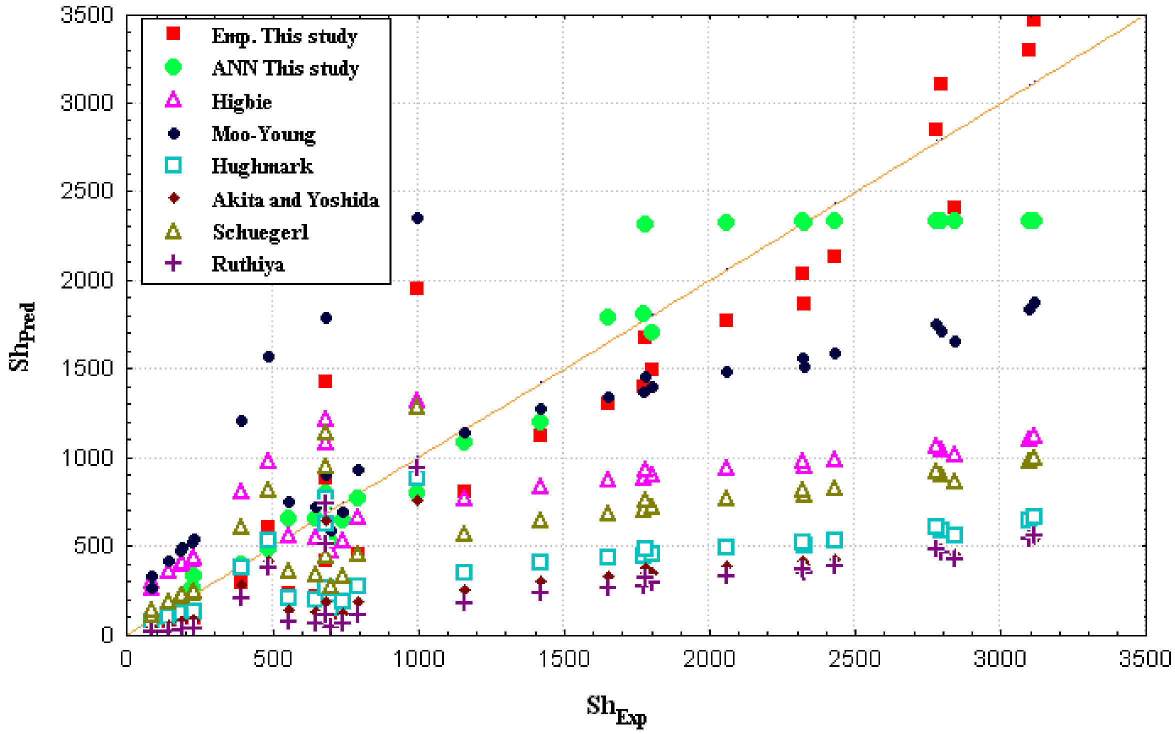


Fig. 12, comparison between the experimental and predicted Sherwood number of different correlations.

Table 5, Various correlations to predicate Sh No.(adopted from Ruthiya, 2005)

No.	Authors	Correlations
1	Higbies (1960)	$Sh = 1.13 Re^{1/2} Sc^{1/2}$
2	Moo-Young and Calerbank (1961)	$Sh = 0.53 Re^{2/3} Sc^{1/2}$
3	Hughmark (1967)	$Sh = 2 + 0.0192 Re^{0.86} Sc^{0.63}$
4	Akita and Yoshida, (1974)	$Sh = 0.6 Re^{1/2} Sc^{1/3} Bo^{3/8}$
5	Schuegerl, (1977)	$Sh = 0.15 Re^{3/4} Sc^{1/2}$
6	Ruthiya, (2005)	$Sh = 0.083 Re^{1/2} Sc^{1/2} Bo^{0.768}$

Table 6, Comparison between the AARE and σ for the different correlations.

No.	Correlations	AARE %	σ %
1	Higbie	68.3	49.2
2	Moo-Young	80.7	78.6
3	Hughmark	56.5	25.9
4	Akita and Yoshida	67.85	22.1
5	Schuegerl	48.9	20.8
6	Ruthiya	79.2	26.3
7	Empirical (This study)	41.2	30.17
8	ANN (This study)	12.79	10.0

CONCLUSIONS

The study of mass transfer parameters led to the following conclusions:

❶ $k_L.a$ increased with superficial gas velocity.

❷ The gas-liquid bubble interfacial area (a) increased as superficial gas velocity increased, while no significant increase of k_L with superficial gas velocity was observed.

❸ The volumetric mass transfer coefficient $k_L.a$ for CO_2-NaOH system increased with increasing the normality of NaOH solution and more increased when pure gas was used

❹. The correlation proposed by using BPNN shows less AARE and σ (12.79% & 10.0%) respectively ,than other empirical correlations found in literature. An empirical correlation was proposed with AARE, σ and R equal to (41.2 %, 30.17% and 93%) respectively. From above, the use of BPNN is a good choice for predicting mass transfer coefficient.

NOMENCLATURE

a	Gas-liquid interfacial area per unit volume of liquid, m^{-1};
A_C	Cross sectional area of the reactor column, m^2 ;
C_A	Concentration of the gas A in the liquid bulk, kmol m^{-3};
C*	Solubility of the gas at equilibrium, kmol m^{-3};
C_L	Concentration of the gas in the liquid bulk, kmol m^{-3};
D_{AB}	Diffusivity of gas A in the liquid B, m^2 s^{-1};

d_b Gas bubble diameter, m ;

D_C Diameter of the reactor column, m;

d_o Orifice diameter, m;

g Gravitational constant, m s^{-2};

H Henry's Law Constant, bar m^3 $kmol^{-1}$;

H_C Clear liquid height, m;

H_D Dispersed liquid height, m;

$K_{o.a}$ Over all mass transfer coefficients, m s^{-1};

k Phase mass transfer coefficient, m s^{-1};

$k_L.a$ Volumetric liquid-side mass transfer coefficient, s^{-1};

N number of input data for train;

N_o Number of openings on the gas sparger;

P Pressure, bar;

P_T Total pressure, bar;

Q Phase flow rate, m^3 s^{-1};

R gas constant: 8.314 KPa.m^3 $Kmol^{-1}$. $^oK^{-1}$;

t Time, s;

T Temperature, ^oK;

U Superficial velocity, m s^{-1};

U_b Bubble rise velocity, m s^{-1};

V Volume, m^3;

GREEK SYMBOLS

ε Phase holdup;

μ Phase viscosity, kg m^{-1} s^{-1};

ν Kinematic viscosity, m^2 s^{-1};

ρ Phase density, kg m^{-3};

σ Standard of deviation ;

σ_L Surface tension of the liquid, Nm^{-1};

υ Molar volume, m^3 $kmol^{-1}$;

SUBSCRIPTS

A Gas specie;

B Liquid specie;

G Gas phase;

i Initial condition or interface;

L Liquid phase;

O Orifice;

T whole column;

DIMENSIONAL NUMBERS

Bo Bond number, $gd_b^2\rho_L/\sigma_L$;

Re Reynolds number, gas $U_G D_c \rho_L/\mu_L$, gas bubble $U_b d_b \rho_L/\mu_L$;

Sc Schmidt number, $\mu_L/\rho_L D_{AB}$;

Sh Sherwood number, $k_L d_b/D_{AB}$;

We Webber number, $\rho_G U_G^2 D_c^4/N_o^2 d_o^3 \sigma_L$;

ABBREVIATIONS

AARE Absolute average relative error;

ANN Artificial neural network;

BPNN Back propagation neural network;

GL Gas-Liquid;

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