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CFD Modeling and Gas Holdup Measurement in Three-Phase Slurry Bubble Column

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Abstract

Gas-Liquid-Solid system as slurry in a reactor have a wide range of applications in industry, a slurry reactor is a vessel containing the catalyst suspended in a liquid phase. In this study, we develop a CFD model to predict the gas holdup at different gas superficial velocities.

The experiments were done in a gas-liquid-solid slurry bubble column to find the gas holdup (ε_G). The experimental data showed a good agreement with CFD results. An empirical correlation has been developed to predict the gas holdup for three-phase slurry with a correlation co-efficient of 0.994; this correlation shows that the gas holdup predicted was in good agreement with experimental values.

Keywords: CFD modeling, Gas holdup, Three-phase and slurry bubble column.

نمذجة بأستخدام ديناميك الموائع الحسابي و قياسات عملية لمعدل احتجاز الغاز في العمود الفقاعي ذو العجينة السائلة

الخلاصة

نظام الطور الثلاثي (غاز-سائل-صلب) فـي مفاعـل العجينة السائلة تطبيقات صناعية واسعة.ومفاعل العجينة السائلة عبارة عن وعاء يحتوي على العامل المساعد بشكل عالق في الطور السائل.في هذه الدراسة تم تطوير موديل رياضي (ديناميك الموائع الحسابي) يتم من خلاله حساب معدل احتجاز الغاز داخل العمود عند سرع مختلفة للغاز. وتم قياس معدل احتجاز الغاز عملياً ايضاً وتم مقارنة نتائج الموديل مع النتائج العملية ووجدت المقارنة بينهما جيدة.كذلك تم استنتاج معادلة تجريبية لمعدل احتجاز الغاز وتم مقارنتها مع النتائج العملية بمعامل ارتباط ٠.٩٩٤.

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1. Introduction:

Gas–liquid–solid fluidization systems have been applied extensively in industry for physical (e.g., sand filter cleaning and granular material drying), chemical (e.g., hydrogen peroxide production and methanol synthesis), petrochemical (e.g., reside hydro treating and hydro treating of tar sands), and biochemical (e.g., treatment of lactose wastewater and bioleaching of metals from ores) processing (Fan, 1989). The interest in the application of three-phase fluidization systems has promoted continued research and development efforts in these systems. Examples are biological operation for human viral vaccine for chemical processes where gas–liquid mass transfer is the rate limiting step, it is important to be able to estimate the gas holdup as this relates directly to the mass transfer (Schweitzer et al., 2001). Considerable work has been carried out on the gas holdup in three-phase fluidized columns. Various aspects of these fluidized beds have been reviewed by several investigators (Fan, 1989; Lee et al., 2001; Safoniuk et al., 2002;), which include the importance of gas holdup and various factors affecting it.

Fluidised bed systems are of great interest in chemical process industry, pharmaceuticals production, mineral processing, energy related processes etc. Computational fluid dynamics (CFD) of multiphase flow processes provides a new tool for design and optimisation of multiphase flow systems such as fluidised reactors. CFD has during the last decades shown promising results and will probably become a useful tool in design of chemical reactors in near future, Mathiesen (2000).

Before the advent of CFD techniques, reactor modeling for chemical and biotechnological purposes was mainly carried out by means of highly simplified, semi-empirical parameter-fitting models. This was due to the fact that with computational resources available until just a short time ago, calculations with more precise models would have taken up a prohibitive amount of time thus being way too expensive for any application of interest.

While the limited range of a model's applicability always has to be kept in mind, in the field of two- and three-phase bubble column and airlift loop reactor modeling (and the adjoining area of fluidized bed modeling a number of approaches have gained large popularity due to their comparatively general validity (Schl¨uter et al., 1998). Namely these models are:

- Cell models: These models assume circulation cells inside the reactor which are responsible for back mixing processes (Dassori ,1998).
- The one-dimensional dispersion model: This model assumes that two-

and three-phase flow processes can be modeled as a superposition of convective and dispersive flow where the latter is described in analogy to Fick's first law of diffusion (Krishna et al., 2000, Liu, 1999, Schl¨uter et al., 1998, Sommer and Bohnet, 1996, Sommer, 1997).

- The two-dimensional dispersion model in cylindrical coordinates: This model includes radial effects in addition to axial dispersion. In cylindrical coordinates it can be formulated as follows (Schl¨uter, 1992).

$$\frac{\partial e_a}{\partial t} = D_{ax,a}\cdot\frac{\partial^2 e_a}{\partial^2 x} - u_{ax,a,c}\cdot\frac{\partial e_a}{\partial x} + \frac{1}{r}.D_{rad,a}\cdot\frac{\partial e_a}{\partial r} + D_{rad,a}\cdot\frac{\partial^2 e_a}{\partial^2 r} \quad ....(1)$$

Where:-

$D_{ax,l}$= 1.23 $D_c^{1.5}$ $U_g^{0.5}$ (Towell, G.D. et al. 1972)

$b_{r,l}$= 0.01 $D_{ax,l}$ (Camacho, R.F. 2004)

- Mechanical power balance models: These models calculate liquid circulation velocities from pneumatic power input into the reactor due to gas sparging. This is accomplished by solving force balances including pressure loss and gravitational terms (Zehner and Benfer, 1996).

Computational Fluid Dynamics (CFD) is an engineering tool which has gained large popularity during the last years. As opposed to the semi-empirical models described above, CFD aims at solving the (complete or simplified) fundamental physical equations that describe a flow phenomenon.

The most general form of these equations has been given by Navier and Stokes more than 150 years ago, therefore the set of equations has been named Navier-Stokes equations (Anderson, 1995).

These equations encompass mass, momentum and energy balances; they have to be adapted to the specific problem under consideration by additional closure laws (Feistauer., 1997).

While CFD has been very popular among car manufacturers and in the air and space industry (Griebel, 1995), chemical engineers have only recently become aware of the large potential it bears for the development and improvement of process equipment. This is mainly due to the fact that with modeling flow around a car body or an airplane wing, only single-phase flow has to be considered

(Cockx et al. 1999) reported on CFD calculations for an industrial-scale drinking water ozona-tion tower. They included ozone mass transfer into their calculations and computed the ozone concentration in the liquid phase. By adding baffles and moving the contactor inlet to a different position, they could achieve a 100 % efficiency increase of the disinfection process.

CFD modeling results using CFX-4.2 for a randomly packed distillation column was presented by (Yin et al. 2000). They compared their results to measurement data obtained at different operating conditions from a 1.22-m-diameter 3.66 m high packed bed that was equipped with several sizes of pall rings. Good agreement with the predictions was achieved giving rise to the hope that CFD will become a useful tool for the scale-up of this class of apparatus as well. Similar computations have been carried out for semi-structured catalytic packed beds by (Calis et al., 2001) using CFX-5.3. They found that pressure drop in such beds can be predicted with an error of less than 10 % compared to measurement results; still for such precision, very fine discretization grids (up to three million grid cells) and correspondingly high computational power is necessary.

(Erdal et al., 2000) reported on modeling of bubble behavior in gas-liquid cyclone separators.

Using CFX-4.1 they could determine the percentage of bubbles that unwontedly leave the reactor through the bottom liquid outlet and show the influence of correct modeling of turbulent dispersion on this so-called bubble carry-under effect.

Reducing gas hold-up has been identified as a key objective to improve the performance of Syncrude's LC-FinerSM unit. Redesign of the liquid recycle pan in the freeboard region, aided by multiphase CFD simulation and tests in a kerosene cold model experimental system, led to reduced gas hold-ups. The addition of an anti-foam agent did not provide any improvement (Mcknight, C.A. et al. 2008).

2. Experimental

The experimental setup is shown in Figure (1). The main components are: a column made up by two cylindrical sections of Plexiglas of 0.20 m of inner diameter and an entrance cone, a self-metering pump, two plastic feed tanks, filter devices, a rotameter to measure the gas flow rate, and a pressure transducer connected to a data acquisition system.

The three-phase solid, liquid and gas are Silica particles (particle size =38μm), tap water and oil free compressed air, respectively. Accurately weighed amount of material was fed into the column and adjusted for a specified initial static bed height. Water was pumped to the fluidizer at a desired flow rate using water rotameter. The air was then injected into the column through the air Spurger at a desired flow rate using air rotameter.

The gas holdup was calculated by two methods. The first method was the disengagement of the gas, in which two volumes are measured: the total volume when two phases are present in the system during the operation of the bubble column and the volume when the valves that fed the bubble column are closed suddenly, and the gas go out from the bubble column (Anderson, J. D. 1995).

$$e_G = \frac{V - V_o}{V} \qquad \text{.... (2)}$$

The second method was through the pressure drop, where the friction and acceleration contribution to total pressure drop were neglected. The acceleration contribution was neglected because no changes in cross-sectional area and phase are present, while friction contribution was neglected due to the size of the diameter compared to the traditional pipes as it is made by the majority of researchers; however, latter a calculation of two-phase friction factor was made to verify this assumption(Anderson, J. D. 1995).

$$e_G = \frac{r_L - \Delta P / gH}{r_L - r_G} \qquad \text{...... (3)}$$

3. Computer Simulation:

Computational fluid dynamics (CFD) software offers a promising option for the study of slurry reactor hydrodynamic. As our first step, we used computer simulations to calculate bed expansion and gas holdup where gas holdup is an important factor in the reaction rate because holdup affects interfacial surface area and therefore mass transfer coefficient and reaction rate. Gas holdup is one of the variables that need to be maximized to have a high performance bubble column.

The first step in developing the computer simulation is to create geometry and meshing, the geometry of the column was simple to made.

It was basically a vertical cylinder with an inlet at the bottom and outlet at the top. When the model had been developed the boundary conditions of the system was supplied. These include the sides of the cylinder as wall, and the inlet at the bottom as a velocity inlet, and the outlet on top. The boundary conditions used as follows:

At r=0 , U=Umax , $e_G = e_G$ max (in the centre) ,

at r=R , U=0 , $e_G = e_G$ min (at the walls) .

4. Results and Discussion:

Experiments were conducted with the gas and liquid flow rates which varied from 0.001to 0.0462 m/s and from 0.02123 to 0.16985m/s, respectively. The temperature was maintained at 25±3^{0}C. To ensure steady in operation at least five minutes were allowed. Readings for bed expansion and pressure drop were noted down. Each experiment was repeated three times to have an accurate reading.

Gas holdup increased with increasing gas superficial velocity as shown in figures (2, 3). At higher velocities the gas bubbles is smaller, then the interfacial area increased and the gas holdup as a fraction of gas in liquid increased too.

Figure (4) shows the agreement between the CFD results and experimental data with an average error of 10.2%.

Conceivable variables on which the gas holdup in the present system may depend are: gas velocity (u_g), liquid velocity (u_l), particle size (dp), column diameter (Dc), expanded bed height (He), static bed height (Hs), diameter of the sparger orifice (do), density of gas (ρ_g), density of liquid (ρ_l), density of solid (ρ_s), viscosity of gas (μ_g), viscosity of the liquid (μ_l), surface tension of liquid (σ_l) and gravitational constant (g). The large number of possible variables on which the dispersed phase holdup depends has been reduced to a pertinent few, since many of these variables are interrelated or are maintained as constant.

Therefore, if a theoretical relation exists between the true fractional gas holdup, εg, and the physical characteristic, and flow variables of the system, then εg may be written in the following form:

$$e_g = f[u_g, u_l, r_g, r_l, r_s, m_g, d_p, H_s D_c, g] \quad ....(4)$$

The dimensional analysis carried out indicates that the fractional gas holdup may be simplified to Eq. (4) as,

$$\varepsilon_g = f\,[Frg]^a\,[Rel]^b[Hr]^c[dr]^d \quad ......(5)$$

In order to establish the functional relationship between εg and the various dimensionless groups in Eq. (5), multiple linear regression analysis has been used to evaluate the constant and coefficients of the equation, assuming the power law functional relationship. It can be seen that the following equation, which yields the regression coefficient of 0.994 and a standard deviation of percentage error 2.57, presents the best possible correlation among the family of equations.

$$\varepsilon_g = 6.23[Frg]^{0.38}\ [Rel]^{-0.175}[Hr]^{0.06}\ [dr]^{0.088} \quad ......(6)$$

The values of gas holdup predicted by Eq. (6) have been plotted against the experimental values of fractional gas holdup in Fig.(5). Very close agreement between the experimental and calculated values from the developed correlation is seen. This has been possible due to the repeated experimentation and rejection of odd data points. The correlation (Eq. (6) is highly significant at 99% confidence level.

5. Conclusions

Gas holdup characteristics are one of the important design parameters for gas–liquid–solid three-phase slurry system since the rate of gas–liquid mass transfer is influenced by the gas holdup. In this paper an attempt has been made to predict gas holdup from measurement of bed pressure drop for air–water–solid particles in the fluidization regime. Detailed experimental investigations have been carried out to study the effect of gas velocity.

We develop a CFD model to predict the gas holdup values at different gas superficial velocities. The data of gas holdup is compared with data from

CFD model and this compariion is in a good agreement.

A correlation has been developed to predict the gas holdup for three-phase system with a correlation co-efficient of 0.994. It has been found that the gas holdup predicted was in good agreement with experimental values. A maximum of 6.5% deviations was found in all flow conditions.

6. References

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Nomenclature

D Column inner diameter (m).
Dc Column diameter (m).
$D_{ax,\alpha}$ Axial dispersion coefficient of phase (m^2/s).
$D_{rad,x}$ Radial dispersion coefficient of phase (m^2/s).
dp Particle diameter (μm).
Fr Froude number of the *gas* phase.
g gravitational acceleration (m/s^2).

H Height of column (m).
H_s Height of solid particle (m).
P Pressure drop (Pas.).

r Radius of column (m).
R_e Reynolds number.
t Time (s).
u_g Superficial gas velocity (m/s).
u_l Superficial liquid velocity (m/s).
V Total volume of liquid (m^3).

Greek symbols

α Index denoting a continuous phase.
ε Phase holdup.
μ Newtonian viscosity (Kg/m.s).
ρ density at atmospheric conditions, (Kg/m^3).

Subscripts

G gas phase.
L Liquid phase.

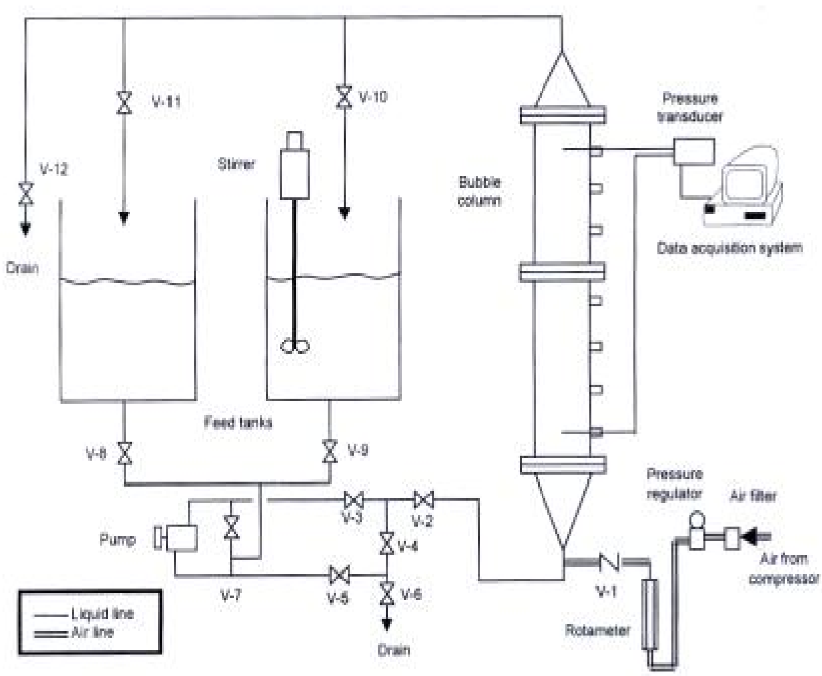

Figure (1) Experimental setup

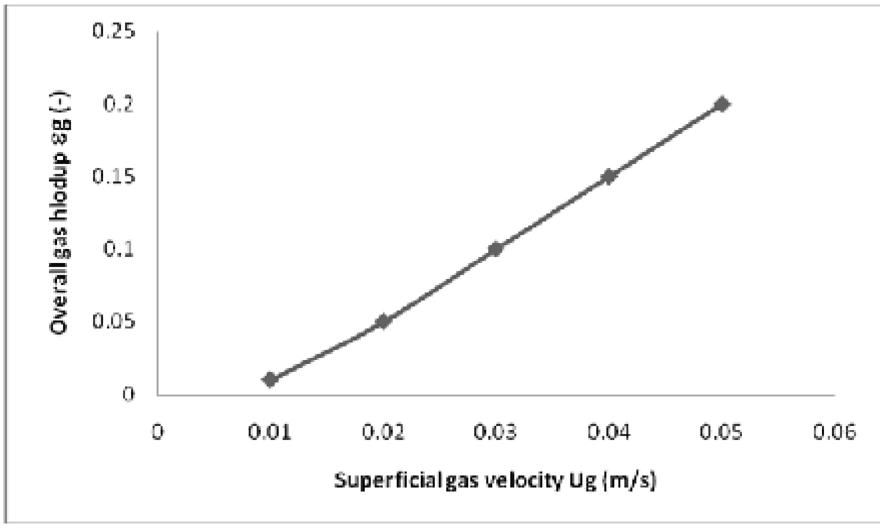

Figure (2) Overall gas holdup vs. superficial gas velocity

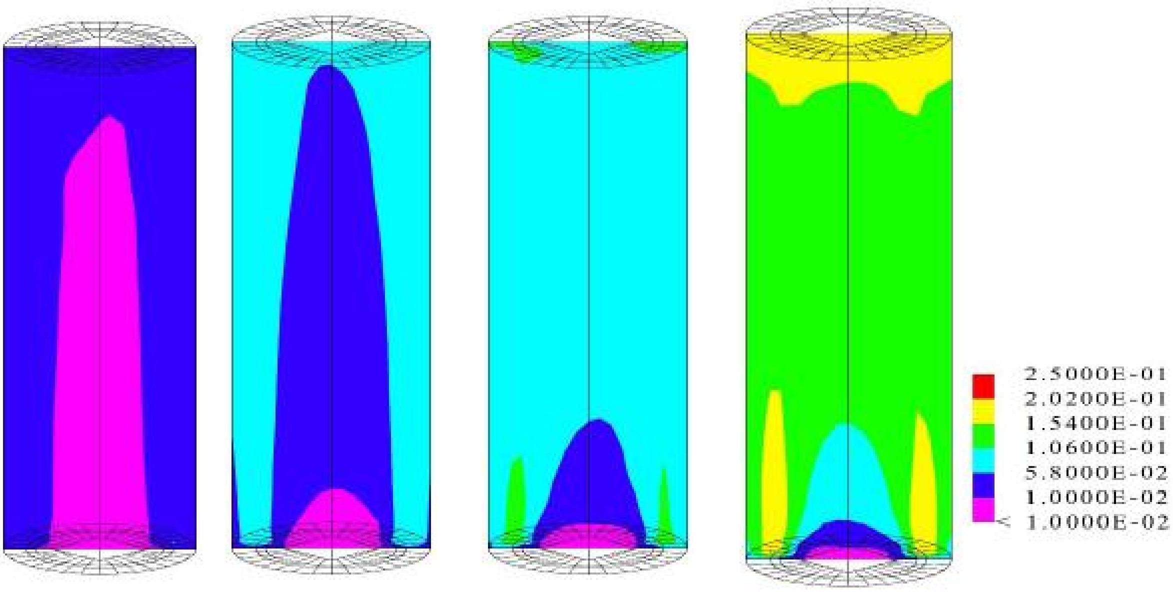

Figure (3) Effect of superficial gas velocity on gas holdup
[velocities from left to right are 0.01, 0.02, 0.03 and 0.04 m/s].

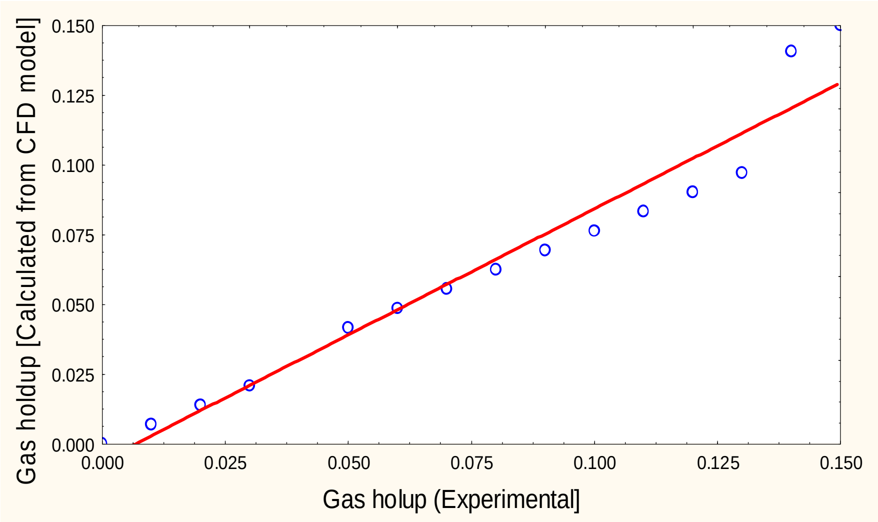

Figure (4) Comparison of experimental and calculated values of fractional gas holdup from CFD model for superficial gas velocity (u_g =0.02m/s).

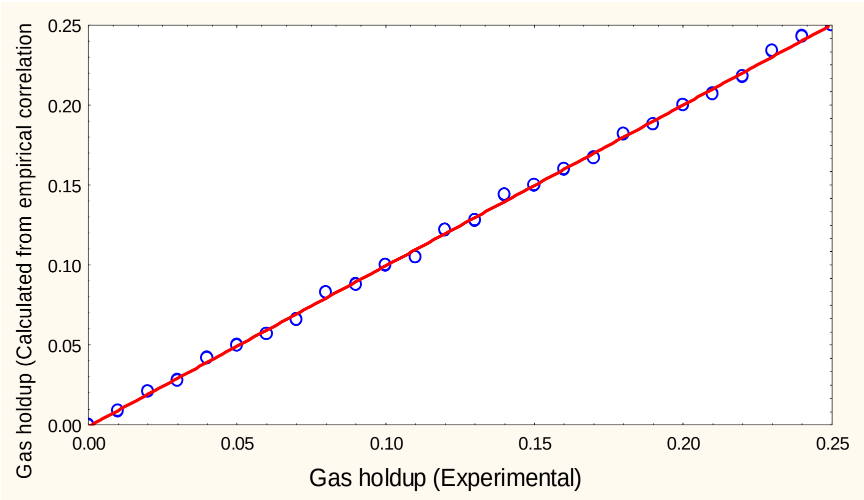

Figure (5) Comparison of experimental and calculated values of fractional gas holdup from Eq. (6)