DEVELOPING CORRELATION FOR PREDICTION OF GAS HOLDUP USING GENETIC ALGORITHM

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Abstract:

This paper deals with the prediction of the overall gas holdup ε_g in slurry bubble column depending on wide range of databank of around 69 measurements collected from the open literature. Correlation for gas holdup was derived using combination of dimensionless analysis and Genetic Algorithm. The correlation takes in consideration the physical properties of liquid and gas that effect on gas holdup and therefore effect on the design of slurry bubble column. Also a comparison between the correlation driven from Genetic Algorithm and a new correlation driven using Quasi-Newton method was made and found that the Average Absolute Relative Error (AARE) was 10.8 % and 16.1%, respectively. This shows that the use of Genetic Algorithm is improve the prediction of gas holdup in slurry bubble column.

Key Word: Genetic Algorithm, gas holdup, slurry bubble column.

تطوير علاقة للتنبؤ بمتغير التحميل الغازي باستخدام الخوارزمية الجينية

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الخلاصة:

يتعامل هذا البحث مع التنبأ بمعامل حجم الغاز إلى حجم الفراغ ε_g في مفاعل التفقيغ ذو الملاط بالاعتماد على حوالي ٦٩ تجربة عملية تم استخراجها من الأدبيات العلمية المرموقة. تم الحصول على علاقة لهذا التنبأ من خلال مزواجة الخوارزمية التطورية ومجاميع غير طولية . يأخذ هذا التنبأ بنظر الاعتبار الخواص الفيزياوية للغاز والسائل والتي تؤثر على معامل حجم الغاز الى حجم الفراغ ε_g والتي تؤثر فيما بعد على تصميم هذا النوع من المفاعل. تم إجراء مقارنة بين هذا التنبأ

وبين تنبأ أخر تم الحصول عليه بواسطة استخدام طريقة كيوسي- نيوتن لإيجاد علاقة رياضية وكانت نتيجة هذه المقارنة هو لصالح استخدام الطريقة الخوارزمية التطورية حيث حصلت هذه الطريقة على اقل معدل خطأ (١٠.٣ %) من الطريقة الأخرى (١٦.١ %). وهذا يبين مدى أهمية استخدام طريقة الخوارزمية التطورية.

Symbols used

a, b ,c, d, e and z	Constants.
Ar	Archimedes number,
Ca	Capillary no., ,
Cs	volumetric solid concentration, vol %,
d_b	Gas bubble diameter, m,
Eo	Eotvos number,
Fr	Froude number,
Mo	Morton number,
R	The cross-correlation coefficient,
Re	Reynolds no., ,
U_g	gas velocity, m/s,
ε_g	Gas holdup,
ρ_g	Gas density, $kg/m^{3,}$
μ_g	Gas viscosity, Pa.s,
ρ_L	Liquid density, kg/m^3,
σ_L	Liquid surface tension, N/m,
μ_L	Liquid viscosity, Pa.s,

Introduction

Slurry bubble column are widely used in chemical, biochemical, fuel and environmental engineering, and many industries. The use of slurry bubble column in industries is due to their simple construction, low operating cost and high – energy efficiency. Major important technology figures prominently in processes for converting natural gas to liquid fuels and light olefins using Fisher –Tropsch synthesis (Albijanic et.al. 2006). Bubble columns are an attractive reactors for various multiphase processes, especially for processes involving highly exothermic reactions. These reactors are operated in semi-batched or continuous mode. For this reason, the hydrodynamics of such reactors are controlled mainly by the gas flow. Overall gas holdup is one of the important parameter for slurry bubble column design and scale up. It is defined as the fraction of the reactor dynamic volume occupied by the gas (Mouza et. al. 2005). The behavior of gas holdup has been attributed to many different factors, including the physical properties of gas/liquid/solid phase, gas velocity, and solid loading (Shah, 1979). Albijanic et. al. (2006), studied the gas holdup in slurry bubble column reactor operated with diluted solution of alcohols and developed a correlation depends on physical properties of liquid such as viscosity and density and surface tension. Ruthiya (2005) studied the gas holdup in slurry bubble column especially the influence of particles on gas holdup and found that the rate of decrease of gas holdup with increasing slurry concentration in the heterogeneous regime lower compared to the rate of decrease of gas holdup in the transition regime. Mouza et. al.(2005) gave a new correlation based on dimensionless groups(Fr, Ar and Eo) for the prediction of gas holdup in the homogeneous regain. Also he found that the viscosity have an influence on bubble coalescence and hinders breakage. Also he found that an increasing of surface tension increase bubble formation by promoting breakage and demoting coalescence. Shaikh et. al. (2003) studied the gas holdup in slurry bubble column and gave a correlation using Artificial Neural Network to predict the gas holdup using dimensionless groups (Re, Fr, Eo, and Mo). The correlation has the lowest AARE when they compared to selected correlations. Ruzicka et.al. (2003) studied the effect of viscosity on gas holdup, and found that the gas holdup decrease with increasing viscosity. Vendu and Krishna (2003) studied gas holdup in slurry bubble column for air/ethanol system with three different concentrations. They found that the increasing of solid concentration tends to decrease gas holdup. This decrease due to the increase of coalescence of small bubbles to form larger bubbles. Shirsat et. al. (2003) observed that as the effective column height increases, the gas holdup also increases due to the increase in the residence time of the bubbles in the contactor. Michele et. al. (2000) used CFD method to predict gas holdup depending on superficial gas velocity solid loading and sparger geometry. DeSwart et.al. (1996) studied the hydrodynamics of slurry bubble columns, and found that increasing slurry concentration reduces the total gas holdup and this reduction is to be largely attributed to the destruction of the small bubble population which have bubble diameters smallest than 10 mm. Increasing slurry concentration increases the size and distribution of the large bubbles.

Artificial techniques brought a new sight to the characterization of gas holdup in slurry bubble column. To the best of our knowledge, the pioneer of the use of these techniques is Shaikh et.al.(2003) and Behkish (2004), both authors used back propagation neural network for prediction of gas holdup.

However, correlations still keep the lock of experimental data. Proper functions require significant computational effort when they are nonlinear and involve large number of parameters. For this reason, Genetic Algorithms bring efficient solutions by avoiding local minima. Moreover, it improves the robustness toward the uncertainties on the correlation coefficients, due to their adaptive and stochastic aspects.

The main object of this study is to predicate the gas holdup using the Genetic Algorithm techniques which is done using Statistica 7 from StatSoft, Inc., and a comparison between the above correlation and another correlation done using another method (Quasi- Newton) was done.

Genetic Algorithms

Genetic algorithm is a particular class of evolutionary algorithms, which are adaptive search techniques for approximating solutions of optimization and prediction problems. They are based on a biological metaphor which simulates processes in natural systems that are necessary for evolution, specifically those that follow the principles first proposed by Charles Darwin of the survival of the fittest. As such, they represent an intelligent exploitation of a random search within a defined search space to solve a problem. A population of abstract representations (chromosomes) of solution candidates (individuals) for an optimization problem evolves toward better solutions. Traditionally, solutions are represented in binary systems as an array of bits, but different encodings are also possible, such as integer or real encodings. The evolution begins from a population of completely random individuals (initialization) and happens in generations. In each generation, the fitness of the whole population is evaluated. Multiple individuals are stochastically selected (selection) from the current population according to their fitness, and mutated (mutation) or recombined (crossover) to form a new population (reproduction). The latter is then used in the next iteration. The algorithm stops when a solution is found satisfying minimum criteria or when a fixed number of iterations are reached. When applying genetic algorithm, one has to define at least a genetic representation of the solution domain (encoding) and at the same time a fitness function to evaluate the defined solution domain. In other words, one needs to fix the encoding of the solution as an array of bits, integers or floats in such a way that their parts are easily aligned due to their fixed size. Besides, at the encoding stage, one has to take into account the crossover and mutation operator complexity, which depends on the solution representation. Indeed, in some situations, in addition to problems associated with encoding and with evaluation definitions, one can face the problem of the definition of crossover and mutation operators in order to keep the validity of the solution. Furthermore, the fitness function has to be defined over the genetic representation in order to measure the quality of the represented solution. The fitness function is always problem dependent (Melanie, 1998).

Once the genetic representation of the solution is known and the corresponding fitness function is defined, the genetic algorithm starts initializing a population of solutions randomly. Then the algorithm improves it by repetitive applications of crossover, mutation and selection operators **Figure (1).**

1. Collection of Data

A set of 69 experimental data of different systems were collected from literatures for different workers. The data collected for slurry bubble column reactor operated with different liquids and different slurry concentration. Table (1) summarizes the sources of data.

The physical properties such as density, surface tension and viscosity were included in the data base. Most of slurry bubble column are operated with low liquid velocities, which have been reported to have little or no effect on over all gas holdup (Shetty et. al. 1992), so it is not included in the correlation.

2. Dimensionless Groups

Most of workers on slurry bubble column reactors predicted the gas holdup using correlations based on dimensionless groups. The following criteria guide was used to choose the input dimensionless groups:

a. The dimensionless groups should be as few as possible.

b. Each group should be highly cross-correlated to the output parameter.

c. The input groups should be weakly cross-correlated to each other.

So in this study Reynolds number, densities of gas to liquid ratio, viscosities of gas to liquid ratio, volumetric solid concentration, and finally the Capillary number (which were used by (Hikita et. al., 1988) and (Zou et. al., 1988)), where used to predict gas holdup in our work.

3. Statistical Analysis

The statistical analysis of prediction results is based on the following criteria:

a. The average absolute relative error (ARRE) should be minimum.

$$AARE = \frac{1}{N}\sum_{1}^{N}\left|\frac{y_{pred.} - y_{\exp.}}{y_{\exp.}}\right| \qquad ①$$

b. The cross-correlation coefficient, R between input and output should be around unity.

$$R = \frac{\sum_{1}^{N}\left(y_{\exp.} - y_{\exp.(mean)}\right) - \left(y_{pred.} - y_{pred.(mean)}\right)}{\sqrt{\sum_{1}^{N}\left(y_{\exp.} - y_{\exp.(mean)}\right)^2}\sqrt{\sum_{1}^{N}\left(y_{pred.} - y_{pred.(mean)}\right)^2}} \qquad ②$$

Results and Desiccation

a. Gas holdup Prediction Using Genetic Algorithm

Using the Statistica Neural Network 7 (SNN) a correlation has been developed to predicate the gas holdup by applying the 69 experimental data point collected (section 4), putting the population at 100, generations at 100 and mutation rate at 0.1 as shown in **Figure (2)**. **Table (2)** shows the minimum and maximum of dimensionless groups used.

Table (3) shows the model summary used to predict the gas holdup using SNN. The final predicted gas holdup has been drawn against the experimental gas holdup **Figure (3)**.

b. Gas holdup Prediction Using Quasi- Newton Method

Using the Statistica 99 and Quasi-Newton method (QN) a correlation has developed to predicate the gas holdup by applying the 69 experimental data point collected using the following form:

$$\varepsilon_g = a + \mathrm{Re}^b + \left(\frac{\rho_g}{\rho_L}\right)^c + \left(\frac{\mu_g}{\mu_L}\right)^d + \mathrm{Cv}^e + \mathrm{Ca}^z \qquad ③$$

The result from the program is shown below **Table (4)**.

The equation 3 will be:

$$\varepsilon_g = -6.09 + \mathrm{Re}^{0.0837} + \left(\frac{\rho_g}{\rho_L}\right)^{-0.168} + \left(\frac{\mu_g}{\mu_L}\right)^{0.189} + \mathrm{Cv}^{-0.0189} + \mathrm{Ca}^{-0.015} \quad ④$$

Figure (4) shows the relation between the experimental and predicated gas holdup using the QN method.

Comparing between the correlations obtained using SNN and QN are shown in **Figure (5)**, which leads to conclude that Genetic Algorithm is more accurate than Quasi-Newton method. Moreover the comparing between these correlations on statistical analysis basis leads to above the conclusions. **Table (5)** shows the mentioned comparing.

Conclusions

In this paper, a new presentation of predicating gas holdup in slurry bubble column was made using Genetic Algorithm and this correlation was compared with a correlation obtained using Quasi-Newton method. This comparing leads to one conclusion that using Genetic Algorithm is better than using of empirical correlations by means of results of statistical analysis done her. This work identified Reynolds number, gas to liquid densities ratio, gas to liquid viscosities ratio, volumetric solid concentration and Capillary number as expressive dimensionless groups to predicate the gas holdup in slurry bubble columns. Hence the developed Genetic Algorithm correlation should be useful in the scale up of slurry bubble columns.

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Table (1) Data sources of experimental points

No.	Reference	System	No. of Exp.
1	Koop et.al. (2004)	Air/paraffin oil/Alumina catalyst	43
2	Vendu and Krishna (2003)	Air/Ethanol/Raney cobalt catalyst	26

Table (2) Maximum and minimum for dimensionless groups.

Variable	Reynolds No.	Density Ratio	Viscosity Ratio	Volumetric Solid Concentration	Capillary No.	Gas holdup
Maximum	2.485	0.002	0.013	0.25	3469.56	0.229
Minimum	0.016	0.0016	0.002	0.01	25.03	0.014
Mean	0.8293	0.0017	0.0061	0.0996	640.8	0.1025

Table (3) Model summary of genetic algorithm.

Profile	Train error	Input	Hidden (1)	Hidden (2)	Output
5:5-6-1:1	0.02965	5	6	0	1

Table (4) The result of using QN method.

Parameter	a	b	c	d	e	z
Estimated	-6.09	0.0837	-0.168	0.189	-0.0189	-0.015

Table (5) Comparing between SNN & QN methods.

Correlations	AARE %	R
SNN	10.8	0.988
QN	16.1	0.977

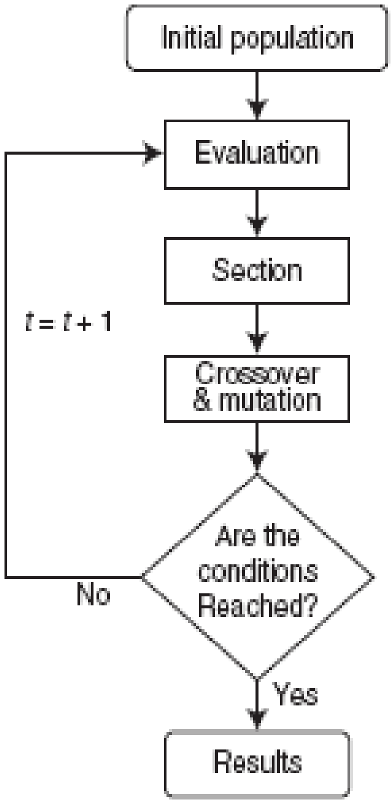

Figure (1), Genetic Algorithm block diagram

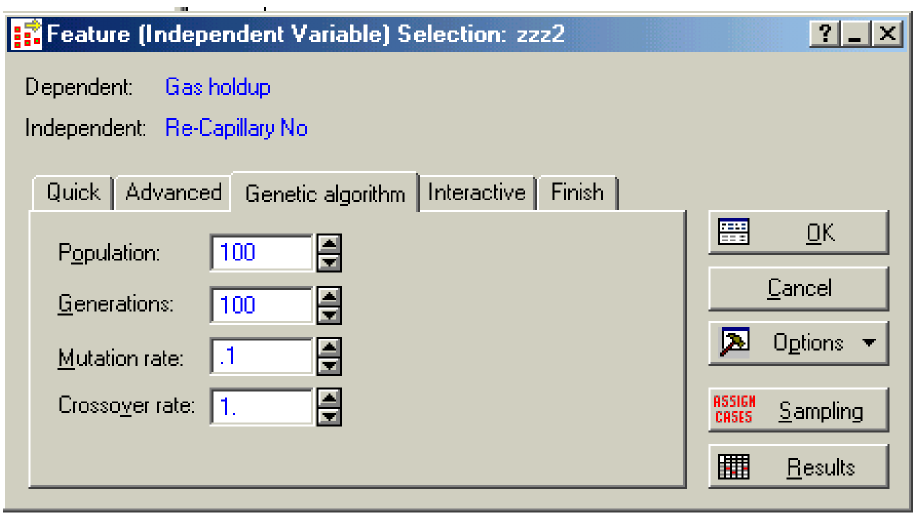

Figure (2), Dialog box used in SNN.

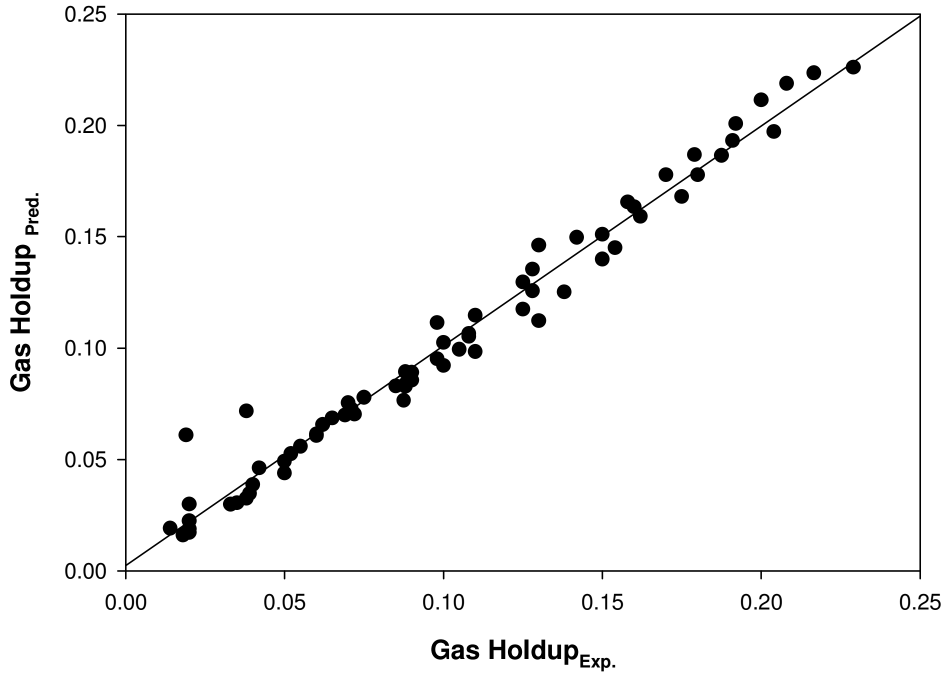

Figure (3), Experimental gas holdup verses predicated gas holdup using SNN.

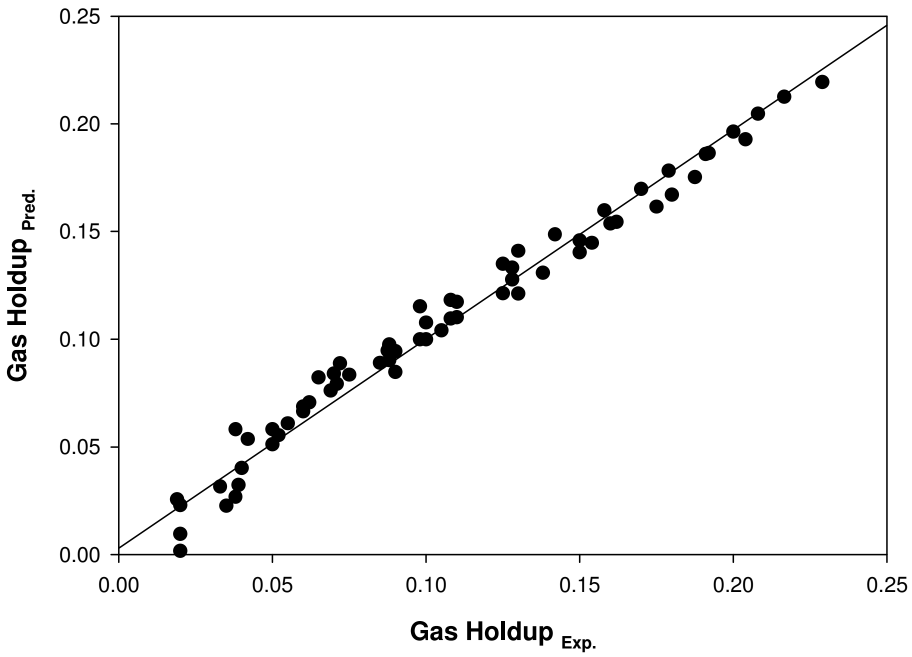

Figure (4), Experimental gas holdup verses predicated gas holdup using QN

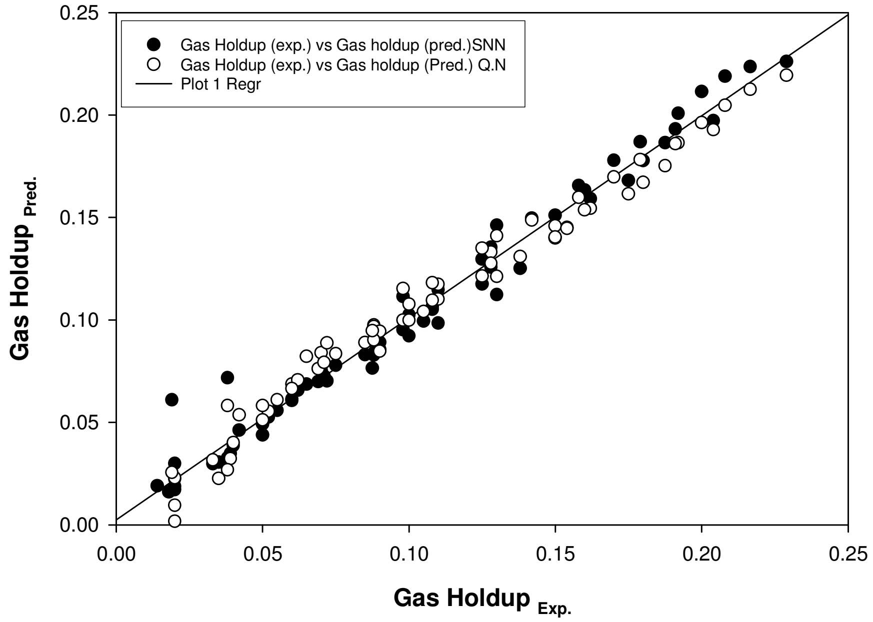

Figure (5), Experimental gas holdup verses predicated gas holdup using SNN & QN.