Application of New Inflection Point Method
for Hydrodynamics Study in Slurry Bubble Column Reactors

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ABSTRACT: *Bubble column reactors are used in a wide variety of applications such as multiphase bioreactors, catalytic slurry reactors, and absorption processes. The superficial gas velocity-gas holdup relationship and transition point are two important parameters for characterizing the hydrodynamics of a bubble column reactor. In this study, systematic investigation of a nitrogen - water - glass beads bubble column was conducted using the Taguchi experimental design method. The L_{16} (45) orthogonal array was selected for experiments design. Results showed that the order of importance of parameters is as follows: bed porosity, the ratio of height to diameter, and superficial gas velocity. A novel mathematical model was developed using the experimental data and based on 4th order polynomial. This model was successfully used to obtain the transition point with a high accuracy. The results of the mathematical method were in close agreement with those of the drift flux method. For liquid level of H=12D and slurry content of 13 vol%, transition velocity of 2.98 cm/s was calculated using the presented method, while a velocity of 3.14 cm/s was obtained from the drift flux method.*

KEY WORDS: *Bubble column, Slurries, Mathematical modeling, Hydrodynamics, Inflection point, Taguchi method.*

INTRODUCTION

Proper design and scale-up of Slurry Bubble Column Reactors (SBCRs) depend largely on the accurate prediction of the gas holdup and flow regime transition point. For example, mass and heat transfer coefficients depend strongly on the local fluid dynamics and are mostly calculated using correlations in which gas holdup plays an important role. Many correlations have been proposed to determine the transition point and the relation between gas holdup and superficial gas velocity. However, these methods are not accurate for certain liquids and are not applicable for both homogeneous and heterogeneous flow regimes. The main purpose of this work is

to introduce a novel mathematical model to determine transition point independent of the liquid type and properties.

Conventional correlations

Gas holdup in slurry bubble columns depends mainly on gas velocity. There are many correlations in literature to quantify this relation [1-3]. Some of these correlations contain a transitional gas holdup at a corresponding transitional superficial gas velocity to describe the dependence of gas holdup to superficial gas velocity.

Various empirical methods have been used to determine the flow regime transition. Dynamic Gas Disengagement (DGD) method and change in the liquid height due to induced gas bubbles are used to determine flow regimes [4]. In both methods, the plotted gas holdup against the superficial gas velocity graph exhibits either an extremum or a significant break-up which is considered as the transition point. These two methods do not clearly show the transition.

The drift-flux model is a widely accepted method for analyzing gas holdup in bubble columns. It was first proposed by *Richardson & Zaki* (1954) by plotting $u_b.\varepsilon_g(1-\varepsilon_g)^{2.39}$ against ε_g [5]. A change in the flow pattern was designated by a change of slope in the curve. *Zuber & Findlay* (1965) modified the classic drift flux theory for the heterogeneous regimes by plotting U_g/ε_g against $(U_g + U_l)$ [6]. Flow patterns can be correctly identified in water but in some liquids such as water/butanol borders between regimes are less clear [7]. Drift-flux analysis of *Wallis* (1969) consists of plotting $U_g (1-\varepsilon_g)$ against ε_g for the homogeneous regime [8]. Generally, these methods suffer from a lack of accuracy because the differences between slopes are very small when the transition occurs.

Dependence of the gas holdup on the superficial gas velocity can be expressed by the following power-law expression [8]:

$$\varepsilon_g = aU_g^n \tag{1}$$

Initially, the gas holdup seems to increase sharply and almost linearly with the superficial gas velocity in the homogeneous flow regime where the exponent n in Eq. (1) is generally reported to be in the range of 0.7-1.2 [3,9,10]. The gas holdup then reaches a maximum where the transition from homogeneous to heterogeneous flow regime occurs, and consequently a non-linear increase

with the superficial gas velocity beyond that point is observed. The exponent n in the heterogeneous flow regime is reported to be in the range of 0.4-0.7 [9, 10]. The range of the exponent n in Eq. (1) suggests that the effect of superficial gas velocity on gas holdup in both homogeneous and heterogeneous flow regimes depends strongly on the operation variables, physical properties of the system, as well as the design characteristics of the column.

Moshtari et al. (2009) found that Eq. (1) for a system of water and air is as follows [11]:

$$\varepsilon_g = 0.45U_g^{0.954} \qquad \text{Homogeneous flow regime} \tag{2}$$

$$\varepsilon_g = 1.335U_g^{0.449} \qquad \text{Heterogeneous flow regime} \tag{3}$$

Ivan et al. (2009) introduced a simple correlation to predict the gas holdup, liquid circulation time, down comer liquid velocity and volumetric mass transfer coefficient in dilute alcohol solutions (CN wt %) in bubble columns and draft tube airlift reactors with a single orifice sparger as [12]:

$$Y = P_1 U_g^{P_2} \left(1 + C_N\right)^{P_3} \tag{4}$$

Where, Y represents the gas holdup and $P_1 = 1.58$, $P_2 = 0.86$ and $P_3 = 0.18$

Taguchi method

Taguchi method is a powerful tool for determining the optimum test criteria. It assumes that engineering optimization contains three phases: system design, parameter design and parameters variation design. The method uses orthogonal arrays to obtain acceptable results with a smaller number of experiments. One of the important advantages of Taguchi method is analysis of qualitative and discrete factors. The most important step in Taguchi design method is to choose control parameters. Appropriate orthogonal array would then be selected based on the selected factors and their levels, and the experiments would be performed according to the proposed array [13-15]. The next step is the analysis of variance (ANOVA) on the experimental data. This method helps to determine the influence of different parameters and their contributions on the experimental results. Moreover, this method presents the optimum experimental conditions and predicts the results based on the desired criteria [16].

EXPERIMENTAL SECTION

The bubble column was composed of three Pyrex® cylindrical sections (D=15cm, H= 80 cm) that were joined by aluminum flanges. Gas holdup was calculated using manometer pressure drop data. Fig. 1 represents schematic of measurement set up.

According to Fig. 1, pressure is equal in two arms of manometer. Then we have the following equations.

$$Patm + \rho_D g \hat{z}_1 + \rho_L g (h_1 - \hat{z}_1) = \tag{5}$$

$$Patm + \rho_L g \hat{z}_2 + \rho_L g (h_2 - \hat{z}_2) + \rho_m g (h_1 - h_2)$$

$$\rho_D \hat{z}_1 + \rho_L h_1 - \rho_L \hat{z}_1 = \tag{6}$$

$$\rho_D \hat{z}_2 + \rho_L h_2 - \rho_L \hat{z}_2 + \rho_m (h_1 - h_2)$$

$$(\rho_D - \rho_L) \hat{z}_1 = \tag{7}$$

$$(\rho_D - \rho_L) \hat{z}_2 + \rho_L (h_2 - h_1) + \rho_m (h_2 - h_1)$$

$$(\rho_D - \rho_L)(\hat{z}_1 - \hat{z}_2) = \tag{8}$$

$$\rho_L (h_2 - h_1) - \rho_m (h_2 - h_1)$$

$$(\rho_L - \rho_D) d\hat{z} = -(\rho_L - \rho_m) dh_m \tag{9}$$

$$\frac{dh_m}{d\hat{z}} = \frac{\rho_L - \rho_D}{\rho_m - \rho_L} \tag{10}$$

For the term ρ_D we have the Eq. (11).

$$\rho_D = \rho_L (1 - \varepsilon) + \rho_G \varepsilon \tag{11}$$

Form Eqs. (10) and (11) we have the Eqs. (12) and (13).

$$\frac{dh_m}{d\hat{z}} = \frac{\rho_L - \rho_G}{\rho_m - \rho_L} \tag{12}$$

$$\varepsilon = \frac{\rho_m - \rho_L}{\rho_L - \rho_G} \frac{dh_m}{d\hat{z}} \tag{13}$$

According to Eq. (13), it's the accuracy of measuring dh_m that determines the accuracy of Eq. (13). In this method, the error is calculated from the resolution of the manometer ruler (1mm). Then the error of measuring gas holdup would be 0.1%.

Manometer connections were provided at four different heights along the column. The bottom segment was attached to a chamber that contained gas inlet and drain valve (Fig. 2).
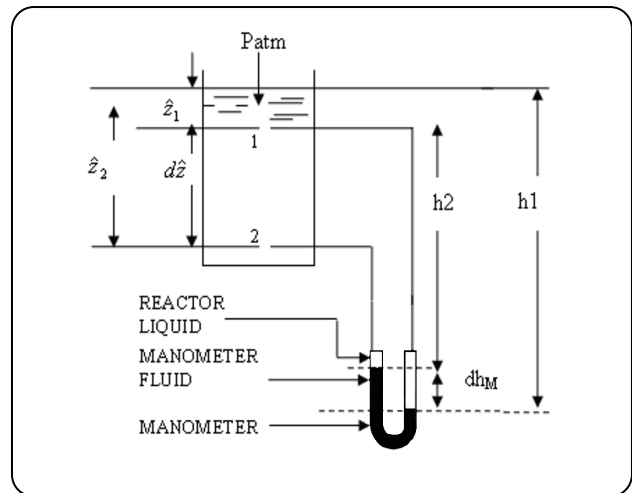

Fig. 1: Schematic of U- shaped manometer.

A sintered glass gas sparger was used in this chamber. According to the Fig. 2 nitrogen gas after passing the inlet valve enters the hopper shaped space under the sintered glass plate and after passing this plate enters the bubble column in the bubble form. The column was loaded with small glass beads as the solid phase. Table 1 shows size distribution of the glass beads. All experiments were carried out with distilled water and nitrogen gas at the ambient pressure and temperature (1 bar, 295 K). The gas was delivered through a regulator and two calibrated rotameters for low and high ranges of the gas flow rate. The error of measuring Ug with the typical values of up to 5cm/s is 2.8%. Pressure differences were taken at different liquid heights.

Three main factors namely solid content, superficial gas velocity and column height to diameter ratio were studied in order to investigate the gas holdup and the regime transition point.

RESULTS AND DISCUSSION

Experiments were conducted in two stages. In the first stage, Taguchi's method of experimental design was employed to obtain importance of the parameters, as well as their optimum values. Next, a new mathematical model was used to obtain the transition gas holdup, transition superficial gas velocity, and their analyzing.

Design of experiments
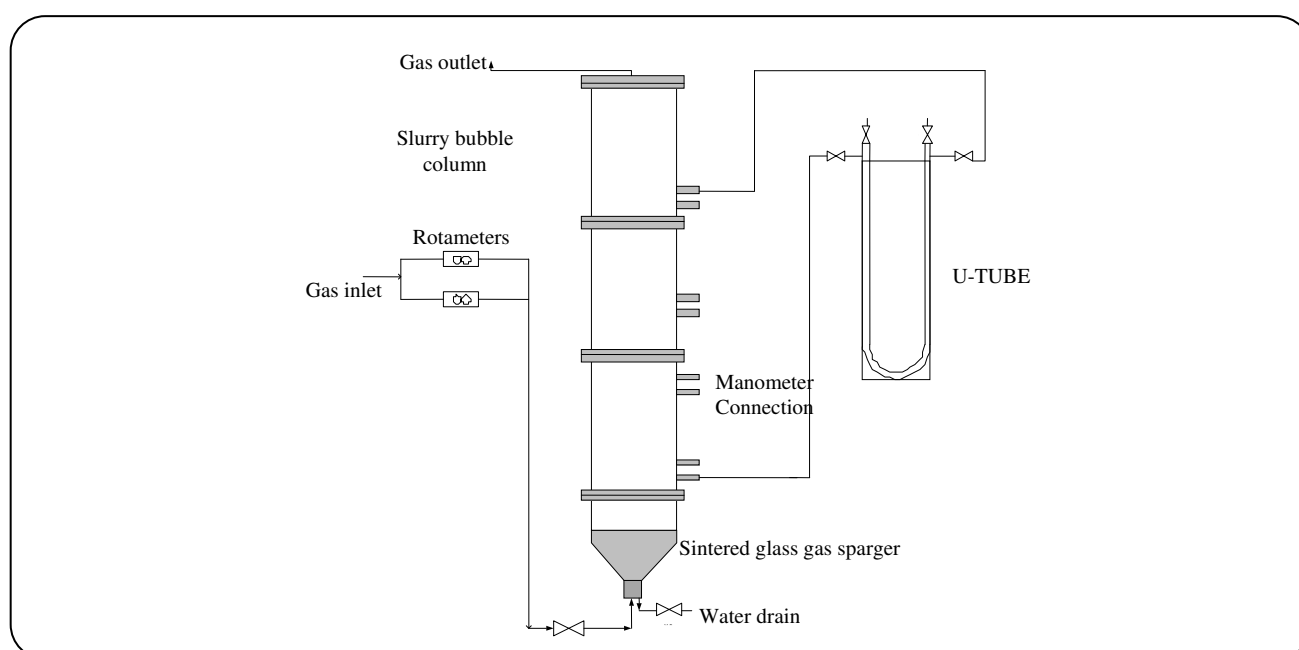*Experiment design for the first section*

Three main factors were considered, as mentioned before. These factors and their levels are presented in Table 2.

Table 1: Glass Beads Size Distribution.

Particle Size(μ_m)	Weight Percent
75 < dp<150	82.1
63 < dp<75	12.8
45 < dp<63	5.1

Table 2: Parameters & Levels- 1st Design

Parameter	L_1	L_2	L_3	L_4
ε_s	0	0.13	-	-
H/D	8	10	12	-
U_g (cm/s)	0.853	1.792	2.73	3.14

Fig.2. Schematic of experimental set up.

A L16 (45) orthogonal array was selected by applying the Taguchi method. Upgrading and downgrading methods were used to make the array appropriate for the case study of this work. The final orthogonal array with the desired levels is presented in Table 3. The experiments were performed according to the rows in Table 3 and the results are presented in the last column of this table. The main effects were obtained and presented in Table 4. It can be concluded from Table 4 that the solid content is the most effective factor and that the superficial gas velocity and H/D are the next important parameters respectively. From the analysis of variance (Table 5),

contribution of each factor was determined separately. The experimental error was about 6%, which is in the acceptable range of less than 15% [16].

Experimental design for second section

For the second section, the factors and their levels were the same as the previous design, but the superficial gas velocity was studied at eight levels. The new configuration of factors and their levels are presented in Table 6.

Like the previous design a L_{16} (45) orthogonal array was selected and the method of upgrading and

Table 3: L_{16} (45) Orthogonal array- 1st design.

L_{16}	1	2	3	4	5	Result
1	1	1	1	0	0	0.0313
2	1	2	2	0	0	0.087
3	1	3	3	0	0	0.114
4	1	1	4	0	0	0.204
5	2	1	3	0	0	0.066
6	2	2	4	0	0	0.101
7	2	3	1	0	0	0
8	2	1	2	0	0	0.0139
9	1	1	3	0	0	0.148
10	1	2	4	0	0	0.219
11	1	3	1	0	0	0.043
12	1	1	2	0	0	0.0941
13	2	1	4	0	0	0.115
14	2	2	3	0	0	0.073
15	2	3	2	0	0	0.01
16	2	1	1	0	0	0

Table 4: Main effects - 1st design.

	L_1	L_2	L_3	L_4	ΔL
ε_s	0.11755	0.047363			0.070188
H/D	0.084038	0.12	0.04175		0.07825
U_g	0.018575	0.05125	0.10025	0.15975	0.141175

Table 5: Analysis of variance - 1st design.

Parameter	f_i	SS_i	V_i	SS'_i	P (%)
ε_s	1	0.106777	0.106777	0.106777	36.57995
H/D	2	0.103866	0.051933	0.103866	35.58273
U_g	3	0.099149	0.03305	0.099149	33.9668
error	9	-	-	-	6.12948

Table 6: L16 (45) Orthogonal array- 2nd design.

L_{16}	1	2	3	4	5	Result
1	1	1	1	0	0	0.0313
2	1	2	1	0	0	0.052
3	1	3	2	0	0	0.0623
4	1	1	2	0	0	0.0607
5	2	1	3	0	0	0.014
6	2	2	3	0	0	0.006
7	2	3	4	0	0	0.0384
8	2	1	4	0	0	0.0439
9	1	1	5	0	0	0.111
10	1	2	5	0	0	0.173
11	1	3	6	0	0	0.114
12	1	1	6	0	0	0.148
13	2	1	7	0	0	0.09
14	2	2	7	0	0	0.087
15	2	3	8	0	0	0.0996
16	2	1	8	0	0	0.115

downgrading was used to change the number of levels in the columns. The final orthogonal array is presented in Table 7. The experiments were carried out according to the orthogonal array and the results are listed in the last column of Table 7. The analysis of variance showed that the order of importance of factors was as follows (Table 8): the solid content, the ratio of height to diameter in reactor, and the superficial gas velocity. Experimental error of about 13% was achieved which is in the acceptable range.

New 4th order polynomial correlation

Experimental values for the gas holdup were correlated by a fourth order polynomial (Eq.(14)). The results were then compared with those from the drift flux method.

$$\varepsilon_g = a\, U_g^{\,4} + b\, U_g^{\,3} + c\, U_g^{\,2} + d\, U_g + e \qquad (14)$$

In this equation, U_g is the superficial gas velocity in the homogeneous or the transient region below the second transition point. The inflection point of the polynomial (Eq.(14)) is used as the transition velocity between homogeneous and transient flow regimes. The inflection point of the Eq. (14) was calculated as follows:

$$\frac{\partial^2 \varepsilon_g}{\partial U_g^{\,2}}\bigg|_{U_g = U_{g.t}} = 0 \qquad \left(b^2 \geq \frac{8}{3}ac\right) \qquad (15)$$

According to Eq. (15), the inflection point method is applicable when there is an inflection point in the homogeneous or the transient region $\left(b^2 \geq \dfrac{8}{3}ac\right)$.

Fig. 3 is an example of the drift flux velocity vs. gas holdup. This figure was obtained for a water column with a height of H=8D and a slurry content of 13 vol%. As it can be found from the drift flux plot, the gas holdup corresponding to the transition occurs at a gas velocity of 2.734 cm/s.

Fig. 4 is an example of gas holdup against superficial gas velocity for the liquid level of H=12D and slurry

Table 7: Parameters and levels- 2nd design.

Parameter	L_1	L_2	L_3	L_4	L_5	L_6	L_7	L_8
ε_s	0	0.13	-	-	-	-	-	-
H/D	8	10	12	-	-	-	-	-
U_g (cm/s)	0.853	1.322	1.792	2.265	2.497	2.73	2.919	3.14

Table 8: Analysis of variance- 2nd design.

Parameter	f_i	SS_i	V_i	SS'_i	P (%)
ε_s	1	0.095482	0.095482	0.095482	32.71037
H/D	2	0.093204	0.046602	0.093204	31.93003
U_g	7	0.065073	0.009296	0.065073	22.2929
error	5	-	-	-	13.0667
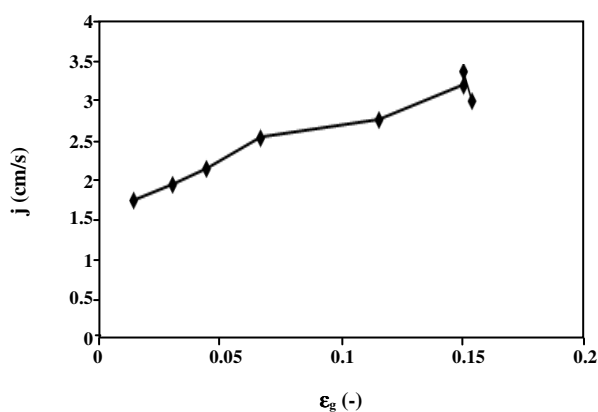
Fig. 3: The drift flux velocity against gas holdup for a standing water column height of H=8 D and particles content of 13 vol%.

Fig. 4: Gas holdup against gas velocity for H=12 D, εs =0.13 and related fourth order fitted plot.

content of 13 vol%. This figure also shows a fourth order curve describing the fitted data. The corresponding equation for this graph is as follows:

$$\varepsilon_g = -0.0190\ U_g^4 + 0.1942\ U_g^3 - 0.7233\ U_g^2 + 1.2273 U_g - 0.7877 \qquad (16)$$

As Eq. (16) shows, higher order terms of the polynomial have smaller coefficients. Consequently, at low superficial gas velocities, only the lower order terms of the expression are significant. This is in agreement with the Eq. (1) in which the power of the superficial gas velocity is around one. As the superficial gas velocity

increases, the higher order terms will become more important.

From this method for a liquid level of H=12D and a slurry content of 13 vol%, a transition velocity of 2.98 cm/s was calculated while a value of 3.14 cm/s was obtained from drift flux method. Application of this mathematical method does not depend on visual observation of the slope change used in the drift flux method.

Gas holdup

In SBCRs, the volumetric solid concentration greatly affects the hydrodynamics. The solid particles in the bubble column reactors are typically in the micron size
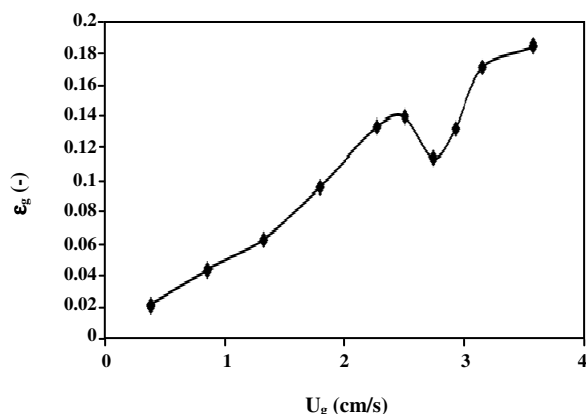
Fig. 5: Gas holdup against gas velocity for H=12 D and zero particles content.

Fig. 6: The influence of glass particles content on gas holdup for the liquid level of H=12 D.

range and are suspended in the liquid phase to form a slurry. Consequently, their concentration in the liquid phase changes the physical properties of the slurry, namely the density and viscosity. Several investigators have reported that an increase in the solid content decreases the total gas holdup [17-20]. The decrease of gas holdup with the solid concentration was attributed to the increase of pseudo-viscosity of the slurry phase, which enhances formation of large gas bubbles [21-23].

Fig. 5 is a representative example of the gas holdup against the gas velocity for H=12D and zero slurry content. The data points in the low ranges of velocity and holdup belong to homogenous flow regime. The data points in the high ranges of gas velocity and holdup belong to the churn-turbulent regime. The intermediate data points show the approximate range of the velocity transition.

The homogeneous flow regime generally occurs at low to moderate superficial gas velocities. It is characterized by uniformly sized small bubbles traveling vertically with minor axial oscillations. There is practically no coalescence and break-up. With increasing the superficial gas velocity, Due to coalescence all the bubbles will be large. The large bubbles have higher rise velocity than small bubbles, therefore residence time of large bubbles decreases and causes decreasing the rate of increasing gas hold up.

Influence of glass particle content up to 17 vol % was studied on the regime transition and the gas holdup. The slurry content ε_s is expressed as the volume fraction of solids in the gas-free slurry. Fig. 6 shows the relation between the gas holdup and the gas velocity when
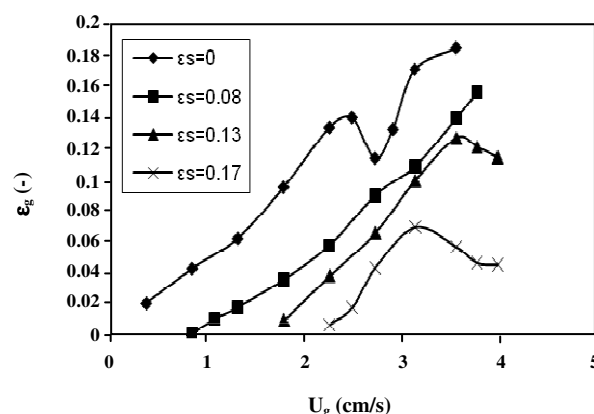
the slurry bubble column reactor contains glass particles. It can be observed from this figure that for a liquid level of H=12D the maximum gas holdup near the first transition point decreases at high slurry content. At lower slurry content, you can see a change between uniform bubbles size distribution in homogenous regime to a wide size distribution of bubble sizes in the heterogeneous regime and resulting sharp decrease in gas holdup.

Note the sharp maximum in the total gas holdup near the regime transition point for slurry content smaller than 13 vol%. The behavior of the slurry bubble column is close to that of a solid free bubble column. At higher slurry content, the influence of solids concentrations is dominant.

In the homogeneous regime, therefore, the gas holdup decreases with increasing slurry content due to increasing bubble diameters of the small-bubble population. This phenomenon also manifests itself in the heterogeneous flow regime and there is not any sharp change in gas holdup.

Some investigators reported no obvious change in the gas holdup when H/D ratios were above 5 - 6 [24,25]. Figs. 7a and 7b show dependence of gas holdup on gas velocity in the slurry bubble column reactor with the particle contents of 0 vol% and 13 vol% at different column heights. The liquid level has a very small influence on the gas holdup at lower superficial gas velocities. The maximum gas holdup values clearly decrease with increase in the liquid level. The same trend has also been reported earlier [26].

According to the gas-liquid theories [27], the gas hold-up increases linearly with the gas velocity while in the bubbly regime with a velocity of 0 cm/s producing

Table 9: The influence of glass particles content on regime transition for liquid level of H =8 D.

Solid Content (vol %)	Drift Flux Method		Inflection Point Method	
	Ug_t	εg_t	Ug_t	εg_t
0	1.792	0.0941	1.86	0.0989
8	2.734	0.0788	2.608	0.0771
13	2.734	0.0662	2.48	0.0541
17	2.734	0.0188	2.845	0.026907

Table 10: Comparison of inflection point and drift flux methods for reports of some investigations.

	Drift Flux Method		Inflection Point Method	
	U_{g_t}	ε_{g_t}	U_{g_t}	ε_{g_t}
Vandu C.O.et al.,2004[27]:air, porous catalyst, paraffin oil(ε_s=0.05)	0.0206(m/s)	0.064	0.024(m/s)	0.0804
*Letzel H.M. et al.,*1997[28]:air, water system	0.106(m/s)	0.0733	0.132(m/s)	0.150
U. Parasu Veera and Joshi J.B., 2000 [29]: air butanol system	0.0573(m/s)	0.170	0.0458(m/s)	0.138
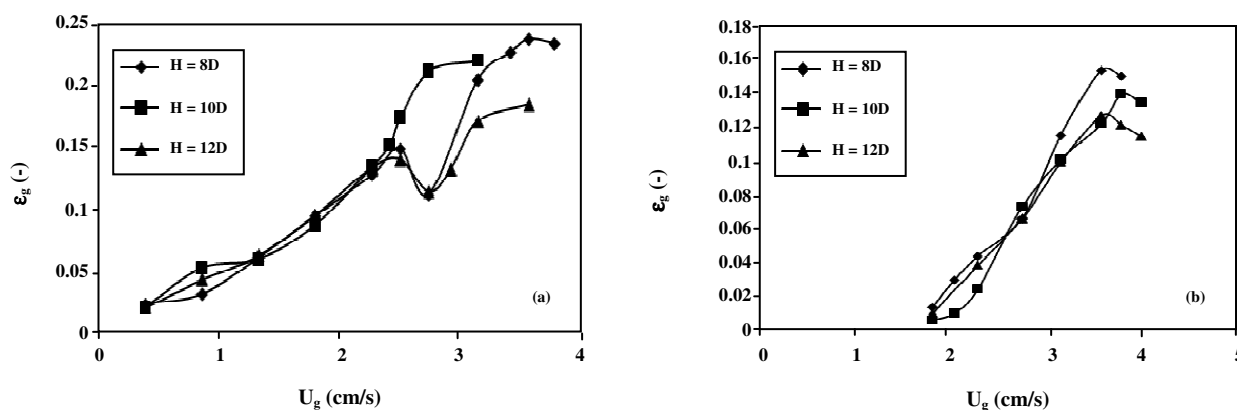
Fig. 7: The influence of liquid level on gas holdup, Particles content: εs =0 (a); εs =0.13 (b).

no holdup [28]. This is observed in the zero particle content case. For the case of 13 vol% particles content, a gas velocity of around 1.8 cm/s is required to fluidize the particles accumulated at the bottom of the column. Below this gas velocity, there is no bubble inside the column and the gas holdup is assumed to be zero.

Regime transition

The stability of the homogeneous regime was expressed by the values of the gas flow rate and the holdup at the first transition point [U_{g_t}, ε_{g_t}]. The transition points were determined using the inflection point and drift- flux method. The effect of the solid

particle content was especially visible on the transition point. The transition points for the glass particle contents up to 17 vol% and a liquid level of H=8D are shown in Table 9. The results obtained from both the drift flux and the inflection point methods are shown in this table. According to Table 9, the results of these two methods are in a good agreement. Table 10 shows the transition points obtained from the results presented by some investigators [29-31]. The results are in an agreement too. For air, butanol system the transition velocity obtained from drift flux method is not so clear but can be exactly clear from inflection point method.
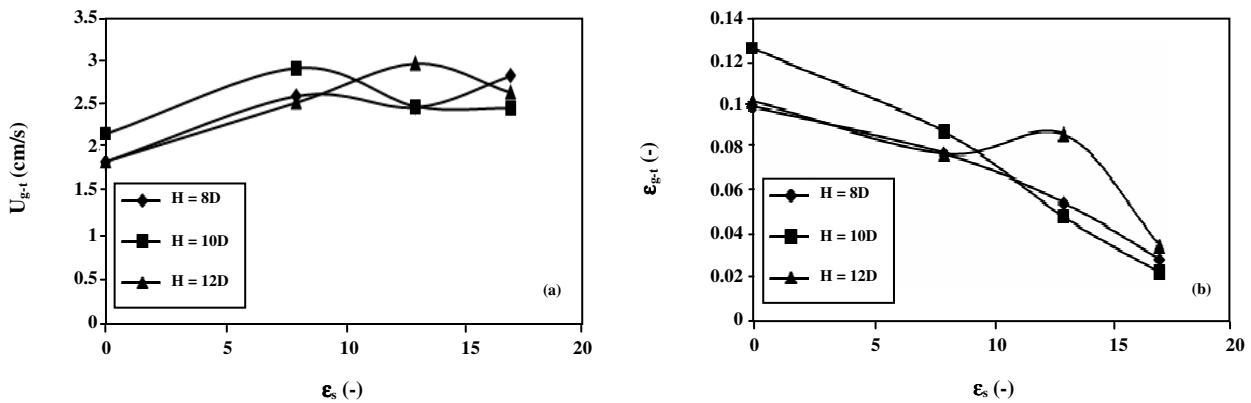
Fig. 8: The effect of particles content on the transition superficial gas velocity (a) and Transition gas holdup (b).
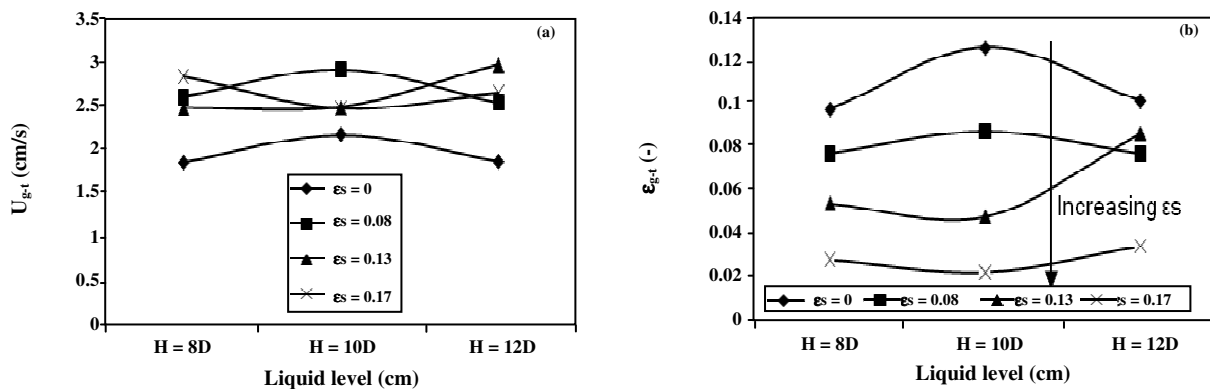

Fig. 9: The effect of column height on the transition superficial gas velocity (a) and the transition gas holdup (b).

Figs. 8a and 8b show the relationship between the transition point and the particle content at different column heights. According to Fig. 8, at low solid loadings, the transition superficial velocity initially raises with increase in the particle content and for the higher solid loadings, a small reduction in the transition superficial velocity is observed with the increase in particle content.

The regime transition point shifts to a lower gas holdup with increasing the solid loading. These results suggest that particle content can play a dual role in the homogeneous regime stability: low particle contents up to 8vol% stabilize the homogenous regime, while high particle contents over 8vol% destabilize.

This is in agreement with the experimental observations of *Mena et al.* (2005) for air-alginate beads-distilled water slurry systems [32] that they showed a same behavior for their system for the particle content up to 3vol% and over.

Figs. 9a and 9b show the influence of liquid level on the transition superficial gas velocity and the transition gas holdup. According to Fig. 8, there is no significant change in the transition superficial gas velocity and the transition gas holdup by increasing liquid level. This is in agreement with results obtained by *Ruzicka et al.* (2001) for the H/D ratios above 5 - 6[26].

CONCLUSIONS

Effects of the liquid level, the gas flow rate and the particle content on the gas holdup and regime transition point were studied for nitrogen-water-glass particles with particles contents of up to 17 vol% using inflection point and drift flux methods. Taguchi method was used for experimental design using two configuration of a L16 (45) orthogonal array. The following conclusions can be made from this work:

1- Experimental results for gas holdup against superficial gas velocity are expressed satisfactorily with a fourth order polynomial correlation. Inflection point of the fourth order polynomial correlation is considered as the transition point and the results obtained from this method and the drift flux method agree fairly well.

2- Maximum gas holdup values after transition decrease by increasing the liquid level. The liquid level has a very small effect on the gas holdup at lower superficial gas velocities.

3- The glass particle content has a stabilizing effect at lower contents, while high contents tend to destabilize the reactor flow regime.

4- With H/D ratios above 5 used in this study, there is no significant change in the transition point by increasing the liquid level.

5- In gas holdup measurements, the solid content is proved to be the most important parameter followed by H/D and the superficial gas velocities at the next importance levels.

Nomencluture

j	Drift fulx velocity,cm/s
U_g	Superficial gas velocity, cm/s
U_l	Liquid velocity, cm/s
U_{g_t}	Superficial gas velocity at regime transition, cm/s
u_b	Single bubble velocity in an infinite medium
V_g	Gas volume
V_l	Liquid volume
dp	Solids particle diameter, μm
fi	Degree of freedom
SSi	Sum of squares
SS'i	Pure sum of squares
Vi	Variance
P	Factor contribution

Greek Letters

ε_g	Gas holdup
ε_s	Weight fraction of glass particles in the slurry phase
ε_{g_t}	Gas holdup at regime transition, dimensionless

Subscripts

G	Rreferring to gas phase
l	Referring to liquid phase
m	Referring to manometer liquid
s	Referring to solids

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