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Prediction of Gas Holdup in Bubble Columns Using Artificial Neural Network*

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Abstract A new correlation for the prediction of gas hold up in bubble columns was proposed based on an extensive experimental database set up from the literature published over last 30 years. The updated estimation method relying on artificial neural network, dimensional analysis and phenomenological approaches was used and the model prediction agreed with the experimental data with average relative error less than 10%.
Keywords bubble column, gas holdup, artificial neural network, correlations

1 INTRODUCTION

Bubble columns are very important gas-liquid reactors which are widely used in industry due to their high interfacial areas, high heat transfer and mass transfer rates, high liquid residence time, simple construction and low operating cost.

Gas holdup is one of most important parameters of hydrodynamics in bubble columns, it influences heat and mass transfer rates and reaction rate, and it is a key parameter in the design of bubble columns. There are many correlations for prediction of gas holdup in bubble columns reported in the literature[1]. However all the correlations are obtained under limited experimental conditions and it is very difficult to extrapolate the correlations to a wide range of operating conditions, physical properties and reactor structures. Hence, it is important to develop a general correlation for prediction of gas holdup in bubble columns under a wide range of conditions. The purpose of this research is to predict the gas holdup in bubble columns using neural network fitting based on back propagation model in artificial neural network.

2 GAS HOLD UP DATABASE

Table 1 describes the gas hold up database in terms of ranges of liquid properties, operation conditions and gas-liquid systems.

More than 3000 experimental data are collected from the literature published over last 30 years for different gas-liquid systems. A wide range of liquid and gas velocities, fluid physical properties, and column geometries is included.

Table 1 Description of bubble column database

Physical properties of fluids	Operating conditions	Dimensionless groups
$684\,\mathrm{kg\cdot m^{-3}} < \rho_L < 1462\,\mathrm{kg\cdot m^{-3}}$	$0.00128\,\mathrm{m\cdot s^{-1}} < u_G < 0.86865\,\mathrm{m\cdot s^{-1}}$	$0.078 < Re < 5.996\times10^4$
$0.00041\,\mathrm{Pa\cdot s} < \mu_L < 0.232\,\mathrm{Pa\cdot s}$	$0.1\,\mathrm{MPa} < p < 17\,\mathrm{MPa}$	$6.64\times10^{-17} < Fr < 0.513$
$0.0023\,\mathrm{N\cdot m^{-1}} < \sigma_L < 0.074\,\mathrm{N\cdot m^{-1}}$	$293\,\mathrm{K} < T < 356\,\mathrm{K}$	$6.635\times10^{-6} < We < 63.628$
$0.102\,\mathrm{kg\cdot m^{-3}} < \rho_G < 252.862\,\mathrm{kg\cdot m^{-3}}$	$0.045\,\mathrm{m} < D_c < 0.61\,\mathrm{m}$	$3.116\times10^{-7} < Ca < 0.04134$
$0.000013\,\mathrm{Pa\cdot s} < \mu_G < 0.012\,\mathrm{Pa\cdot s}$		$1.755\times10^{-11} < Mo < 0.1082$
		$275.411 < Bo < 124840.3$
		$4.47\times10^5 < Ga < 6.197\times10^{12}$
		$1.073\times10^{-8} < St < 0.297$
		$275.411 \times Eo < 124840.3$
		$0.007 < \varepsilon_G < 0.581$

Liquids tested: Dichloroethane, *n*-heptane, cyclohexane, *n*-octanol, Paratherm NF heat transfer fluid, ethanol/water(75/25,by mass), reaction solvent, isopar G, trichloroethylene, tetradecane, paraffin oil, carboxymethyl cellulose (0.7%, 1.1%, 1.6%, by mass), isopropanol (0.0, 0.01%, 0.2%, by volume), DEA/water/ETG (20%,40% ,60%, by volume), soltrol-130, 0.01, 0.02, 0.03, 0.05, $0.051\,\mathrm{mol\cdot L^{-1}}$ Na_2SO_4, $0.145\,\mathrm{mol\cdot L^{-1}}$ NaCl, $0.202\,\mathrm{mol\cdot L^{-1}}$ KCl, $0.037\,\mathrm{mol\cdot L^{-1}}$ $BaCl_2$

Gases used: N_2, H_2+N_2 (1:1, 5:1), H_2, He, Ar, CO_2, N_2/CO_2, Air

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3 ARTIFICIAL NEURAL NETWORK METHOD

Artificial neural network is a complex network system composed of many simple units connected with each other. It is widely used in many fields because of its many merits such as self-study, non-linear descriptive ability, *etc.* In chemical engineering, it has been successfully used in predicting the pressure drop, liquid holdup, mass transfer, and other properties in trickle flow reactors[2]. However, it has not been found in the literature for prediction of gas hold up in bubble columns with artificial neural network technology.

3.1 Force analysis

A force analysis was performed to identify the most meaningful forces that impact the gas hold up.

Plausible forces to be considered are as follows:

(a) gas inertial forces, scaling as

$$F_{i,\mathrm{G}} = \rho_{\mathrm{G}} u_{\mathrm{G}}^2 \tag{1}$$

(b) gas viscous forces, scaling as

$$F_{\mathrm{V,G}} = \frac{\mu_{\mathrm{G}} u_{\mathrm{G}}}{D_{\mathrm{c}}} \tag{2}$$

(c) liquid and gas gravitational forces, scaling as

$$F_{\mathrm{g,L}} = \rho_{\mathrm{L}} g D_{\mathrm{c}} \tag{3}$$

and

$$F_{\mathrm{g,G}} = \rho_{\mathrm{G}} g D_{\mathrm{c}} \tag{4}$$

respectively, and

(d) capillary force,

$$F_{\mathrm{C,L}} = \frac{\sigma_{\mathrm{L}}}{D_{\mathrm{c}}} \tag{5}$$

Dimensional analysis was used to search for the best set of dimensionless groups that would intervene in the final hold up correlations. A number of sets of dimensionless numbers were tested by trial and error method resulting in the most relevant groups listed in Table 1.

3.2 Neural regression

Three layer feed forward neural network models were designed (Fig. 1), using NNfit software[3] to derive the desired gas hold up correlations. The neural architectures are described by generic equation

$$\boldsymbol{H}_j = \frac{1}{1+\exp\left[-\sum_{i=1}^{I+1} \omega_{ij} \boldsymbol{U}_i\right]} \tag{6}$$

which correlates the network output, S_k, to sets of normalized input variables, $U_{i,k}$. In Eq. (6), $\boldsymbol{U}$ and $\boldsymbol{H}$ define the input and hidden layer vectors, $\boldsymbol{H}_{J+1}$ and $\boldsymbol{U}_{I+1}$ are the bias constants set equal to 1, ω_{ij} and ω_j are the weights or the fitting parameters of the neural network models and J is the number of the nodes in the hidden layer. The network fitting parameters are *a priori* unknown, and they have to be determined using a training algorithm by performing a nonlinear least-squares regression over known pseudo-random sets of input/outputs (70% of the database). The weights are set as to minimize the training error for the training set using a quadratic objective function minimized by the quasi-Newton-Broyden-Fletcher-Goldfarb-Shanno algorithm. A good measure for the extrapolation performance of a well trained neural network is given by the generalization error which should be comparable to the training error in the case of input/output not presented during the learning steps to the neural network (*i.e.*, 30% of the remaining data). For each of gas holdup parameter neural networks, the number of hidden neurons, J, was varied from 3—12. Hidden layers with 3 neurons were found to be the optimal neural architecture leading to the minimum average absolute relative errors and standard deviations for the training and generalization sets.

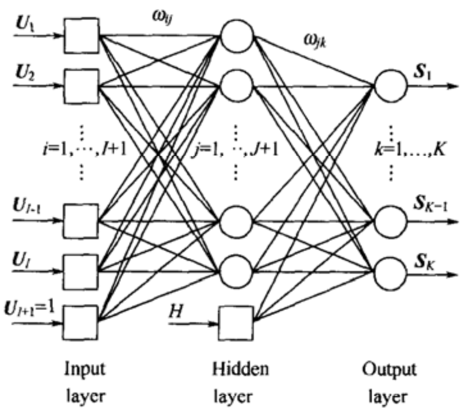

Figure 1 Architecture of the three-layer feed forward neural network

4 RESULTS AND DISCUSSION

Two, four and nine dimensionless parameter groups were employed as inputs using neural network technology respectively to correlate gas holdup, and three different models were obtained. Correlation coefficients, determination coefficients, average absolute relative error(AARE), standard deviation(SD), and ratio of data with error below 15% were used as criteria to compare the three models. The results are summarized in Table 2.

For nine dimensionless parameter groups as inputs, the complete sets of neural network equations for gas holdup are listed in Table 3, and Table 4 lists the fitted weights of each neural correlation.

Predicted *versus* experimental gas hold up is showed in Fig. 2(Fig. 2 does not include all the 3000 set data in the database since parameter of reactor diameter was not reported for some authors, so those data can not be considered for the purpose of regression). It can be seen that the proposed correlation predicted the experimental data well. 92.5% of experimental data *versus* predicted data fall in less than 15% error.

Six correlations reported in the literature[4] were used to predict data from two references[4,5]. The results (listed in Table 5) were compared to that of proposed model by this study. It is shown that a better fitisachievedbytheneuralnetworkcorrelation developed in this work.

The same seven correlations are applied to the total data bank (2174 set data), and the results are listed in Table 6. It is showed that our model has higher accuracy, small standard deviation, and can be applied to a wider range of data than the correlations reported in the literature . Thus, it is a correlation for prediction of gas holdup in bubble column that can be used more generally.

Table 2 Summarized results of different inputs number

	2 inputs	4 inputs	9 inputs
hidden nodes	4	12	11
weight numbers	17	73	122
correlation coeff.			
training group	0.838	0.892	0.946
generalization group	0.836	0.894	0.932
total data	0.836	0.892	0.943
determination coeff.			
training group	0.702	0.795	0.896
generalization group	0.698	0.794	0.869
total data	0.699	0.795	0.888
AARE			
training group	0.101	0.081	0.060
generalization group	0.103	0.095	0.066
total data	0.101	0.085	0.062
SD			
training group	0.162	0.106	0.065
generalization group	0.167	0.137	0.090
total data	0.164	0.115	0.073
ratio of error < 15%	0.817	0.872	0.925

Table 3 Set of equations for the neural network correlations

$$S=\frac{1}{1+\exp\left[-\sum_{j=1}^{J+1}\omega_j \boldsymbol{H}_j\right]},$$

$$\boldsymbol{H}_j=\frac{1}{1+\exp\left[-\sum_{i=1}^{I+1}\omega_{ij}\boldsymbol{U}_i\right]},\quad 1\leqslant j\leqslant J$$

$$S=\frac{\lg\varepsilon_G+2.155}{1.9191}$$

$$\boldsymbol{U}_1=\frac{\lg Re+1.107}{5.885},\quad \boldsymbol{U}_2=\frac{\lg Fr+5.0896}{4.799},$$

$$\boldsymbol{U}_3=\frac{\lg We+4.85183}{6.6555},\quad \boldsymbol{U}_4=\frac{\lg Ca+6.012}{4.628},$$

$$\boldsymbol{U}_5=\frac{\lg St+7.969}{7.443},\quad \boldsymbol{U}_6=\frac{\lg Mo+10.59}{9.625},$$

$$\boldsymbol{U}_7=\frac{\lg Bo-2.44}{2.656},\quad \boldsymbol{U}_8=\frac{\lg Ga-5.65}{7.14},$$

$$\boldsymbol{U}_9=\frac{\lg Eo-2.44}{2.656},\quad \boldsymbol{U}_{10}=1$$

Table 4 Fitting parameters of the neural network correlations for gas holdup

ω_{ij}	1	2	3	4	5	6	7	8	9	10	11
1	1.487	−1.217	0.857	−0.660	−2.286	−0.120	0.582	−2.236	−1.035	−3.527	−0.322
2	2.912	0.444	5.185	−0.902	−0.890	−2.389	0.865	−3.278	−0.230	7.209	0.345
3	1.922	2.364	−0.921	0.500	1.341	5.116	−0.077	−2.754	0.678	−4.487	1.000
4	0.277	0.201	1.061	−0.490	1.415	−2.905	0.263	−0.105	0.732	6.965	0.912
5	0.165	4.128	−4.092	0.841	5.142	5.696	−0.446	−0.643	2.212	−2.463	1.962
6	−3.099	−1.144	−1.405	−0.210	−2.945	−1.849	−0.958	−3.395	2.808	−3.071	1.901
7	−0.578	2.193	4.036	0.122	1.933	−1.447	0.476	−0.253	0.155	1.762	0.370
8	1.413	1.114	1.675	−0.015	2.721	−0.467	1.023	2.360	−1.380	2.674	−0.425
9	−0.653	2.175	3.981	0.076	1.881	−1.361	0.478	−0.331	0.180	1.817	0.356
10	−0.443	−2.068	−3.075	−0.387	−0.381	−1.779	0.405	0.301	0.922	−0.755	1.448

ω_{ij}	1	2	3	4	5	6	7	8	9	10	11	12
	1.659	−3.111	6.106	0.538	−3.880	5.365	0.672	−2.700	1.492	2.016	1.670	−5.911

Table 5(a) Comparison of different correlations *versus* data of Wilkinson *et al.*[4]

	Hikita[6] [1980]	Hammer[7] [1984]	Idogawa[8] [1985]	Reilly[9] [1986]	Idogawa[10] [1987]	Wilkingson[4] [1992]	This work
AARE, %	21.43	15.2	28.77	46.39	53.45	18.30	20.0
MRE, %	52.21	52.05	141.99	149.76	148.63	48.42	76.2
SD, %	69.97	11.34	23.5	31.49	40.58	13.59	17.82

Table 5(b) Comparison of different correlations *versus* data of Reilly *et al.*[5]

	Hikita[6] [1980]	Hammer[7] [1984]	Idogawa[8] [1985]	Idogawa[10] [1987]	Wilkingson[4] [1992]	Reilly[9] [1986]	This work
AARE, %	33.45	21.72	28.81	28.64	31.73	46.66	13.0
MRE, %	107.87	50.27	156.24	148.37	62.84	513.32	64.1
SD, %	5.87	13.51	21.07	23.79	16.38	67.99	10.48

Table 6 Comparison of different correlations versus experimental data

2174 set data	Hikita[6] [1980]	Hammer[7] [1984]	Idogawa[8] [1985]	Reilly[9] [1986]	Idogawa[10] [1987]	Wilkingson[4] [1992]	This work
AARE, %	0.272	0.246	0.355	0.619	0.501	0.254	0.062
MRE, %	2.706	3.349	6.971	11.126	4.999	2.569	0.995
SD, %	0.234	0.203	0.583	1.016	0.507	0.191	0.073

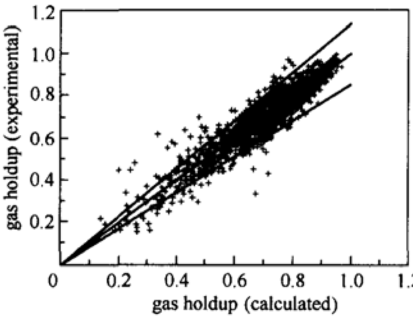

Figure 2 Predicted *versus* experimental gas hold up with 2174 sets of data

5 CLOSING REMARKS

Based on the largest gas-liquid gas holdup database available, a new correlation for prediction of gas holdup in bubble columns was derived with a combination of dimensional analysis and artificial neural networks. The overall results were a significant improvement in predicting the gas holdup in bubble columns. However it is worthy to note that although it is more accurate than some available correlations in literature, the model proposed here is basically a set of interpolation correlations. Hence it is suggested to verify *a priori* that conditions to be predicted fall within the range of the dimensionless groups shown in Table 1.

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NOMENCLATURE

Bo	Bond number ($Bo = gD_c^2\rho_L/\sigma_L$)
Ca	capillsrity number ($Ca = \mu_G u_G/\sigma_L$)
D_c	column diameter, m
Eo	Eoivos number $\{Eo = g\rho_L D_c^2\phi^2\varepsilon^2/[\sigma_L(1-\varepsilon^2)]\}$
Fr	Froude number ($Fr = u_G^2/gDc$)
g	gravity acceleration, m/s
Ga	Galileo number ($Ga = gD_c^3\rho_L^2/\mu_L^2$)
$\boldsymbol{H}$	hidden-layer vector
I, i	number of nodes in inputs
J, j	number of nodes in the hidden layer
K, k	number of nodes in outputs
MRE	maximum relative error
Mo	Morton number ($Mo = g\mu_L^4/(\rho_L\sigma_L^3)$)
p	operating pressure, MPa
Re	Reynolds number ($Re = \rho_G u_G D_c/\mu_G$)
$\boldsymbol{S}$	normalized output variable
St	Stokes number [$St = \mu_G u_G/(\rho_G g D_c^2)$]
T	temperature, K
U	normalized input variable
u_G	gas velocity, m·s^{-1}
We	Weber number ($We = u_G^2\rho_G Dc/\sigma_L$)
ε_G	gas hold up
ρ	density, kg·m^{-3}
μ	viscosity, Pa·s
σ	liquid surface tension, N·m^{-1}
ϕ	sphericity factor
ω	weights

Subscripts

L	liquid phase
G	gas phase
i	number of input
j	number of nodes in the hidden lay
k	number of output

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