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Prediction of bubble size in Bubble columns using Artificial Neural Network

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Abstract

In the literature, several correlations have been proposed for bubble size prediction in bubble columns. However these correlations fail to predict bubble diameter over a wide range of conditions. Based on a data bank of around 230 measurements collected from the open literature, a correlation for bubble sizes in the homogenous region in bubble columns was derived using Artificial Neural Network (ANN) modeling. The bubble diameter was found to be a function of six parameters: gas velocity, column diameter, diameter of orifice, liquid density, liquid viscosity and liquid surface tension. Statistical analysis showed that the proposed correlation has an Average Absolute Relative Error (AARE) of 7.3 % and correlation coefficient of 92.2%. A comparison with selected correlations in the literature showed that the developed ANN correlation noticeably improved the prediction of bubble sizes. The developed correlation also shows better prediction over a wide range of operation parameters in bubble columns.

Introduction

The design and scale-up of bubble columns have gained considerable attention due to complex hydrodynamics and its influence on transport characteristics. Although the construction of these columns is simple, accurate and successful design and scale-up require an improved understanding of multiphase fluid dynamics and its influences. The design and scale- up of bubble column reactors generally depend on the quantification of three main phenomena;

(i) heat and mass transfer characteristics;
(ii) Mixing characteristics;
(iii) Chemical kinetics of the reacting system. Thus the reported studies emphasize the requirement of the multiphase fluid dynamics and its influence on phase hold up, mixing and transport properties (Degaleesan et al 2001). Scale –up problems basically stem from the scale dependency on the aforementioned phenomena. Scale –up methods used in biotechnology and chemical industry range from know-how based methods that are in turn based on empirical guidelines, scale –up rules and dimensional analysis to know why based approaches that begin with regime analysis. This analysis is hydrodynamics (Deckwer and Schumpe 1993). More specifically, in order to design bubble column reactors the following hydrodynamic parameters are required: specific gas-liquid interfacial area, axial dispersion coefficients of the gas and liquid , sauter mean bubble diameter, heat and mass transfer coefficient, gas hold up, physicochemical properties of the liquid medium. In order to estimate these design parameters for the system, experimental studies benefit from specialized measuring devices and accessories.

The fluid dynamic characterization of bubble column reactors has a significant effect on their operation and performance. Bubble populations, their hold up contributions and rise velocities have significant impact on altering the hydrodynamics, as well as heat and mass transfer coefficients. Many literature correlations are proposed to predict sizes of bubbles and most important ones are presented in Table (1).

The average bubble size in a bubble column has been found to be affected by gas velocity, liquid properties, gas distribution, operating pressure and column diameter (Kantarci et al 2005).

Since the early 80s, artificial neural networks (ANNs) have been used extensively in chemical engineering for such various applications as adaptive control, model based control, process monitoring, fault detection, dynamic modeling, and parameter (Bhat and McAvoy 1990). ANN provides a non-linear mapping between input and output variables and is also useful in providing cross- correlation among these variables. The mapping is performed by the use of processing elements and connection weights. The neural network is a useful tool in rapid predictions such as steady- state or transient process flow sheet simulations. Cai et al 1994 applied Kohonen self-organizing neural networks to identify flow regimes in horizontal air-water flow. Leib et al 1995 used a neural network model along with the mixed-cell model to predict slurry bubble column performance for the Fischer-Tropsch synthesis. Piche et al 2001, and Illuta et al 2002 used an ANN to improve the prediction of various hydrodynamic parameter in packed bed and fluidized bed reactors .Shaikh and Al- Dahhan 2003, Behkish et al 2005 used a Back Propagation Neural Network to predict the hold up bubble columns, while Al-Hemiri and Ahmedzeki 2008 used the same type of network to predict the heat transfer coefficient in bubble columns.

Building on these studies, the focus of this work is to develop a unified correlation for the bubble size prediction in the homogeneous region in bubble columns which can be useful for design engineers. This correlation is derived from the experimental data bank collected from the open literature.

Building ANN

ANNs are being applied to an increasing number of real-world problems of considerable complexity. It is a massively parallel distributed processor that has a natural propensity for storing experimental knowledge and making it available.

In the present work, a multilayer neural network has been used, as it is effective in finding complex non- linear relationships. Training was accomplished using NeuroSolutions by Excel version 5, supplied by NeuroDimension, Inc. copyright 1997-2005.

MLP (Multi-layer perceptron) is known as a supervised network because it requires a desired output in order to learn. The goal of this type of network is to create a model that correctly maps the input to the output using historical data so that the model can then be used to produce the output when the desired output is unknown. This type was used which is multilayered FeedForward Network (MLFF), trained with static back propagation (Bp) of error using the generalized Delta rule [MATLAB, 2003]. Bp was one of the first general techniques developed to train multi-layer networks, which does not have many of the inherent limitations of the earlier, single -layer neural nets. The Bp algorithm is an iterative gradient algorithm designed to minimize the mean-squared error between the desired output and the actual output for a particular input to the network [Lendaris, 2004]. Basically, Bp learning consists of two passes through the different layers of the network: a forward pass and backward pass. During the forward pass the synaptic weights of the network are all fixed. During the backward pass, on the other hand, the synaptic weights are all adjusted in accordance with an error-correction rule [Lippmann, 1987]. This algorithm may be found elsewhere [Lendaris, 2004].

Bp is easy to implement, and has been shown to produce relatively good results in many applications. It is capable of approximating arbitrary non-linear mappings. The success of Bp methods very much depends on problem specific parameter settings and on the topology of the network [Leonard 1990].

Training a Back-Propagation Network

The steps for back- propagation training can be shown as follows (Leonard, 1990):

1. Initialize the weights with small, random values.
2. Each input unit broadcasts its value to all of the hidden units.
3. Each hidden unit sums its input signals and applies its activation function to compute its output signal.
4. Each hidden unit sends its signal to the output units.
5. Each output unit sums its input signals and applies its activation function (hyperbolic tan in the present simulation)to compute its output signal.
6. Each-output unit updates its weights and bias.

Development of ANN based correlation

Database generation

Collecting of the data is the preliminary step for building ANN. In this model 230 experimental data points (for bubble diameter in the homogeneous region in bubble column) were collected from literature spanning the years (1956-2005). The source of data which is the past experimental work of different systems is given Table (2). Different geometries of bubble columns with various liquids (water, solutions of ethanol, buthanol, NaOH, and glycerol), were included in the data bank.

The input parameters to the network were selected from the most important parameters affecting bubble diameter. Therefore, six parameters were chosen as the input layer given in Table (3) with the range taken for each.

The output to the network (the desired parameter) is the bubble diameter for bubbles in the homogeneous region.

ANN Design

Training was accomplished using NeuroSolutions by Excel version 5, from NeuroDimension, Inc. copyright 1997-2005. Multilayered feedforward network. type was used and trained with static backpropagation of error. 75% of the collected data (230) was set for training and the rest is for testing. The ANN topology consists of three layers; the first is the input layer with six neurons (PEs) representing the six aforementioned parameters. The second consists of one or two hidden layers which is the varying part in this work , each with different number of neurons. The selection of the number of hidden layers and the number of neurons (perceptrons or PEs)in each hidden layer is the target for such research and it is troublesome. For the purpose of finding the best architecture of the network, the testing MSE, %AARE and the correlation coefficient (%R) which should be around unity, are calculated and compared for each topology and for each type of ANN. Testing is made for the 25% part of the collected data which are not seen by the network

The size of the mean square error (MSE) can be used to determine how well the network output fits the desired output, but it doesn't necessarily reflect whether the two sets of data move in the same direction. For instance, by simply scaling the network output, we can change the MSE without changing the directionality of the data. The correlation coefficient (R) solves this problem.

By comparing the results of ANN models, which have different number of PEs in each hidden layer, the optimal ANN structure has been obtained. All trials were made initially using a hyperbolic tangent (tanh) activation function, constant momentum rate (The acceleration parameter used to improve convergence) of 0.7 and 5000 number of iterations (how many times the network sees the whole data).

Results and Discussion

(i) One hidden layer

First trials were made using one hidden layer. The number of processing elements were changed using constant parameters of activation function of (tanh), momentum rate of (0.7) and 5000 iterations. Results for selected ANN structures of one hidden layer are listed for comparison in Table (4).

The number of processing elements in the hidden layer was plotted against MSE, correlation coefficient and %AARE. These relations are shown in Figures 1,2 and 3.

(ii) Two hidden layers

In order to find a better performance of the network, many topologies of two hidden layers were also examined. Different numbers of processing elements in each layer were applied and the results of MSE, %AARE and correlation coefficient were compared. Some selected structures are listed for comparison in Table (5).
By examining Table (5), it would be obvious that the performance of ANN structure using two hidden layers is improved in comparison with one hidden layer. The structure of [6-12-12-1] is found the best. Further investigation was made for the optimum ANN structure of [6-12-12-1] by changing the momentum rate. It was found that the momentum rate of 0.7 (by default) still gave the best performance for AAN model. Results are given in Table (6).

The numbers of processing elements in the second hidden layer were varied to see the effect on the performance of the network. Results given in Table (7), showed that [6-12-12-1] is the best structure among others.

Therefore, after careful training of the network, testing showed that ANN structure of [6-12-12-1] using the activation function of (tanh), momentum rate of 0.7 and after 5000 iterations, had correlated the bubble diameter in the homogenous region in bubble columns successfully. The result of prediction is plotted with experimental values as shown in Figs (4) and (5).
Statistical analysis based on the test data is calculated to validate the accuracy of the output for pervious correlation model based on ANN. The structure for each model should give the best output prediction, which is checked by using statistical analysis. Results are given in Table (8).
The proposed model of ANN was compared with literature correlations. These correlations showed poor agreement between the prediction and experimental bubble diameter values. Results are given in Table (9) and its graphical representation is shown in Fig (6). The problem facing ordinary correlation (when used for reproducing other experimental data) is that it is restricted to their systems and range of variables studied, leading to high percentage of error.
Artificial neural network had proved that it is powerful tool in solving complex non-linear relationships when ordinary correlations fail to simulate experimental data.

Table 1 Correlations for bubble size (Kantarci et al 2005)

Researcher	Correlation
Miller (1974)	$d_b = \left[\frac{6\sigma\, d_o}{g(\rho L - \rho g)}\right]^{1/3}$
Moo-Young and Blanch (1981)	$d_b = 0.19 d_o^{0.48}\, \mathrm{Re}_o^{0.32}$
Leibson et al (1956)	$d_b = 0.18 d_o^{1/2}\, \mathrm{Re}_o^{1/3}$
Kumar and Kuloor (1970)	$V_b = \left(\frac{4\pi}{3}\right)^{1/3}\left(\frac{15\mu Q}{2\rho L g}\right)^{3/4}$
Bhavaraju et al (1978)	$\frac{d_b}{d_o} = 3.23\left(\frac{4\rho Q}{\pi\,\mu\, d_o}\right)^{-0.1}\left(\frac{Q^2}{d_o^2 g}\right)^{0.21}$

Table 2 Database References.

No.	Researcher(s)	System
1	Van den Hangel (2005)	Air-water, d_T=0.052m, 0.02m.
2	Mews and Wiemann (2004)	Air-water , d_T=0.15m, perforated plate.
3	Hillmer (1993)	d_T=0.15m, d_o=0.003m,
4	Shah et al (1985)	Air-water and different concentrations of aqueous ethanol , d_T=0.1m, d_o=0.001m.
5	Miayhara (1983)	Air-water, d_T=0.05m, perforated plate.
6	Kumar et al (1976)	Air-water, kerosene, aqueous glycerol and 2N NAOH, d_T=0.01m,single orifice d_o=0.00153m and perforated plate.
7	Koide et al (1966)	Air-water, (53and 80% by vol.) glycerin d_T =0.15m, perforated plate.
8	Towell et al (1965)	Air-water, d_T= 0.406m ,perforated plate.
9	Tadakiet (1963)	d_T =0.01m, d_o=0.001m
10	Leibson et al (1956)	Air-water and aqueous butanol, d_T=0.2m, d_o=(0.0016-0.003)m.
11	Van Krevelen and Hoftijzer(1950)	Air-water, d_T= (0.02-0.06m), single orifice of different sizes.

Table 3 Range of the input parameters

	Parameter	Range
Input	Superficial velocity	0.00012- 0.01995 m/s
	Orifice diameter	0.000419 – 0.02m
	Column diameter	0.026-0.2 m
	Liquid density	787.2-1211 kg/m^3
	Liquid viscosity	0.00088-0.035 Pa.s
	Liquid surface tension	0.0745- 0.0072 N m
Output	Bubble diameter	0.00204 -0.00925 m

Table 4 Different ANN structures using one hidden layer.

Case	*ANN Structure*	*MSE*	*%AARE*	*%R*
1	6-4-1*	5.22 x 10^{-7}	12	75.8
2	6-8-1	6.35 x 10^{-7}	13.8	73.6
3	6-10-1	6.3 x 10^{-7}	13.1	73
4	6-12-1	5.19 x 10^{-7}	11.78	77
5	6-14-1	6.88 x 10^{-7}	13.9	71
6	6-16-1	7.38 x 10^{-7}	14.48	69.6
7	6-20-1	6.7 x 10^{-7}	13.4	70

* refers to the number of neurons in the [input- hidden-output] layer

Table 5 ANN structure using two hidden layers.

Case	ANN Structure	MSE	%AARE	%R
1	6-4-4-1	3.58E-7	10.8	86.8
2	6-8-8-1	2.6E-7	8.8	90.6
3	6-10-10-1	2.69E-7	8	90.3
4	***6-12-12-1***	***2.2E-7***	***7.3***	***92.2***
5	6-15-15-1	3.1E-7	9.1	88.7
6	6-25-25-1	3.55E-7	8.7	87

Table 6 Different momentum rates for the [6-12-12-1] ANN model

Momentum	MSE	%AARE	%R
0.5	3.29E-7	9.2	88
0.7	***2.2E-7***	***7.3***	***92.2***
0.8	3.03E-7	8.68	89
1.0	3.77E-7	9.88	86.5

Table 7 ANN structure with different PEs in the second hidden layer.

Case	ANN structure	MSE	%AARE	%R
1	6-12-4-1	2.65E-7	8.86	90.7
2	6-12-8-1	3.79E-7	8.7	86
3	***6-12-12-1***	***2.2E-7***	***7.3***	***92.2***
4	6-12-16-1	3.3E-7	9.03	88
5	6-12-20-1	3.3E-7	8.02	87.9

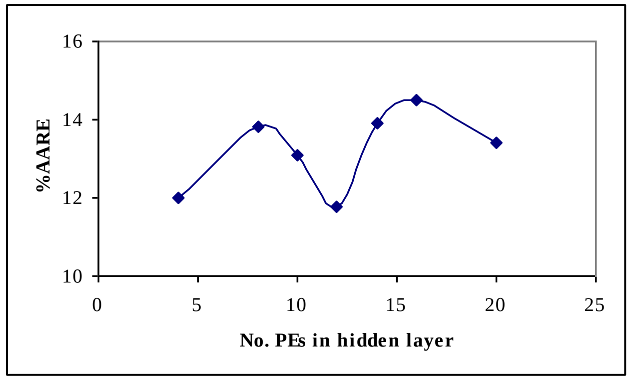

Fig.2 %AARE vs. No. of processing elements in hidden layer.

Table 8 Statistical analysis for the proposed model.

Performance	***db***
MSE	2.20721E-07
NMSE	0.151403968
MAE	0.000343427
Min Abs Error	9.19866E-06
Max Abs Error	0.001536108
R	0.92209016

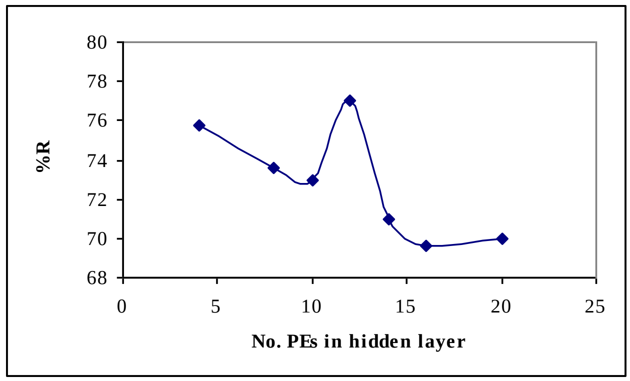

Fig.3 % R vs. No. of processing elements in hidden layer.

Table 9 Comparison the present results with previous work

Correlation	**AARE%**	**%R**
Miller(1974)	37	13.4
Moo-Young and Blanch(1981)	51	20
Bhavaraju et al (1978)	79	30
ANN(present study)	7.3	92.2

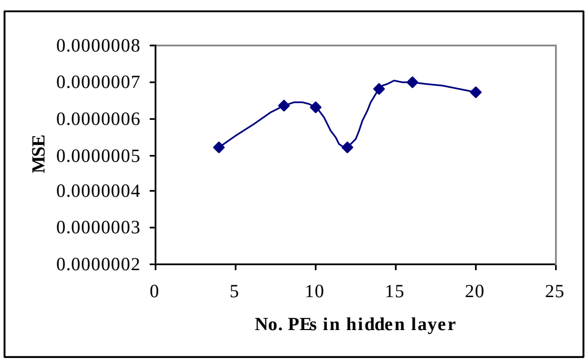

Fig.1 MSE vs. No. of processing elements in hidden layer.

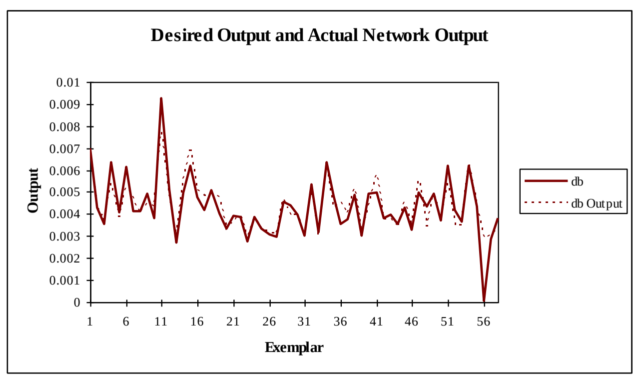

Fig.4 Desired (measured) and the actual (predicted) values vs. testing exemplars.

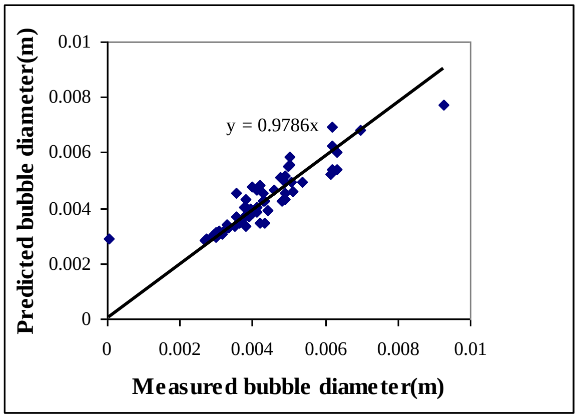

Fig.5 Predicted bubble diameter versus desired values for ANN structure of [6-12-12-1]

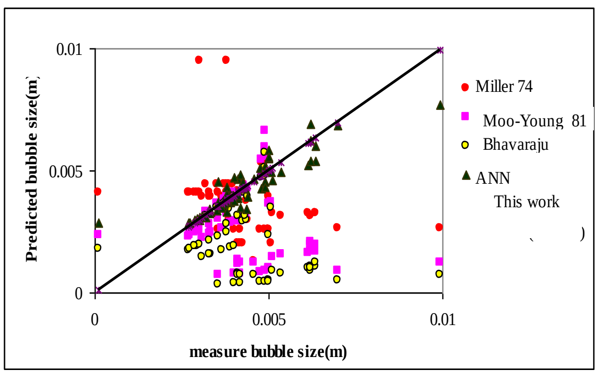

Fig.6 the predicted values by ANN with previous work.

Conclusions

From the present study of using ANN in predicting the bubble size in the homogenous region in bubble columns. It is concluded that ANN structure of [6-12-12-1] was chosen as the best to implement the target of the present study. MLP architecture of six inputs in the first layer (gas velocity, column diameter, diameter of orifice, liquid density, liquid viscosity and liquid surface tension) with 12 PEs in the 1st hidden layer and 12 PEs in the 2nd hidden layer, and one output in the third layer which is the desired output of bubble size. Momentum rule was 0.7, hyperbolic tan activation function, and 5000 numbers of iterations were used. ANN predicted well the diameter of bubbles which is better than those, obtained for the selected literature correlations; it yielded a minimum AARE of %7.3 and a correlation coefficient of 92.2%.

NOMENCALATURE

AARE: Average Absolute Relative Error.

$$AARE = \frac{1}{N}\sum_{1}^{N}\left|\frac{x_{prediction} - x_{experimental}}{x_{experimental}}\right|$$

Where: N, here, is the number of data points.
x is bubble diameter.

Bp : Back Propagation.
MAE : Mean absolute error.
Max Abs Error : Maximum absolute error.
Min Abs Error : Minimum absolute error.
MLFF : Multilayered FeedForward Network.
MLPs : Multi-layer perceptron.
ANN : Artificial Neural Network.
d b : Diameter of bubble(m).
MSE : Mean square error

$$MSE = \frac{1}{2p}\left[\sum_{p}\sum_{k}(d_k^p - o_k^p)^2\right]$$

Where p is the number of patterns in training set
k is the number of iterations.

d_k^p is the desired output.

o_k^p is the actual output.

NMSE : Normalized mean square error defined as:

$$NMSE = \frac{PN\ MSE}{\sum_{j=0}^{p}\frac{N\sum_{i=0}^{N} d^2_{ij} - (\sum_{i=0}^{N} d_{ij})^2}{N}}$$

Where P=No. output PEs
N=No. exemplars in the data set
MSE= Mean square error.
dij= Desired output for exemplar I at PEs j.

PEs : Processing elements (neurons).

R : The correlation coefficient

$$R = \frac{\sum_{i=1}^{N}(x_{experimental(i)} - \bar{x}_{experimental})(x_{prediction(i)} - \bar{x}_{prediction})}{\sqrt{\sum_{i=1}^{N}(x_{experimental} - \bar{x}_{experimental})^2}\sqrt{\sum_{i=1}^{N}(x_{prediction} - \bar{x}_{prediction})^2}}$$

$\bar{x}_{experimental}$: Bubble diameter mean of experimental points.

$\bar{x}_{prediction}$: Bubble diameter mean for prediction points.

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التنبؤ بقطر الفقاعات في الابراج الفقاعية ياستعمال الشبكة الاصطناعية الذكية

ندى سعدون احمد زكي / جامعة بغداد كلية الهندسة / قسم الهندسة الكيمياوية / بغداد / العراق.

الخلاصة:

يوجد في الادبيات المنشورة عدد من الموديلات الرياضية التي تستعمل للتنبؤ بقطر الفقاعات في عمود الفقاعات ولكن تفشل هذه الموديلات عند تطبيقها لمدى واسع من الظروف المختلفة. ولهذا وبالاستناد الى عدد من المعلومات (بحدود 230) جمعت من الادبيات المنشورة، تم الحصول على موديل لقطر الفقاعة في المنطقة المتجانسة للبرج الفقاعي باستعمال الشبكة الاصطناعية الذكية. تم انتخاب مجموعة عوامل مؤثرة وتم تصنيفها الى ستة مجاميع لغرض استعمالها كمدخلات الى الشبكة. هذه العوامل هي : سرعة الغاز وقطر العمود وقطر الثقوب وكثافة السائل ولزوجة السائل والشد السطحي للسائل. لقد اثبت التحليل الاحصائي ان للموديل نسبة الخطا % AARE تساوي 7.3 ومعامل ارتباط 92.2%. لقد تم المقارنة مع موديلات منتخبة في الادبيات وتبين بوضوح نجاح شبكة ال ANN في التنبؤء بقطر الفقاعات لمدى واسع من الظروف التشغيلية.