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Simulation Study of Mass Transfer Coefficient in Slurry Bubble Column Reactor Using Neural Network

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Abstract

The objective of this study was to develop neural network algorithm, (Multilayer Perceptron), based correlations for the prediction overall volumetric mass-transfer coefficient (k_La), in slurry bubble column for gas-liquid-solid systems. The Multilayer Perceptron is a novel technique based on the feature generation approach using back propagation neural network. Measurements of overall volumetric mass transfer coefficient were made with the air - Water, air - Glycerin and air - Alcohol systems as the liquid phase in bubble column of 0.15 m diameter. For operation with gas velocity in the range 0-20 cm/sec, the overall volumetric mass transfer coefficient was found to decrease with increasing solid concentration. From the experimental work 1575 data points for three systems, were collected and used to predicate k_La. Using SPSS 17 software, predicting of overall volumetric mass-transfer coefficient (k_La) was carried out and an output of 0.05264 sum of square error was obtained for trained data and 0.01064 for test data.

Keyword: *slurry bubble column reactor, mass transfer coefficient, neural network*

1. Introduction

Slurry bubble columns (SBC) are widely used in the chemical and petrochemical industries to carry out catalytic hydrogenation or oxidation reactions. SBCs are the preferred type of reactors especially for highly exothermic processes, when efficient interphase contacting is needed and when significant phase back mixing is not detrimental to the operation. These three-phase reactors are characterized with simplicity in construction, low operating cost, excellent heat and mass transfer and variable residence time. SBCs offer several advantages, such as nearly isothermal operation, good interphase contacting, large catalyst area, good productivity, operational flexibility, low pressure drop, possibility of online catalyst addition, and low pore diffusion resistance. The SBC is currently the best suited reactor for Fischer-Tropsch synthesis and conversion of natural gas to fuels and chemicals. This type is also considered for both direct and indirect coal liquefaction, waste water treatment as well as biotechnological applications. In SBCs, there is an intense and intimate contact between a gas-phase component, a liquid-phase component and a finely dispersed solid [1, 2].

The design and efficient exploitation of multiphase reactors require knowledge of their hydrodynamics and mass- and heat-transfer characteristics, e.g., pressure drop, phase holdups, mass- and heat-transfer coefficients, etc. Rigorous treatment from first principles of multiphase flow problems remains a difficult task and has not yet attained sufficient maturity to take over the correlation-based approaches. Artificial neural networks (ANNs), as correlation tools, hav gained wide acceptance in the field because of their inherent ability to map nonlinear relationships that tie up independent variables (either as dimensional inputs, e.g., pressure, diameter, etc., or as dimensionless inputs, e.g., Reynolds, Weber, and Froude numbers, etc.) to the reactor characteristics to be predicted, i.e., dimensional or dimensionless output [3]. (ANN) is the most commonly and widely used data-driven modeling technique. For modeling of the parameters for bubble column reactors, ANN has been used by Shaikh and Al- Dahhan (2003) [4] for correlating the overall gas hold-up in bubble column reactors. Recently, support vector regression (SVR) rigorously based on statistical learning theory data has gaoined popularity for driven modeling. The focus of this study is to develop neural network algorithm (Multilayer Perceptron), based correlation for the prediction over all mass transfer coefficient in slurry bubble column. The input layer has nine nodes, including gas holdup, gas velocity, solution concentration, solid concentration, solution density, solution viscosity, solution surface tension, geometry ratio and diffusivity. The output layer has one node, which is the mass transfer coefficient.

2. Model of ANN

An ANN can be considered as a black box consisting of a series of complicated equations for the calculation of outputs based on a given series of input values. ANNs consist of collections of connected processing elements or neurons. The function of a neuron can be mathematically expressed as:

$a = f\,(wp + b)$

where p is the neuron input, which is multiplied by weight w, and then is summed by a bias b, a the neuron output and f is called the activation or the transfer function. Neural networks are computer algorithms inspired by the way information is processed in the nervous system. An ANN is a massively parallel distributed processor that has a natural propensity for storing experimental knowledge and making it available [5]. It was n reported that multilayer ANN models with only one hidden layer are universal approximators. Multilayer Perceptron, back propagation network used in this paper is shown in Fig. 1. wj,i represents the weights between the input layer vectors and hidden layer vectors, and vk,j represent the weights between the hidden layer vectors and output layer vectors.

The calculated prediction error based on the following criteria:

- Sum of Square Error (SSE):

This method based on the following equation:

$$SSE = \sum_{1}^{n} (experimental\ value\ -\ predicted\ value)^2$$

- Relative Error (RE)

$$RE = \frac{Experimental\ value - Predicted\ value}{Experimental\ value}$$

3. Experimental Work

Experiments were carried out in a column of 0.15 m in diameter and of 1.6 m in height. Perforated plate sparger was used in the column. Tap water, Glycerin with 33 wt %, 50 wt % and 66 wt %, and alcohol solution with 0.3 wt %, 0.6 wt % and 1.5 wt % were used as the liquid phase. The physicochemical properties (Table 1) were calculated from values and correlations given in Perry [6]. The aspect ratio (Static liquid height/Diameter of column) was 2,4 and 6. PVC particles (density 1025 kg/m^3, diameter 3 mm) was used as solid phase with 25 kg/m^3, 50 kg/m^3, 75 kg/m^3, and 100 kg/m^3 concentration in the column. The operation was batch with respect to liquid phase. The rate of air-flow sparged continuously was measured by a calibrated rotameter. The gas hold-up was obtained by the volume expansion method. The volumetric mass transfer coefficients were determined by the dynamic method. The material balance of the oxygen dissolved in the liquid phase is [7]:

$$\log \frac{C_f - C_o}{C_f - C_i} = \frac{k_L a}{2.303(1-\varepsilon_g - \varepsilon_s)} . t \qquad \ldots(1)$$

where ε_g and ε_s are gas hold up and solid hold up respectively, C_o and C_f are initial and final concentration of oxygen respectively, C_i represents the concentration of oxygen at any time in the bubble column. Plotting of the left hand side of equation (1) versus (t) will give the average slop term ($k_L a$ /2.303(1- ε_g- ε_s)), then $k_L a$ can be calculated. The change in the dissolved oxygen concentration was monitored using a fast dissolved oxygen electrode. Figure (2) shows the schematic diagram of the experimental apparatus.

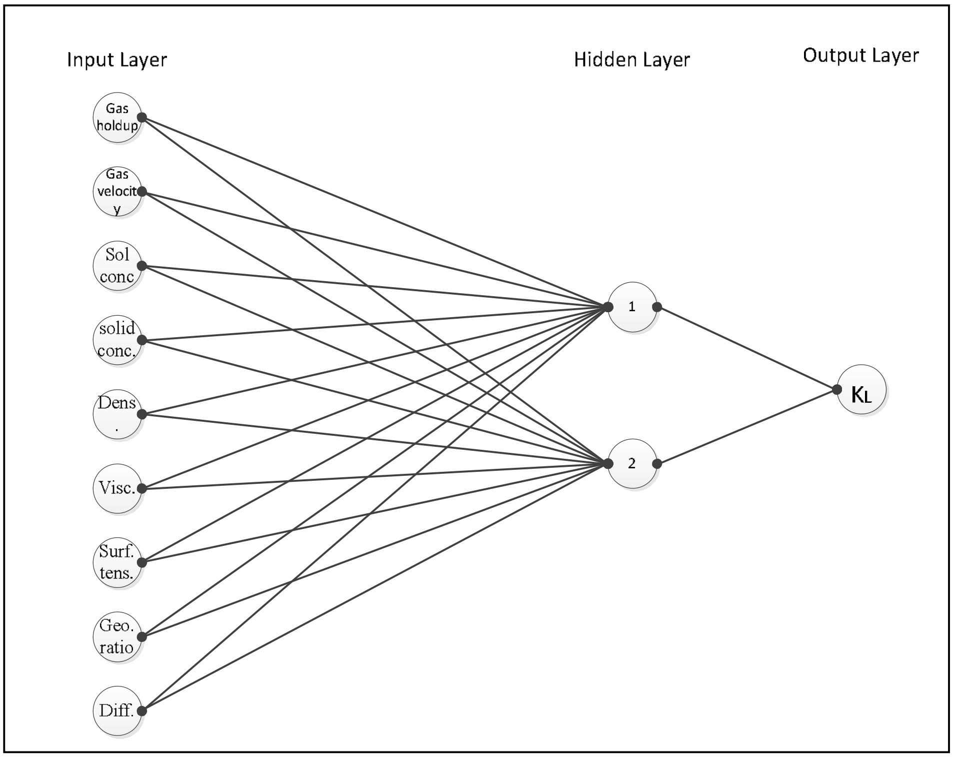

Fig. 1. Multi Layer Perceptron, Back Propagation Network.

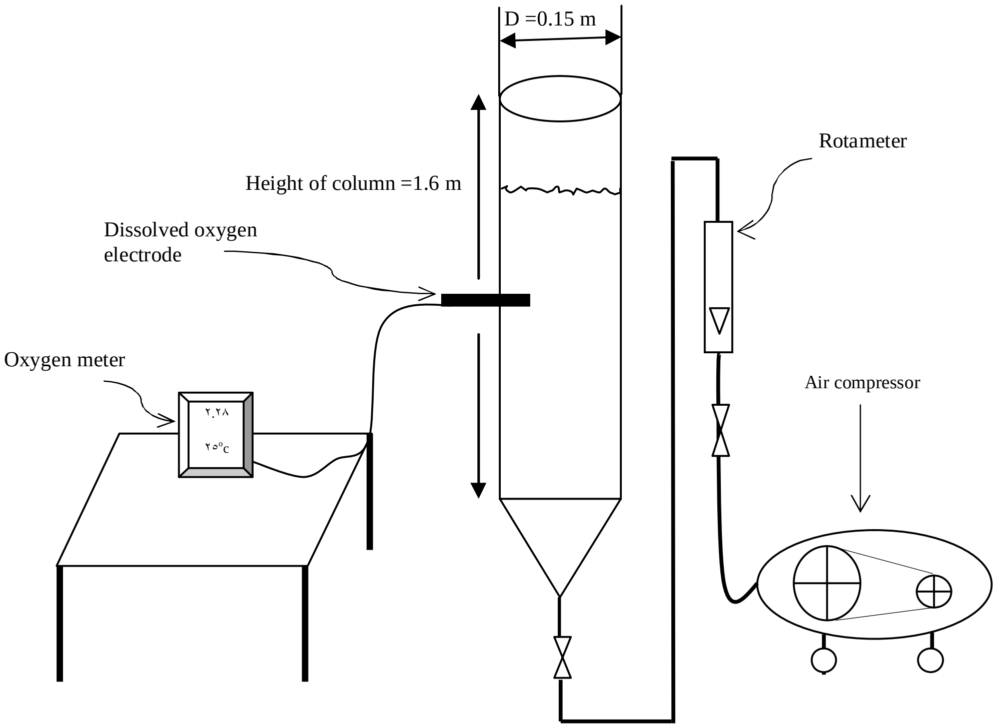

Fig. 2. Schematic Diagram of the Experimental Apparatus.

4. Results and Discussion

From the ranges of the data obtained in experimental work (Table 1), the developed models can be used to predict the mass transfer parameters in slurry bubble column reactor operating under typical conditions (1575 data were used). In this study, the model was used to predict the volumetric mass transfer coefficient, in slurry bubble columns SBC. From SPSS 17®, 78 try and error attempts were done by the option Multilayer Perceptron (MLP) and through using automatic architecture selection option as shown in Figure 3 a & b. Figure 4 shows the data partition's used in this prediction (70% of data was trained and 30% for testing).

Table 1,
The Range of Data Obtained in the Experimental Work.

variables	**gas holdup**	**gas velocity**	**solution concentration**
Maximum	0.545455	0.20608	1
Minimum	0.00217	0.02167	0.003
Units	-	m/s	w/w
variables	**density**	**viscosity**	**surface tension**
Maximum	1173	0.0225	0.072
Minimum	991	0.0009	0.0009
Units	Kg/m^3	Pa.s	N/m
variables	**Aspect ratio**	**Diffusivity*10^{-9}**	
Maximum	6	20.807	
Minimum	2	0.048	
Units	-	m^2/s	
variables	**Solid concentration**		
Maximum	100		
Minimum	0		
Units	Kg/m^3		

The back propagation neural network (BPNN) selected for predicting k_La has the following topology: (9, 2, 1).The learning rate for the k_La BPNN was 0.25 and 1500 iterations were used during the training and learning process. The values of SSE, and RE of 5.264 and 1.064, respectively (Table 2), were obtained with this BPNN.

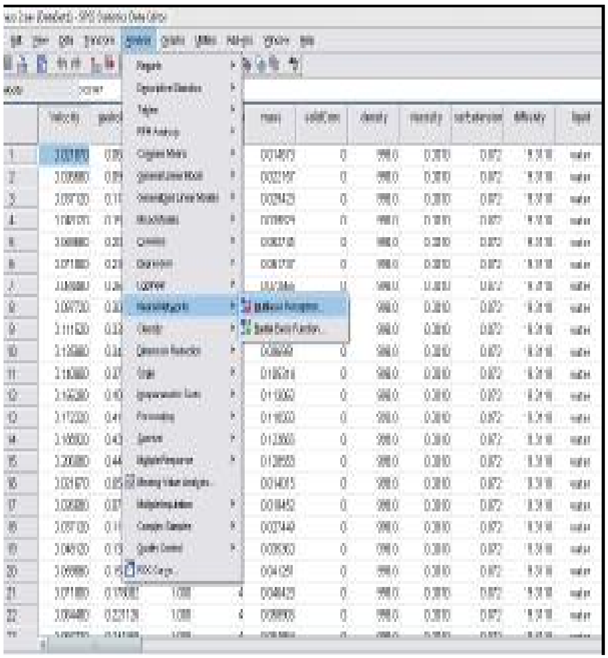

Fig. 3-a. SPSS Statistics Data Editor.

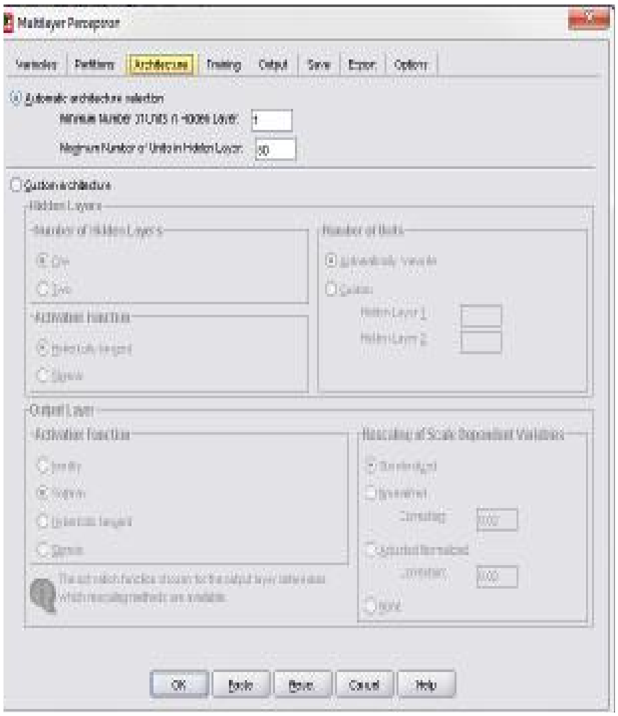

Fig. 3-b. Multi Layer Prediction.

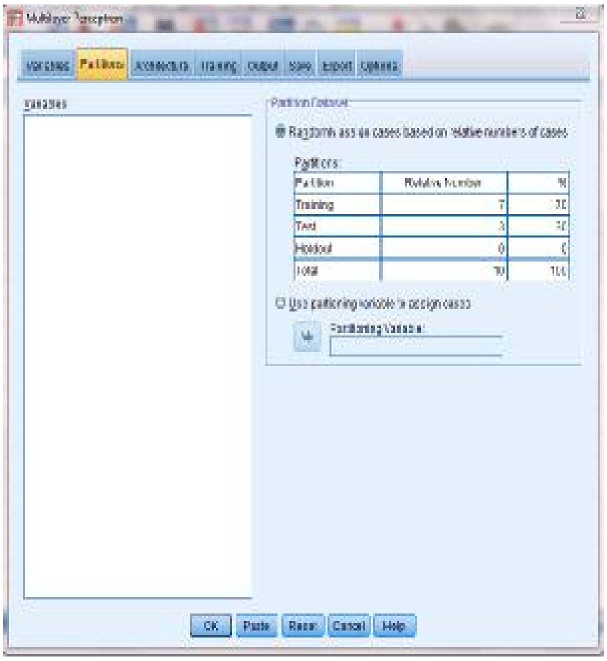

Fig. 4. The Partition Data.

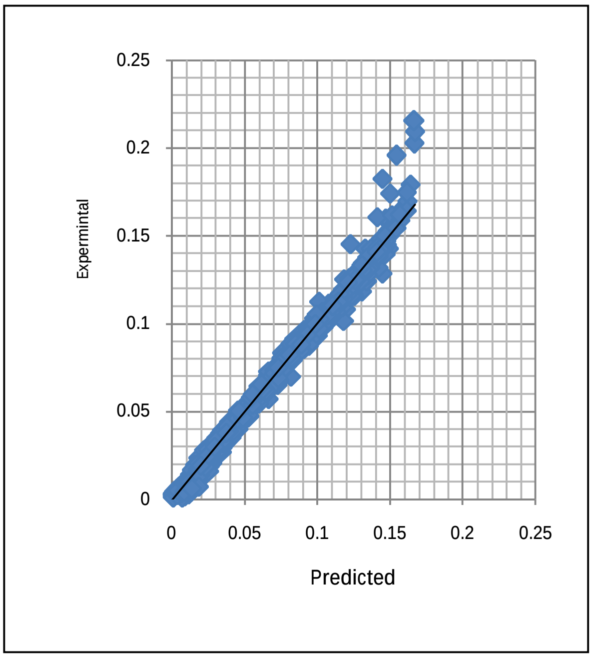

Fig. 5. The Comparison between Experimental and Predicted k_La using BPNN.

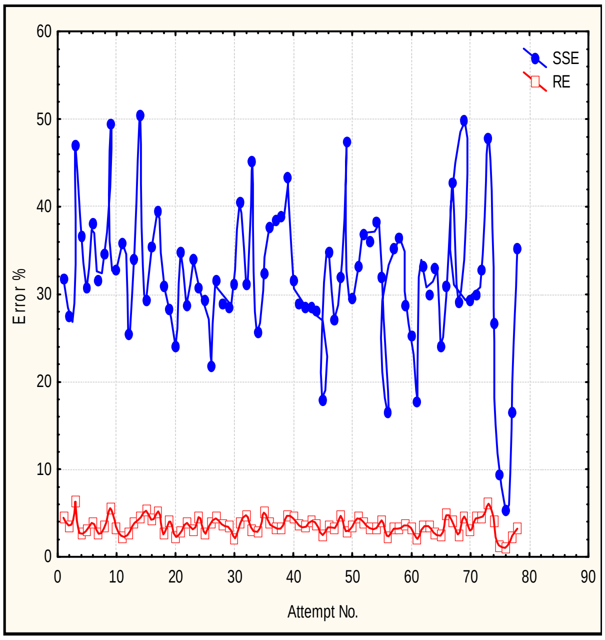

Fig. 6. The Iterations with Errors Counted for Each Iterate.

Table 2,
Model Summary

Training	Sum of Squares Error (SSE)	5.264
	Relative Error (RE)	0.010
	Stopping Rule Used	1 consecutive step(s) with no decrease in error
	Training Time	0:00:01.520
Testing	Sum of Squares Error	1.064
	Relative Error	0.027

Figure 5 shows the comparison between experimental and predicted k_La values using the BPNN. Figure 6 shows the iterations with errors counted for each iterate.

4.1. Effect of Gas Velocity on Mass Transfer Coefficient

Figures 7 to 10 show the relation between gas velocity and mass transfer coefficient for experimental and predicted values. As can be seen in these figures k_La values increase with gas velocity. This increase of k_La can be observed for all solid concentrations and liquid systems. These results pointed out that in the churn-turbulent regimes, as the superficial gas velocity increases the overall mass transfer coefficient increases due to the large bubble holdup increase. In bubbly flow regime, number of bubbles increases with increasing superficial gas velocity leading to increase the gas-liquid interfacial area.

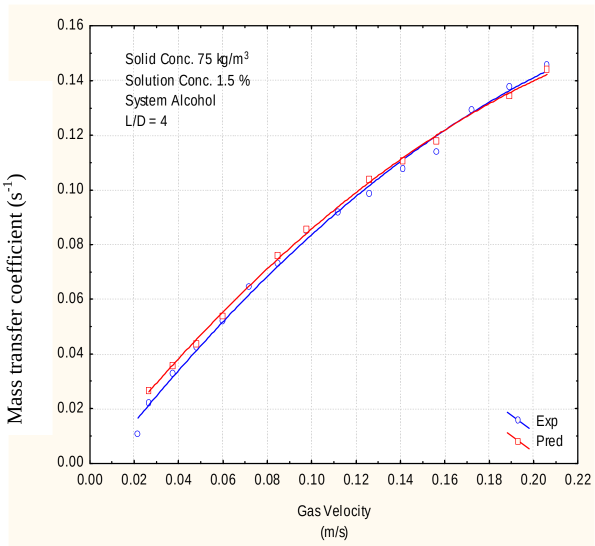

Fig. 7. The Relation between Gas Velocity and Volumetric Mass Transfer Coefficient for Alcohol System, 75 kg/m^3 Solid Concentration.

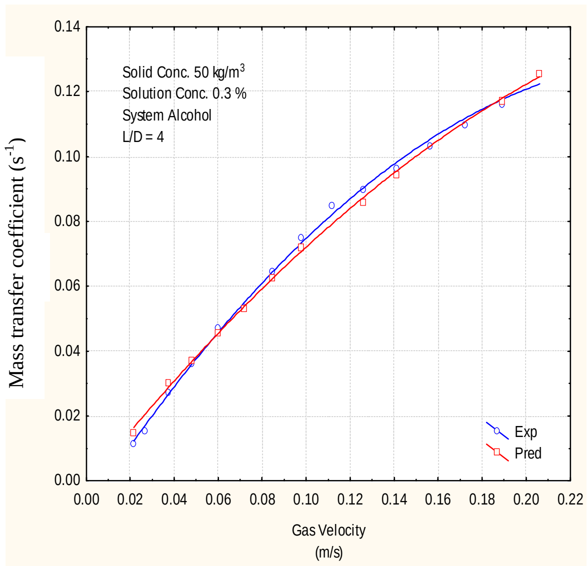

Fig. 8. The Relation between Gas Velocity and Volumetric Mass Transfer Coefficient for Alcohol System, 50 kg/m^3 Solid Concentration.

These results are in agreement with Krishna and Van Baten (2003) [8] and Verma and Rai (2003) [9]. These figures compare the predictions of the proposed simulation with the experimental data. It can be seen that the proposed ANN correlation agrees reasonably with the experimental data.

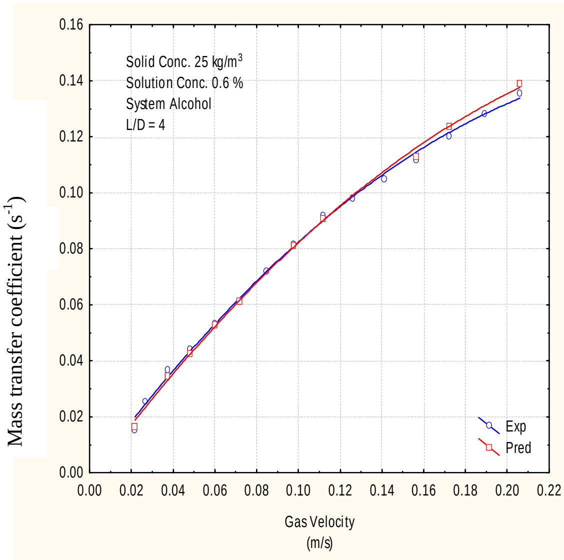

Fig. 9. The Relation between Gas Velocity and Volumetric Mass Transfer Coefficient for Alcohol System, 25 kg/m^3 Solid Concentration.

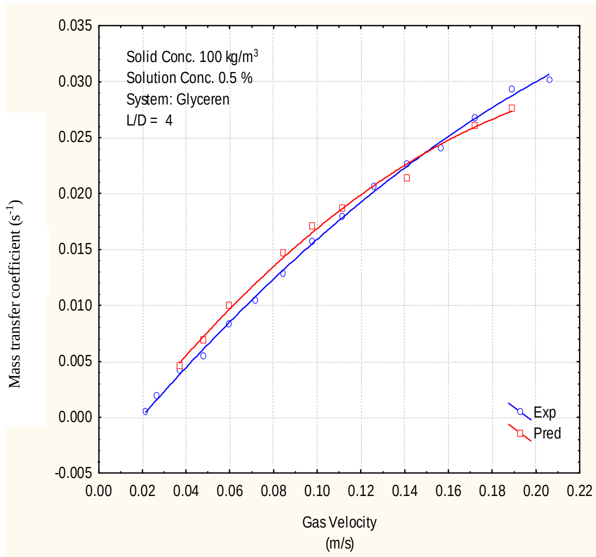

Fig. 10. The Relation between Gas Velocity and Volumetric Mass Transfer Coefficient for Glycerin System, 100 kg/m^3 Solid Concentration.

4.2. Effect of Gas Holdup

Figures 11 to 13 show a comparison between the predictions obtained using the ANN correlation and experimental data for air-water and air-alcohol systems at different solid concentrations and gas velocity. The trend shown by the ANN correlation is in a good agreement with experimental work. These figures show that, the volumetric mass transfer coefficient k_La increases with increasing gas holdup. These results pointed out that higher gas holdup led to increase gas-liquid interfacial areas leading to a higher mass transfer coefficient k_La.

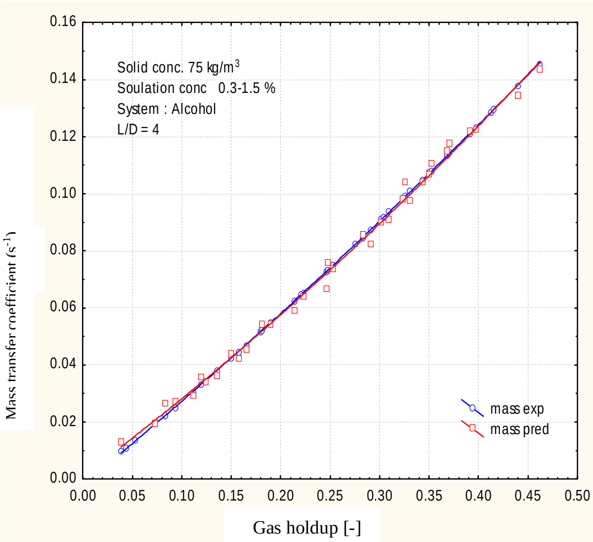

Fig. 11. The Comparison between ANN Correlation and Experimental Data for Air-Alcohol System at 75 kg/m^3 Solid Concentration.

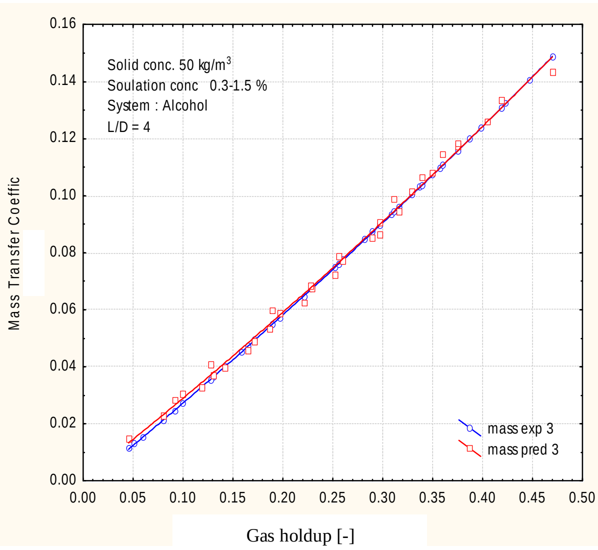

Fig. 12. The Comparison between ANN Correlation and Experimental data for Air-Alcohol System at 50 kg/m^3 Solid Concentration.

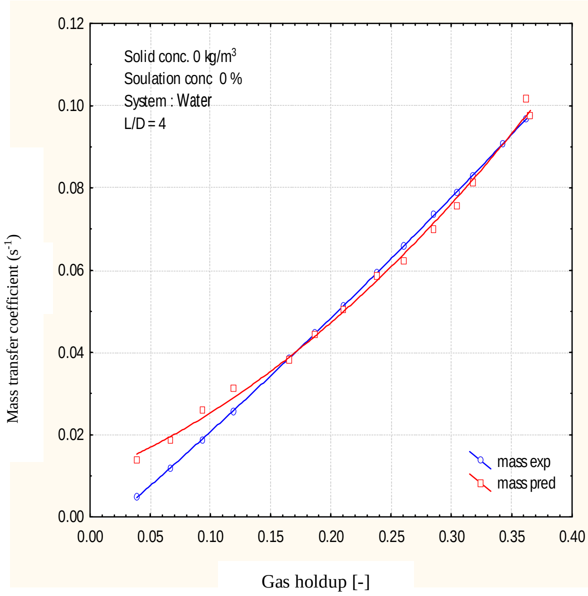

Fig. 13. The Comparison between ANN Correlation and Experimental Data for Air-Water System.

4.3. Effect of Solid Concentration

The experiments performed with addition of solid showed that, the volumetric mass transfer coefficient k_La decreases with increasing solid concentration as shown in Fig. 14, 15 and 16, whereas, the gas-liquid interfacial area decreases with increasing solid concentration. The decrease of mass transfer coefficient with increasing solid concentration is attributed to decrease of small bubble and increase large bubble size due to the bubble coalescence tendencies and they limited the mass transfer coefficient. These results are in agreement with Vandu and Krishna (2004) [10] and Koide et al. (1984) [7].

Figures 15 and 16 shows a good agreement of ANN predictions with the experimental data.

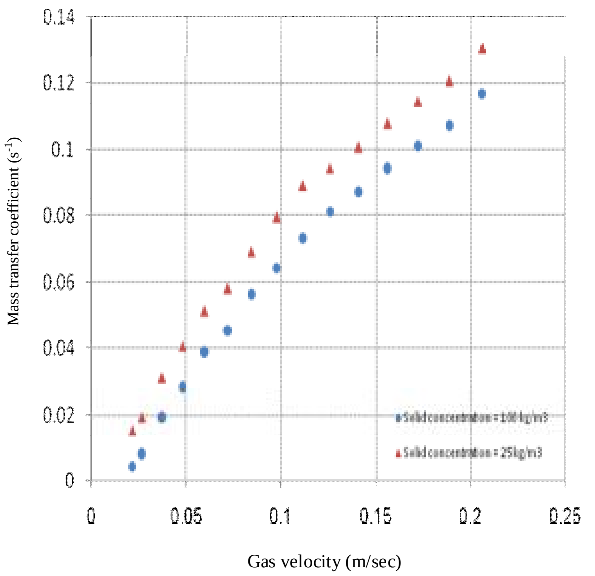

Fig. 14. Effect of Solid Concentration on Mass Transfer Coefficient for 0.3 % Alcohol System and L/D=4.

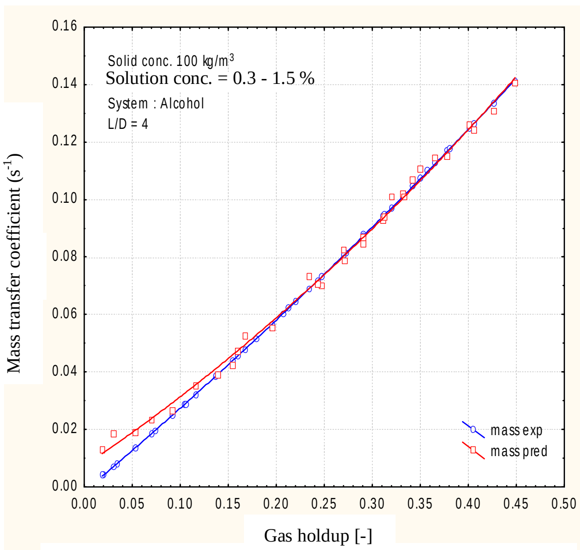

Fig. 15. The Comparison between ANN Correlation and Experimental Data for Air-Alcohol System at 100 kg/m³ Solid Concentration.

4.4. Effect of the Type of Liquid Phase

To check the effect of liquid physical properties, ANN predictions were carried out at different liquid viscosities and liquid surface tension. The experiments performed with viscous media (Glycerin systems) showed that the volumetric mass transfer coefficient decreases with increasing liquid viscosity as shown in Fig. 17. It was pointed out that, higher viscosity led to increase of the volume fraction of large bubbles, leading to much lower gas-liquid interfacial areas while k_La values increased in the presence of alcohol as shown in Fig. 18 and 19. The increase of k_La with the presence of alcohol is attributed to creation of small bubbles and reduced bubble coalescence due to the surfactant. As a result, the presence of small bubbles should be preferred and the presence of large bubbles should be avoided for effective mass transfer rates, these results are in agreement with Ozturk et al. (1987) [11] and Behkish et al. (2002) [12].

In these figures, the predictions of proposed simulation fit the experimental data reasonably well.

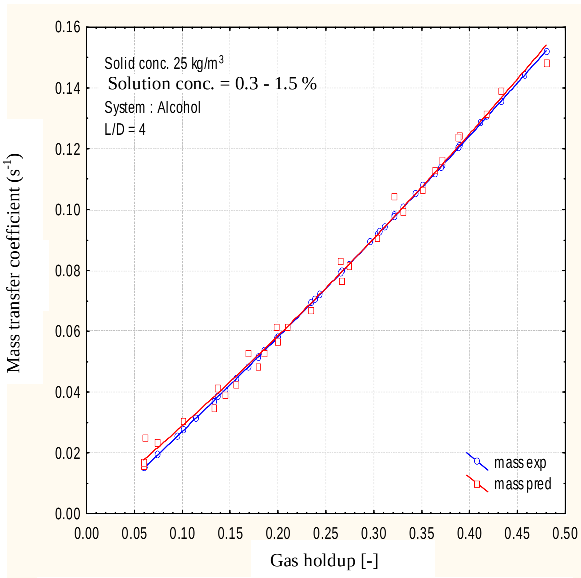

Fig. 16. The Comparison between ANN Correlation and Experimental Data for Air-Alcohol System at 25 kg/m³ Solid Concentration.

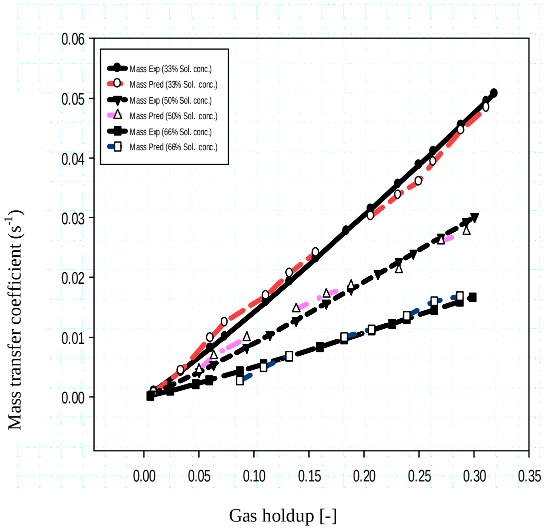

Fig. 17. Effect of Liquid Viscosity on Volumetric Mass Transfer Coefficient.

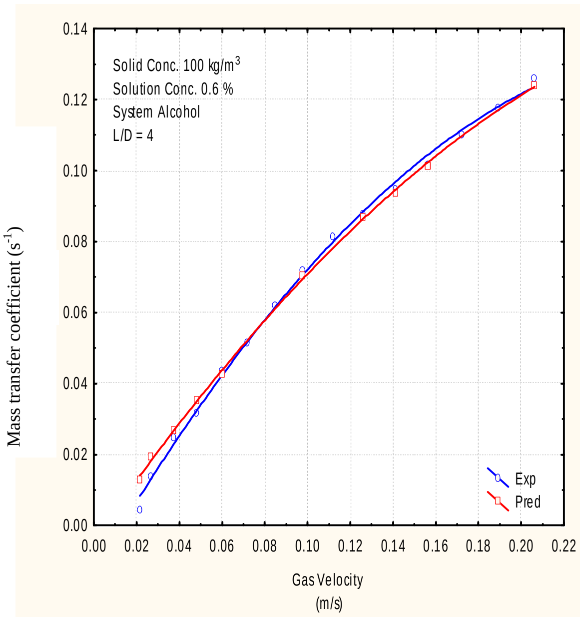

Fig. 18. The Relation between Gas Velocity and Volumetric Mass Transfer Coefficient for Alcohol System, 100 kg/m^3 Solid Concentration.

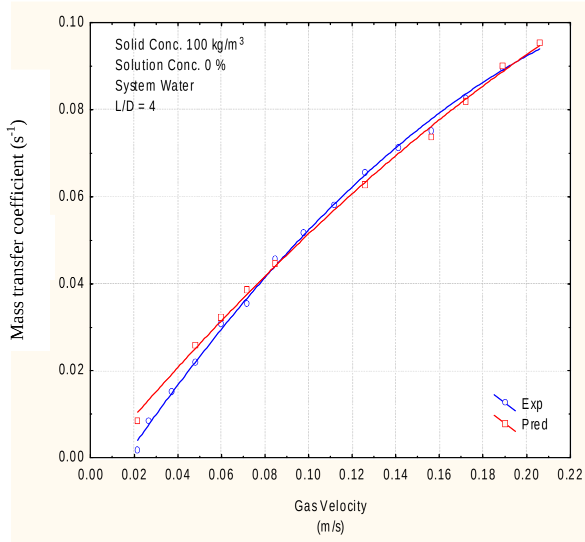

Fig. 19. The Relation between Gas Velocity and Volumetric Mass Transfer Coefficient for Water System, 100 kg/m^3 Solid Concentration.

5. Conclusion

1. It can be concluded that the volumetric mass transfer coefficient, k_La increases with increasing gas velocity and gas holdup whereas decreases with increasing solid concentration and liquid viscosity. It is also concluded that the presence of surfactants increase k_La, due to the presence small bubbles.
2. The ANN model for prediction of mass transfer coefficient is developed successfully in this work. In this model, the number of nodes in the input layer, hidden layer and output layer are 9, 2 and 1 respectively. The nodes in the input layer are including gas holdup, gas velocity, solution concentration, solid concentration solution density, solution viscosity, solution surface tension, geometry ratio and diffusivity. The node in output layer is Mass transfer coefficient.
3. The sum of square error and relative error are used to assess the performance of ANN model. This ANN model demonstrated a good statistical performance with the sum of square error and relative error of (5.264% and 1.064% respectively) which are very low values relative to the range of the experiments.

6. References

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دراسة محاكاة معامل انتقال الكتلة في العمود الفقاعي ثلاثي الأطوار باستخدام الشبكات العصبية الصناعية

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الخلاصة

هدف هذه الدراسة كان تطوير خوارزمية الشبكة عصبيةِ، (Perceptron متعدّد الطبقة) و اعتماد علاقات معامل انتقال الكتلة الحجمي (k_La) في مفاعل العمود الفقاعي ثلاثي الاطوار (سائل-غاز-صلب). (Perceptron) متعدّد الطبقة هو تقنية مبتكرة و معتمدة على ميزة نظرية الجيلِ باستخدام شبكة التوليدِ العصبية العكسية. تم قياس معامل انتقال الكتلة في عمود فقاعي ذي قطر ٠.١٥ م وباستخدام ثلاثة انظمة وهي (هواء وماء) , (هواء وغليسرين) و (هواء وكحول). تم تشغيل العمود الفقاعي بسرع غاز تراوحت من ٠ الى ٢٠ سم/ثانية و وجد بأن معامل انتقال الكتلة قد تناقص بزيادة تركيز الصلب في العمود. تم الحصول على ١٥٧٥ نقطة من التجارب العملية للأنظمة الثلاثة واستعملت هذه النتائج العملية للتكهن بقيم k_La باستخدام برنامج (SPSS 17) و تم الحصول على معامل انتقال الكتلة الحجمي (k_La) المتوقع من البرنامج و بمربع خطأ مقداره (٠.٠٥٢٦٤) للبيانات التدريبية و(٠.٠١٠٦٤) لبيانات الإختبار.