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MODEL BASED IN NEURAL NETWORKS FOR THE PREDICTION OF THE MASS TRANSFER COEFFICIENTS IN BUBBLE COLUMNS. STUDY IN NEWTONIAN AND NON-NEWTONIAN FLUIDS.

E. Alvarez, J. M. Correa and C. Riverol
Department of Chemical Engineering. University of Vigo. 36200-Vigo. Spain.

J.M. Navaza
Department of Chemical Engineering. University of Santiago. 15706-Santiago. Spain.

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ABSTRACT

A comprehensive study for the prediction of the volumetric transfer coefficient k_La with Newtonian and Non-Newtonian fluids in bubble columns is the objective of this work. The evaluation of the hydrodynamic characteristics of the bubble columns and delineated the different hydrodynamic regimes considering column geometry, gas flow, liquid height and type of fluid (Newtonian and non-Newtonian) suggest a general applicability of the proposed model. A new learning pattern based in the design parameters of the bubble columns is proposed. © 2000 Elsevier Science Ltd

Introduction

Numerical simulation is being recognized as a primary tool for improving the performance of process equipment Mangatz et al. [1]. In particular, for scale-up of chemical reactors a reliable the fluid dynamic of bubble column model is of great benefit. Dynamical numerical simulation is thus on the agenda of most big chemical companies and many scientific research laboratories. Traditionally, the design and scale-up of reactors were largely based on multiphase and multidimensional dispersion models Mangatz et al. [1], Shah et al. [2] and Yadneshwar et al. [3]. In these models, the design parameters were evaluated by empirical correlations, which are applicable to narrow operating ranges. Due to the advent of more powerful computers and a better understanding of the multiphase flows in recent years. The objective of this work is evaluated and simulate the hydrodynamic characteristics of the bubble columns

and delineated the concentration to different conditions of column geometry, gas flow, liquid height and type of fluid (Newtonian and non-Newtonian).

Description of Learning Algorithm

Because of the limited space available in this paper, the reader is referred to Mill et al [4] for details on the conventional weight update equation and its terms. For the single pattern presentation method above, the equation describing the weight update can be expressed recursively. At time-step k each weight $w_{ij}(k)$, connecting, the input of node i on each layer to the output of node j on the preceding layer, is updated using

$$w_{ij}(0) = \varepsilon_{ij} \tag{1.a}$$

$$w_{ij}(k) = w_{ij}(k-1) + \alpha \cdot \xi_i(k) + \beta(w_{ji}(k-1) - w_{ji}(k-2)) \tag{1.b}$$

where ε_i is the back-propagated error value corresponding to the input to the sigmoid function calculated for node i during presentation of the pattern derived from process time-step k. The constants α and β are the learning rate and momentum parameters, respectively and ξ_{ij} is a random variable independently selected for each weight from a distribution with zero mean and small variance. The recursive equation is applied to each weight at each time-step k of the plant operation. The algorithm operates as a first-in first out stack (containing n_p patterns which at each time-step k accepts a new pattern) in n_c cycles to update the weights at each time-step. The algorithm sequence is summarized in the Table 1.

TABLE 1
Learning Algorithm.

Step	Description.
1.	Simultaneously sample inputs and outputs of process.
2.	Shift and update pattern element.
3.	If the pattern is not full, restart at step 1 at next time.
4.	Construct a training pattern from elements of the input pattern of the step 3.
5.	Execute neural network to calculate one-step ahead prediction.
6.	Insert the new pattern into the history –stack.
7.	If the size > n_p, remove the oldest pattern.
8.	Train network for n_c cycles of up to n_p pattern presentation (randomized order)

As presentation pattern the equation used was the following: $(f_g \cdot t/V_L)^{\varepsilon_g}$ where ε_g is the hold-up, V_L is the liquid volume, t time and f_g gas flow that input to the column. As a new idea in this paper, this pattern proposed describes a relation of all design parameters thus as consequence, all the parameters take part in the learning process.

Experimental Procedure

To understand how the convergence of neural network modeling may be improved it is necessary to analyze the way which each of the patterns from the previous experimental data is learned by neural network. Two bubble columns are used in this work: One bubble column of cylindrical section with 6 cm in internal diameter and other of rectangular section with 6 cm in each side. The top plate is flat and has a central orifice, for the inflow of liquid and two off-center orifices for the outflow of gas, and the thermometer respectively. The baseplate has two off-center orifices for outflow of the liquid phase, and a thermometer and a central orifice for inflow of gas through a porous plate. The absorbing liquids used in this work are sucrose, for studied the Newtonian fluids, or of carboxymethylcellulose (CMC), for studied the non-Newtonian fluids) were thermostated to room temperature (25 °C) before entering the contact device. The concentration ranges were (16, 50 and 107 g/l) for sucrose and (0.05 and 0.2%) for carboxymethylcellulose. All the experiments were carried out in batch operation with respect to the liquid, and the level of the liquid in the bubble column was varied between 60 and 90 cm. The gas to be absorbed, CO_2, was passed through a humidifier at 25 °C and entered the bubble column at a constant flow rate measured with a bubble flowmeter. Gas outflow through the top-plate outflow port was measured with another bubble flowmeter before its release into the atmosphere. The amount of CO_2 absorbed into of the solution was determined as the difference between inflow and outflow rates.

Results and Discussion

The volumetric gas-liquid mass-transfer coefficient k_La is one of the fundamental characteristics of gas-liquid reactors. The governing equation for absorption of slightly soluble gases in liquids, assuming constant diffusivity and. mass density can be written as:

$$\frac{\partial C}{\partial t} + (v \cdot \nabla) \cdot C = D\nabla^2 C \qquad (2)$$

where C is concentration of diffusing gas, t time, v is local velocity vector, ∇ is vector operator and D is the coefficient of diffusivity. The volumetric coefficient of liquid phase mass transfer is defined as:

$$\frac{dC}{dt} = k_L a \cdot \left(C - C^* \right) \tag{3}$$

where C* is the value of C in equilibrium. This method of evaluating k_La was based on three assumptions: 1.- The liquid phase was perfectly mixing, 2.- The driving potential for mass transfer was uniform throughout the column and 3.- Response of the CO_2 of the experimental method to a change of the dissolved CO_2 concentration was sufficiently fast. With the use of computer and the Visual Basic v 5.0 software, the learning algorithm and the Eqs. (2) and (3) were programmed. A part of the results of the identification model are shown in the Figs. 1 to 3.

For the space limitation, we selected four figures as the most important because in the Figure 1 are shown the comparisons between the k_La (experimental) and the k_La (calculated) to two height liquids in the rectangular column.

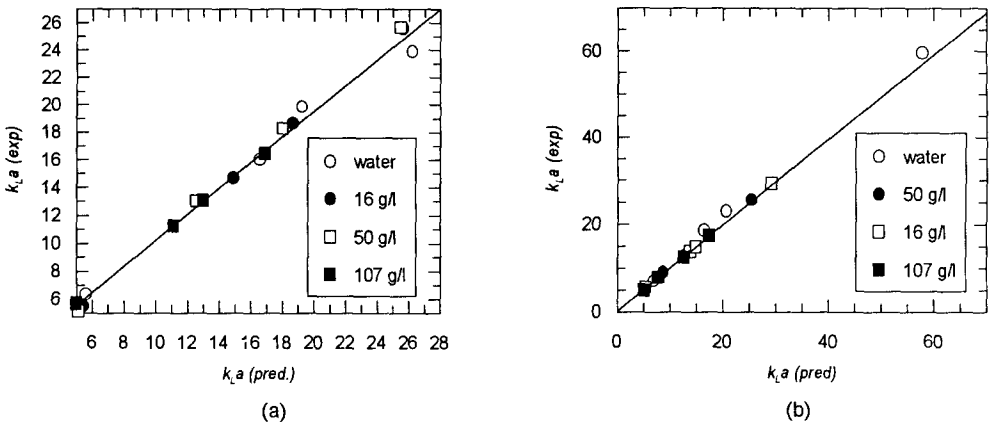

FIG. 1
Values of of k_La in the rectangular column to two liquid heights
(a) 0.70 m; (b) 0.96 m

The Figure 2 shows the result to a liquid height of 0.96 m but in the cylindrical column. The result of the Fig. 1 can be compared with the Fig. 2 and it permits to observe the influence of the geometry in the hydrodynamic and the absorption. Finally, the Figure 3 depicts the results of the CMC in the rectangular column and in the cylindrical column.

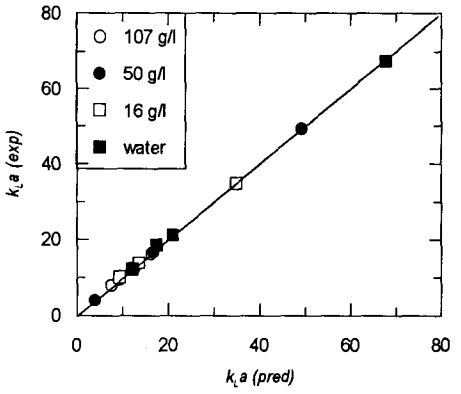

FIG. 2
Values of k_La in the cylindrical column. 0.96m of liquid height.

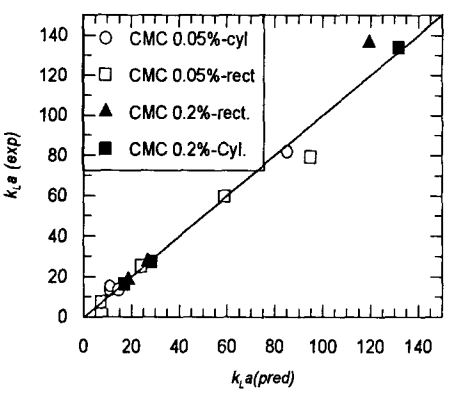

FIG. 3
Comparison of values of k_La in non-newtonian fluids

Even though the system is quite simple 500 learning step was used (with the experimental data). The k_La calculated using the neural network is better than the k_La using the correlations reported in the literature. The % error between experimental and calculated was of 1 % approximately, in the references of this paper and others literature not reported in this paper obtain a error > 4%. Owing to space limitation, no attempt to most details but is important to observe as the neural network with the pattern used can adapt to Newtonian and Non-Newtonian fluids.

Conclusion

This paper has demonstrated a large advance in concentration prediction in bubble columns using neural networks. For the simulation demonstrated, the identification performance is 50 times faster than previously established techniques. In this paper a pattern that search the relation of all the design parameters is proposed.

Nomenclature

ε_i	The back-propagated error value
C^*	Value of C in equilibrium
C	Concentration of diffusing gas

D	Coefficient of diffusivity
t	Time
v	Local velocity vector
ε_g	Hold-up,
V_L,	Liquid volume
f_g	Gas flow that input to the column

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