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Toward a Multiphase Local Approach in the Modeling of Flotation and Mass Transfer in Gas-Liquid Contacting Systems

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1. Introduction

This chapter comprises two major parts: The first part is devoted to the development of a kinetic model of flotation based on the theory of mass transfer in gas - liquid bubbly flows. The second part presents some requirements in order to go forward in implementing multiphase local approach in the modeling of flotation and mass transfer in gas-liquid contacting systems.

The common kinetic models applied to the flotation process are first order and they are validated on the basis of experimental analysis. Classical kinetics model of flotation cannot represent the bubble carrying capacity because their solution supposes that for long contact time, the concentration of the slurry have to vanish whatever the rate of the superficial bubbles loading may be.

The bubble carrying capacity, which can be interpreted as a superficial saturation of the bubbles, cannot be represented by simple first order models. However, saturation phenomena have been observed in some flotation devises. For example the experiments of the flotation column of Bensley et al., (1985) show that, for a given flux of bubbles, the recovery of particles in the slurry may still be constant at a relatively low value whatever the height of the flotation column may be. This is similar to what it happens in common gas-liquid mass transfer devices.

Gas-liquid mass transfer theory indicates that the flux of mass through the gas-liquid interface is proportional to the gas-liquid contact area. It indicates also that the resistance to the interfacial transfer of low solubility gases may be described by a first order kinetics law where the main variable is the difference between the local concentration of the gas in the liquid and the concentration at saturation in the same thermodynamic conditions. For long contact time, this difference vanishes: the mass transfer is stopped up when the concentration of saturation in the liquid is reached. A kinetic model inspired from the theory of mass transfer in gas - liquid medium is presented. This model, developed to describe flotation in a bubble column, is interpreted with regard to the effect of the superficial saturation of the bubbles on the kinetics of flotation.

The second part of the chapter is devoted to local analysis and modeling of gas-liquid turbulent flows. The local description of gas-liquid contacting systems (average velocity, turbulence, void fraction etc.) represents an important scientific challenge and creates a

major interest in many industrial applications especially when transfer phenomena are in concern. Many experimental results in gas-liquid bubbly flows indicate the important effect of the interfacial interactions on the turbulence of the liquid phase, Lance &Bataille (1991). The eulerian-eulerien model of Chahed et al. (2003) insists on two aspects of the interaction between phases : first the turbulent correlations associated with the added mass force are taken into account in the expression of the force exerted by the liquid on the bubbles and second the Reynolds stress tensor of the continuous phase is separated into two parts: a turbulent part produced by the gradient of mean velocity and a pseudo-turbulent part induced by bubbles displacements, each part is predetermined by a transport equation. This two-fluid model allows the prediction of the turbulence and of the void fraction in basic bubbly flows with moderate void fractions. We present the most prominent results, which are commented in order to specify the basic requirements in the elaboration of CFD codes applied to gas-liquid reactors.

2. Mass transfer approach applied to the modeling of flotation

2.1 First order kinetic model of flotation

In flotation in a bubble column, air bubbles are injected in an aqueous phase (slurry) containing a suspension of non-wettable (hydrophobic) and wettable (hydrophilic) particles. As the bubbles move through the slurry, they collect the hydrophobic particles and carry them to the surface, where they form a stable froth. The froth is removed and the floated particles recovered.

As for the description of the kinetics of chemical transformations, the kinetics of flotation is essentially described by first order models. First order models express that the rate of appearance/disappearance of specie in a process of transformation is proportional to its concentration. Applied to flotation, this model, describes the reduction of the concentration in the liquid during the process of flotation in the form:

$$\frac{dC}{dt} = -kC \tag{1}$$

where C is the liquid concentration (mass of particles per unit volume of the liquid) and k the kinetic coefficient (frequency) assumed to be constant. Broadly speaking, for column flotation where we only consider the collection that occurs in the collection zone, the kinetic models are established in order to represent the number of particles that succeed to have a collision with a bubble and to be effectively attached to the gas liquid interface. The kinetic coefficient of the flotation process is thus formulated as the product of three factors representing the frequencies of collision (P_c), of attachment (P_a) and of non-detachment (P_d):

$$k = P_c P_a P_d \tag{2}$$

Many models have been developed in order to determine the factors involved in the modeling of flotation kinetics and excellent reviews have been produced establishing the state of the art in the domain, (Tuetja et al., 1994; Zongfu et al., 2000). These studies show that there is a variety of kinetic models used for flotation; but when confronted to the experiments, the disparity of their results may indicate that the mechanisms involved in flotation phenomena are too complex to be described by relatively simple formulations.

Generally speaking, this kind of model may be validated on the basis of experimental analysis provided that the first order behavior is supported by the experimental data, as in the work of Ahmed and Jameson (1985) for example. Nevertheless, it is reported that the phenomenon of flotation may be limited by bubble carrying capacity, (Finch & Dobby, 1990; Yoon et al, 1993), or by the ability of the bubbles to transport large size particles (Nguyen, 2003).

Similar phenomenon of saturation occurs in gas-liquid mass transfer with this difference that the saturation concerns, in this case, the concentration of the liquid where the gas is dissolved. Indeed gas-liquid mass transfer theories indicates that the resistance to the interfacial transfer of low solubility gases may be described by a first order kinetics law where the main variable is the difference between the local concentration of the gas in the liquid and the concentration at saturation in the same thermodynamic conditions. For long contact time, this difference vanishes: the mass transfer is stopped up when the concentration of saturation in the liquid is reached.

Flotation can be seen as interfacial liquid-gas transfer and one may expect that we can draw on mass transfer theory in gas-liquid flows in order to build kinetic models for flotation which would be capable of reproducing the phenomenon of saturation. The application of mass transfer theory to flotation process has been previously suggested by Jameson et al. (1977) and Ityokumbul (1992).The later proposed, for the collection zone of a flotation column, a kinetic model based on a mass balance at the gas-liquid interfaces where the rate of particle attachment to the bubbles is assumed to be proportional to the particle concentration in the liquid and to the presence of non-saturated bubble surface. Chahed & Mrabet (2008) have built on this model and have proposed a more complete formulation. They also tried to comment some reductions of this formulation in comparison with the common first order model of flotation and with the model proposed by Ityokumbul (1992). In the following, we briefly present some aspects of gas-liquid mass transfer theory than we present the results obtained in the formulation of kinetics of flotation in bubble columns based on mass transfer theory.

2.2 Interfacial mass transfer in gas-liquid flow

To focus on the physical significance of the mass transfer phenomena let us analyze the relatively simple two-film model, figure (1). In the two-film model, the rate of mass transfer due to the diffusion of a gas through a gas-liquid interface can be expressed in two ways according as we consider the liquid side film (thickness δ_L) or that on the gas side (thickness δ_G). In the gas side film, the transfer is based on the partial pressure diving force $P_A - P_A^*$ while in the liquid one it is based on the concentration driving force.

$$\frac{dC}{dt} = K_G a(P_A - P_A^*) = K_L a(C_A^* - C_A) \tag{3}$$

where P_A is the partial pressure of the gas and C_A is the concentration of the dissolved gas in the liquid, C_A^*, is the concentration of the gas in the liquid that will be in equilibrium with P_A and P_A^* is the partial pressure of the gas that will be in equilibrium with C_A ; K_G and K_L are respectively the mass transfer coefficients based on the gas and liquid phases ; and a is the interfacial area which represents the interfacial surface per unit volume of the liquid.

The appropriate equilibrium values A_A^* or C_A^* may be given by Henry's law:

$$P_A^* = HC_A \quad \text{and} \quad C_A^* = \frac{1}{H}P_A \tag{4}$$
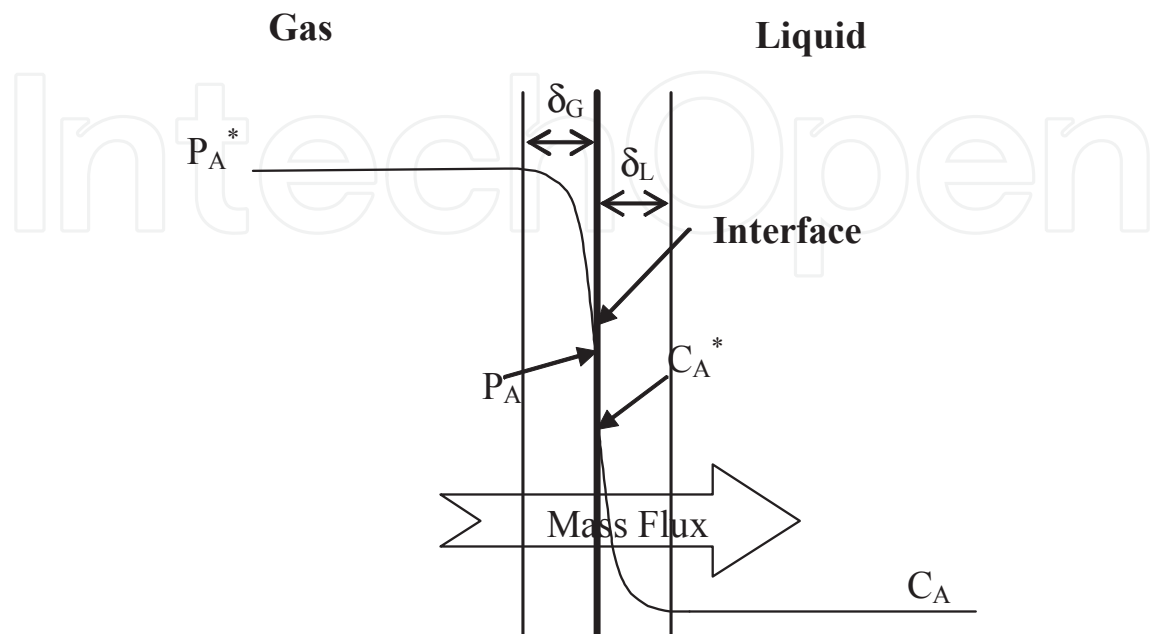
Where H is the Henry's constant

Fig. 1. Schematic representation of double-film mass transfer model

2.3 Mass balance at gas-liquid interfaces in flotation device

The kinetic model of Ityokumbul (1992) is based on a mass balance at the gas-liquid interfaces where the rate of particle attachment to the bubbles is assumed to be proportional to the concentration in the liquid C and to the presence of non-saturated bubble surface. The model considers alos a rate of detachment proportional to the surface load of the bubbles C_b (mass per unit surface). This mass balance is written in the form:

$$\frac{dC_b}{dt} = k_a(C_{mb} - C_b)C - k_dC_b \tag{5}$$

Where C_{mb} represents the maximum surface load of the bubbles that corresponds to the mass of the maximum of particles that bubbles can theoretically carry per surface unit. The model of Ityokumbul introduces two kinetic coefficients: a detachment coefficient k_d which has the dimension of the inverse of time and an attachment coefficient k_a defined so that the product k_aC has the dimension of the inverse of time.

The model has the great advantage of connecting the kinetics of flotation to the presence of interfaces. Indeed, the mass transfer from the liquor is the amount accumulated on the interfaces, so that we can write:

$$\frac{dC}{dt} = -a\frac{dC_b}{dt} = -k_a a(C_{mb} - C_b)C + k_d aC_b \tag{6}$$

Where a is the interfacial area.

In reference to experimental data, Ityokumbul (1992) considers that in ordinary flotation systems, the surface load of the bubbles of the bubbles C_b is still generally small in comparison with the maximum surface load of the bubbles C_{mb}. He deduced that C_b could be neglected and the model (6) degenerates in the form:

$$\frac{dC}{dt} = -k_a a C_{mb} C \qquad (7)$$

Which is identical to first order models generally used to describe the kinetics of flotation. Commenting the model of Ityokumbul (1992), Chahed & Mrabet (2008) assume the hypothesis considering that the surface load C_b is generally small as compared to the maximum surface load C_{mb}, allows to neglect C_b in the first term in the rhs of equation (6), but certainly does not allow, in the general case, to neglect the last term. This term represents the rate of detachment of the particles and when neglected, the model degenerates so much so that it becomes impossible to represent the effect of the surface load of bubble on its potential carrying capacity. In order to avoid this loss of generality, Chahed & Mrabet (2008) proposed to keep the term of detachment but they neglected C_b in the first term of the second member of the mass balance (6) against C_{mb}. In these conditions, the model (6) reduces to:

$$\frac{dC_b}{dt} = k_a C_{mb} C - k_d C_b \qquad \text{and} \qquad \frac{dC}{dt} = k_a a C_{mb}(C_R - C) \qquad (8)$$

Where $C_R = \dfrac{k_d C_b}{k_a C_{mb}}$ is a minimum concentration that we can reach under a given operating condition. This model has a similar formulation than the models used in gas-liquid mass transfer. It shows explicitly that the interfacial transfer is proportional to the interfacial area. This outcome is in concordance with the experimental works of Gorain et al. (1997).

The irreducible concentration C_R depends on the superficial loading condition of the bubble interface. By analogy, C_R represents for flotation what the concentration C* (concentration of the gas in the liquid that is in equilibrium with the partial pressure of the gas) represents for gas-liquid mass transfer. Both determine a certain condition of gas-liquid interface equilibrium. So, we have to build a phenomenological model similar to the Henry's law used in gas-liquid mass transfer in order to derive constitutive relations for the irreducible concentration C_R. The expression of C_R suggests that, for a given operative conditions, C_R depends on the loading condition of the bubble surface in comparison to the maximum load that the bubble can potentially carry per unit of surface area. It is also expected that irreducible concentration will depend on the local conditions (slurry concentration, turbulence, superficial tension, contaminants, etc.)

The model proposed by Ityokumbul (1992) corresponds to a reduction of the model (8) in which the detachment is neglected, equation (7). In this case C_R is zero and there is no limit to the minimum slurry concentration. This corresponds to situations where the bubbles are very lightly loaded ($C_b \rightarrow 0$). If we consider, in first approximation, that the number of particles accumulated by unit of bubbles surface is proportional to d_P^{-2} (d_P is the diameter of the particle), the maximum load C_{mb} is thus proportional to $\rho_P d_p$ (ρ_P is the density of the particle). This result is concordance with the correlation proposed by Finch and Dobby(1990). On the other hand, for spherical bubbles, the interfacial area is given by:

$$a = \frac{6\alpha}{d_b} \cdot \qquad (9)$$

where α is the void fraction that represents the rate of the gas volume and d_b is the bubble diameter. Equation (7) writes:

$$\frac{dC}{dt} = -h\alpha \frac{d_p}{d_b} C \qquad (10)$$

Where h is a constant coefficient. For a given void fraction, equation (10) corresponds to the conceptual first collision model published by Sutherland in a famous paper that introduced the notion of flotation kinetics, Sutherland (1948).

2.4 Modeling of flotation in a bubble column

The kinetic model based on gas-liquid mass transfer theory presented above has been applied to two cases of literature experimental data, Chahed & Mrabet (2008). The first set of experiments is due to Bensley et al. (1985) and concerns the flotation of fine coal particles in a bubble column. The experimental data represent the variation of the flotation recovery as a function of the height of the collection zone in the flotation column. These experiments show that, for the reason that coal particles are very hydrophobic, the most important part of the flotation process takes place in the zone where occurs the first contact between the slurry and the fresh bubbles injected at the bottom of the column. It appears that the bubbles are rapidly saturated and the recovery of the bubble column remained less than 80 % whatever the bubble column height may be. Obviously, the classical first order models with a constant coefficient are inadequate for reproducing the flotation kinetics observed in these experiments.

The second experiment concerns the flotation of less hydrophobic particles (flourite), (Yachausti et al., 1988). The authors reported also experimental data representing the variation of the flotation recovery as a function of the height of the collection zone. In this experiment, we remark that the recovery of flourite is improved as the height of the flotation column is increased. It seems that the flotation process is not terminated by a saturation effect, at least in the range of flotation column heights employed in the experiments; correspondingly, the irreducible concentration is not reached in the experiments. Nevertheless, a trend to a limitation of the flotation can be observed for the highest columns. In both experiments, classical first order models are insufficient and the simulations produced by Chahed & Mrabet (2008) showed how it is pertinent to use mass transfer approach to describe the flotation kinetics in bubble columns. The simulation of the first set of experiments shows that, when the irreducible concentration is suitably adjusted from the experiments, the kinetics of flotation can be adjusted and the model reproduces correctly the experimental results, with an irreducible concentration χ_R^* greater than 20%, figure (2). Note that the collection zone has a height L and the liquid moves through the column with an uniform velocity denoted u_p, $\chi_R^* = \frac{C^*}{C_0}$ represents the concentration of the liquid at the outlet of the column normed by the concentration of the slurry at the inlet.
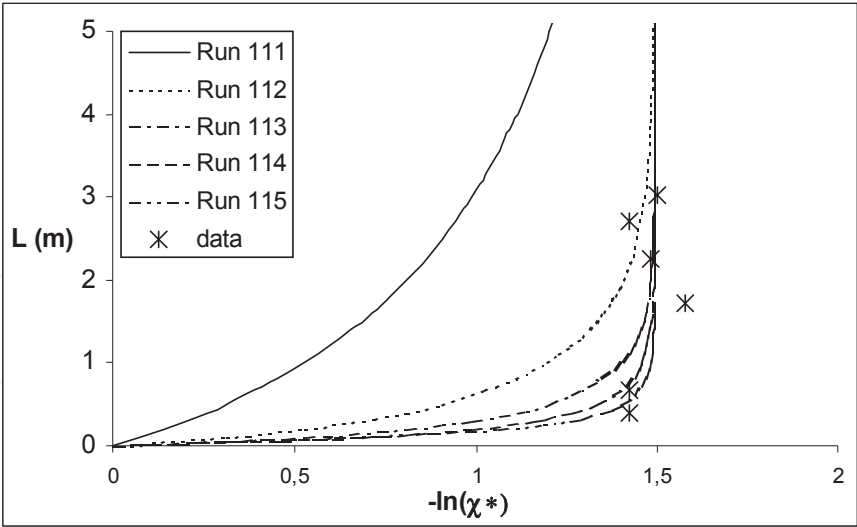
Fig. 2. Effect of the kinetic coefficient on the flotation yield, Simulations with $\chi_R^* = 0.225$,

$\dfrac{k_d}{u_p} = 1$ (Run 111), $\dfrac{k_d}{u_p} = 5$ (Run 112), $\dfrac{k_d}{u_p} = 10$ (Run 113), $\dfrac{k_d}{u_p} = 15$ (Run 114), $\dfrac{k_d}{u_p} = 20$

(Run 115). Experimental data of coal recovery as function of recovery zone height, (Bensley et al., 1985).

The application of the model to the second set of experiments, with an irreducible concentration of order of $\chi_R^* = 2.5\%$ allows quite good reproduction of the experimental results when the kinetic coefficient is suitably adjusted, figure (3).
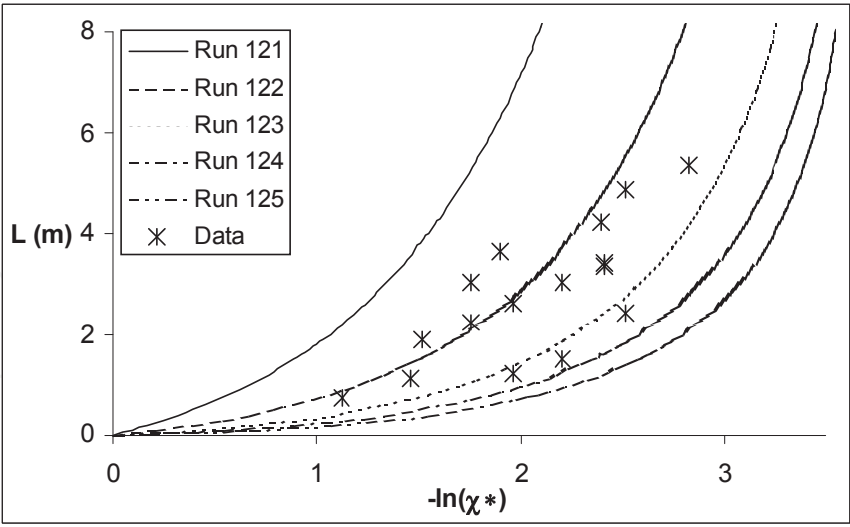

Fig. 3. Effect of the kinetic coefficient on the flotation yield, Simulations with $\chi_R^* = 0.025$,

$\dfrac{k_d}{u_p} = 1$ (Run 121), $\dfrac{k_d}{u_p} = 2.5$ (Run 122), $\dfrac{k_d}{u_p} = 5$ (Run 123), $\dfrac{k_d}{u_p} = 7.5$ (Run 124), $\dfrac{k_d}{u_p} = 10$ (Run

125). Experimental data of flourite recovery as function of recovery zone height, (Yachausti et al., 1988).

3. Local modeling of transfers in gas-liquid bubbly flows

3.1 Mass transfer in gas-liquid flow

There are number of formulations of mass transfer in gas-liquid flow but all of them come down to a general formulation of the general mass flux, including flotation, in the general form:

$$S_c = k_L a(C^* - C) \qquad (11)$$

Where k_L is the transfer coefficient which has dimension of velocity, C^* is the concentration of gas in the liquid at saturation, a is the interfacial area, which is the surface of the interfaces per unit volume, and C_L the concentration far away from the interfaces. In mono-disperse bubbly flows with spherical bubbles, the volumetric interfacial area is proportional to the void fraction and inversely proportional to the bubble diameter ($a = \dfrac{6\alpha}{d}$) which indicates the important role of the bubble diameter and of its distribution in the computation of the local mass transfer.

The experimental and numerical work carried out in recent decades has made significant advances in local modeling of gas-liquid systems, (Lain et al. 1999; Cockx et al., 2001; Buscaglia et al., 2002; Ayed et al., 2007). These studies show the relevance of the approach and open new perspectives of development. Three important questions are prerequisites for the development of general numerical codes for the modeling of transfers in gas-liquid systems bubbly systems. The first question is related to the modeling of the transfer coefficient, the second issue concerns the turbulence modeling in two-phase gas-liquid flows and the third relates to the prediction of the local distribution of the interfaces, this includes the prediction of the local void fraction and of the bubbles size distributions.

a) Gas-liquid mass transfer coefficients

The formulation of gas-liquid mass transfer coefficients involves local time scales in relation with the mechanisms that control the interfacial transfer. The earliest models still commonly used were proposed by Dankwerts (1951) and Hygbie (1935). For instance the Hygbie model involves time scale related to the bubble displacement. If the formulation of the transfer coefficient is theoretically acceptable for simple two-phase flow situations (spherical bubbles in free ascent in a liquid at rest), the effects of turbulence, the deformation of bubbles and the effects of the contaminants are far to be completely controlled.

A significant progress in the study and modeling of the gas-liquid flows has been achieved and many experimental studies have been carried out during the last decades. The experimental data are used in order to provide suitable correlations of the transfer rate (Aisa et al., 1981; Wanninkhof & Gills, 1999). On the other hand basic experiments had established a local description of the interfacial mass transfer at the gaz-liquid horizontal interface in homogeneous turbulence generated by micro-jets, (George et al., 1994) or by oscillating grid, (Reidel et al., 2004). The characteristic scales of transfers in turbulent gas-liquid systems depend on the scales of turbulence in general, but also depend on the specific scales that characterize the bubble and its movement. The problem is more complex considering that the average and fluctuating fields of gas and of the liquid phases are disturbed by the interfacial exchange.

b) Turbulence in gas-liquid bubbly flows

The available experimental results in gas liquid bubbly flows indicate the important effect of the interfacial interactions between phases on the turbulence structure of the liquid phase. The presence of the dispersed phase in the flow alters considerably the liquid turbulence structure by affecting the whole of the turbulence mechanisms e.g. diffusion, production, dissipation, redistribution (Lance & Bataille, 1991).

In particular, the experiments of homogeneous turbulence with a constant shear (Lance et al., 1991) show that the bubbles, in their random movements, induce a supplementary stretching of the turbulent eddies that leads to a more isotropy of the turbulent fluctuations with a reduction of the turbulent shear. With regard to turbulence modeling, this experimental result is of great consequence: it suggests that we have to go up to turbulence closure level so that we may take into account the effect of the bubbles on the redistribution mechanism. In order to attain this objective, second order turbulence modeling is required and in several recent two-fluid models, the turbulence closures are effectively modeled using second order closure modeling (Lance et al. 1991; Chahed et al., 2003; Zhou, 2001; Lopez de Bertodano et al., 1990).

On the other hand, the turbulence structure of the liquid phase was pointed to have an important role in the phase distribution (Drew & Lahey, 1982); more recently it has been proved that the turbulent contributions of momentum interfacial transfer are important in the phase distribution phenomena, (Chahed et al., 2002). Thus one of the previous questions in the elaboration of efficient prediction tools is the accurate predetermination of the turbulence stress tensors in both liquid and gas phases.

c) Void fraction and bubble size distribution in turbulent bubbly flows

Gas - liquid reactors used in the industrial domain often bring about multiphase dense flows (high void fraction in bubbly flows) where transfer and transformation phenomena occur. In these reactors, often with complex geometries, the distribution of the phases is an important factor: transfer and transformation phenomena are in direct relation with the exchange between phases, therefore with the rate of presence of the interfacial area that materializes the contact between the two phases. Indeed, the interfacial area measures the contacting surface by unit volume and it depends on the distribution of the rate of presence of the phases and on the distribution of the sizes of the bubbles.

3.2 Two-fluid model for turbulent bubbly flows : basic equations and closure issues

All of the considerations presented above led to admit that the development of adequate models of transfers in gas-liquid systems should proceed from a comprehensive approach of two-phase flow modeling. With the current progress in the modeling of turbulent gas-liquid two-phase flows, we may expect that a local phenomenological approach of the problem may be useful for developing more suitable modeling of gas-liquid reactors.

Eulerian two-fluid models are based on a classical averaging of the balance equations that express in each phase the mass and the momentum conservation. We consider turbulent gas-liquid bubbly flow with low solubility of the gas in the liquid so that we neglect the effect of the mass transfer on the dynamic of the gas-liquid flow. We consider that without breakup and coalescence, the bubble diameter is still roughly constant.

We note α the void fraction and $\overline{\overline{\mathbf{u}_L}}$, $\overline{\overline{p_L}}$, ρ_L respectively the average liquid velocity, the pressure and the density of the liquid phase. $\mathbf{g}$ is the gravity acceleration and $\overline{\overline{\mathbf{u}}}_R = \overline{\overline{\mathbf{u}}}_G - \overline{\overline{\mathbf{u}}}_L$

is the relative velocity of the bubbles. With the subscript G the variables are related to the gas phase. We consider stationary incompressible bubbly flows and we neglect the effect of the mass transfer on the dynamic of the gas-liquid flow, the averaged balance equations of mass and momentum in the liquid and in the gas are, (Chahed et al., 2003):

$$\nabla \bullet (1-\alpha)\overline{\overline{\mathbf{u}}}_L = 0 \qquad \nabla \bullet \alpha \overline{\overline{\mathbf{u}}}_G = 0 \qquad (12)$$

$$(1-\alpha)\rho_L \frac{D}{Dt}\overline{\overline{\mathbf{u}}}_L = -\nabla \overline{\overline{p}}_L - \nabla \bullet ((1-\alpha)\rho_L \overline{\overline{\mathbf{u'_L}\mathbf{u'_L}}}) + (1-\alpha)\rho_L \mathbf{g} \qquad (13)$$

$$0 = -\alpha \nabla \overline{\overline{p}}_L + \mathbf{M}_G \qquad (14)$$

$$\mathbf{M}_G = -\frac{3}{4}\rho_L \frac{C_D}{d}\left\|\overline{\overline{\mathbf{u}}}_R\right\|\overline{\overline{\mathbf{u}}}_R - 2\rho_L C_L(1-f_{LP}(y^{**}))\overline{\overline{\boldsymbol{\omega}}}_L \times \overline{\overline{\mathbf{u}}}_R$$
$$-\rho_L C_A(\frac{d}{dt}\overline{\overline{\mathbf{u}}}_G - \frac{D}{Dt}\overline{\overline{\mathbf{u}}}_L) - \rho_L C_A \frac{1}{\alpha}\nabla.\alpha(\overline{\overline{\mathbf{u'_G}\mathbf{u'_G}}} - \overline{\overline{\mathbf{u'_L}\mathbf{u'_L}}}) \qquad (15)$$

Where $\quad \frac{D}{Dt} = \frac{\partial}{\partial t} + (\overline{\overline{\mathbf{u}}}_L.\nabla) \;, \; \frac{d}{dt} = \frac{\partial}{\partial t} + (\overline{\overline{\mathbf{u}}}_G.\nabla)$

In the equation of the momentum balance, the acceleration and the weight of the gas are neglected in comparison to the force exerted by the liquid on the bubbles $\rho_G \ll \rho_L$; so the total force exerted on the bubbles is zero as indicated in equation (14). This force contains the non disturbed flow action (pressure term or Tchen force) and the interfacial term $\mathbf{M}_G$.

In the common formulation of the momentum interfacial exchange only the contributions due the average velocities fields of the liquid and the gas phases is considered while the turbulent contributions of the interfacial force are ignored or eventually expressed via a supplementary dispersion term proportional to the void fraction gradient (Lance & Lopez de Bertonado, 1992). In their model Chahed et al. (2002) proposed to take into account beside the average contributions of the interfacial transfer, the turbulent correlations issued from the added mass force and they proved that these turbulent correlations are important in the phase distribution phenomenon, in particular in gas-liquid flow under micro-gravity condition. According to their formulation, the interfacial momentum transfer (4) includes respectively the drag force (drag coefficient C_D), the added mass force (coefficient C_A) that includes the average and turbulent contributions in the liquid and in the gas and the lift force (coefficient C_L) that is expressed with a modified lift coefficient taking into account an eventual wall interaction effect characterised by the function $f_{LP}(y^*)$ where $y^* = \frac{2y_p}{d}$ is the distance y_p from the wall normed by the bubble radius. Considering the expression of the wall force in laminar flow by Antal et al. (1991), a formulation of the function $f_{LP}(y^*)$ is proposed Chahed & Masbernat (2000).

The two-fluid model presented requires closure of the turbulent stress tensors in the liquid and in the gas. The turbulent stress tensor of the gas is related to that of the liquid through a turbulent dispersion model and the turbulent stress tensor of the liquid is computed using a

Toward a Multiphase Local Approach in the
Modeling of Flotation and Mass Transfer in Gas-Liquid Contacting Systems
147

second order closure of the turbulence developed for bubbly flows, (Chahed & Masbernat, 2003)

3.3 Turbulence modeling

The turbulence modeling is based on the decomposition of the Reynolds stress tensor of the continuous phase into two independent parts: a turbulent part $\overline{\overline{\mathbf{u}'_L \mathbf{u}'_L}}^{(T)}$ produced by the gradient of the mean velocity which also contains the turbulence generated in the bubble's wake (where an equilibrium production-dissipation is assumed) and an irrotational part $\overline{\overline{\mathbf{u}'_L \mathbf{u}'_L}}^{(S)}$ induced by bubbles displacements and controlled by the added mass effects. Each part is computed by a transport equation:

$$\frac{D}{Dt}\overline{\overline{\mathbf{u}'_L \mathbf{u}'_L}}^{(S)} = Diff(\overline{\overline{\mathbf{u}'_L \mathbf{u}'_L}}^{(S)}) + \frac{3}{20}\frac{D}{Dt}\alpha \left\|\overline{\overline{\mathbf{u}_R}}\right\|^2 \delta + \frac{1}{20}\frac{D}{Dt}\alpha\overline{\overline{\mathbf{u}_R \mathbf{u}_R}} \tag{14}$$

$$\frac{D}{Dt}\overline{\overline{\mathbf{u}'_L \mathbf{u}'_L}}^{(T)} = Diff(\overline{\overline{\mathbf{u}'_L \mathbf{u}'_L}}^{(T)}) - 2sym\left[\overline{\overline{\mathbf{u}'_L \mathbf{u}'_L}}^{(T)} \bullet \nabla\overline{\overline{\mathbf{u}_L}}\right] + \mathbf{\Phi} - \varepsilon\delta \tag{15}$$

In comparison to second order turbulence modeling in single phase flow, the diffusion and redistribution terms in the transport equation of the turbulent part were modified in order to take into account the interfacial effects. These effects are related to a time scale τ_b that characterizes the relative displacement of the bubbles.

$$Diff(\mathbf{\Psi}) = \frac{C_{S\Psi}}{1-\alpha}\nabla\left[(1-\alpha)(\tau_t\overline{\overline{\mathbf{u}'_L \mathbf{u}'_L}}^{(T)} + \tau_b\overline{\overline{\mathbf{u}'_L \mathbf{u}'_L}}^{(S)})\nabla\mathbf{\Psi}\right] \tag{16}$$

with
$$\tau_t = \frac{trace(\overline{\overline{\mathbf{u}'_L \mathbf{u}'_L}}^{(T)})}{2\varepsilon}, \ \tau_b = C_R \frac{d}{\left\|\overline{\overline{\mathbf{u}_R}}\right\|}$$

$$\mathbf{\Phi}^{(NL)} = -C_1(\tau_t^{-1} + \alpha\tau_b^{-1})\left[\overline{\overline{\mathbf{u}'_L \mathbf{u}'_L}}^{(T)} - \frac{1}{3}trace(\overline{\overline{\mathbf{u}'_L \mathbf{u}'_L}}^{(T)})\right] \tag{17}$$

Where $\mathbf{\Phi}^{(NL)}$ is the non-linear part of the redistribution term $\mathbf{\Phi}$ ($\mathbf{\Phi} = \mathbf{\Phi}^{(NL)} + \mathbf{\Phi}^{(L)}$). The linear part $\mathbf{\Phi}^{(L)}$ and the dissipation rate ε are modeled as in single-phase flow. The reduction of the second order closure of the turbulence furnishes the following turbulent viscosity in bubbly flows, (Chahed et al., 2003):

$$\nu_t = \nu_{t0}\frac{(1+\frac{C_{\mu b}}{C_{\mu 0}}\frac{k_S}{k_0})}{(1+\alpha\frac{\tau_t}{\tau_b})} \tag{18}$$

Where $v_{t0} = C_{\mu 0} \dfrac{k_0^2}{\varepsilon}$ is the equivalent single-phase flow turbulent viscosity,

$k_0 = \dfrac{trace(\overline{\mathbf{u}_L^{'}\mathbf{u}_L^{'}})^{(T)}}{2}$ and $k_S = \dfrac{trace(\overline{\mathbf{u}_L^{'}\mathbf{u}_L^{'}})^{(S)}}{2}$ are respectively the turbulent and the pseudo-turbulent parts of the kinetic turbulent energy in the liquid phase. The two coefficients $C_{\mu 0}$ and $C_{\mu b}$ depend on the turbulence and the pseudo-turbulence anisotropy. The equation (18) expresses two antagonist interfacial effects on the turbulent viscosity: the bubbles agitation induces in one hand an enhancement of the turbulent viscosity and on the other hand a modification of the characteristic scale of the eddies stretching which can reduces the shear stress.

3.4 Transport equation of concentration

Recall that we consider gas-liquid bubbly flow with low solubility of the gas in the liquid. As a result the effect of the mass transfer on the dynamic of the gas-liquid flow is neglected. Without the source term associated with external inputs or reactive exchanges, we consider that the mass transfer is limited to mass flux through the gas-liquid interface we can write, in these conditions, a transport equation of a concentration of the liquid in general form:

$$\frac{DC}{Dt} = Diff(C) + S_c \qquad (19)$$

Where S_c is transfer term through the interface given by equation (11)

3.5 Some results and discussion: Requirements for advanced computation of gas-liquid contacting systems

a) Turbulence modeling

The second order turbulence model presented above predicts correctly the large enhancement of the momentum diffusivity observed in bubbly flow with an important amount of pseudo-turbulence as in mixing layer and wake bubbly flows, (Chahed et al., 2003). On the other hand, the model reproduces the turbulence structure as it is altered by the bubble presence in the boundary layer bubbly flows, figure (4) and pipe bubbly flows figure (5). Figure (4) shows the profiles of the turbulent intensity in the liquid phase produced by the two-fluid model in near wall boundary layer bubbly flow for single phase and two-phase bubblys flows. These profiles are compared to the experimental data of Moursali et al. (1995). Note that y^+ denoted the adimensional distance to the wall $y^+ = \dfrac{u_* d}{\nu}$ where u_* is the friction velocity, d distance to the wall and ν is the kinematic viscocity of the liquid. Figure (5) shows the profiles of the turbulent shear stress produced by the two fluid model in a pipe single phase and bubbly flows. The numerical results are compared to the experimental data of Serizawa (1992). The results of all of these simulations make clear the mechanisms whereby the attenuation of the turbulence in bubbly flows can occurs: the supplementary stretching induced by the bubbles displacements provokes an attenuation of the shear stress, as a result the turbulence production by the mean velocity gradient is reduced and we can note a diminution of the turbulent intensity as observed in some experiences of wall-bounded bubbly flows.

The decomposition of the Reynolds stress tensor in a turbulent and pseudo-turbulent contributions with specific transport equation for each part makes possible the computation of the specific scales involved in each part. The determination of these scales allows to describe correctly the different effects of the bubbles agitation on the liquid turbulence structure.
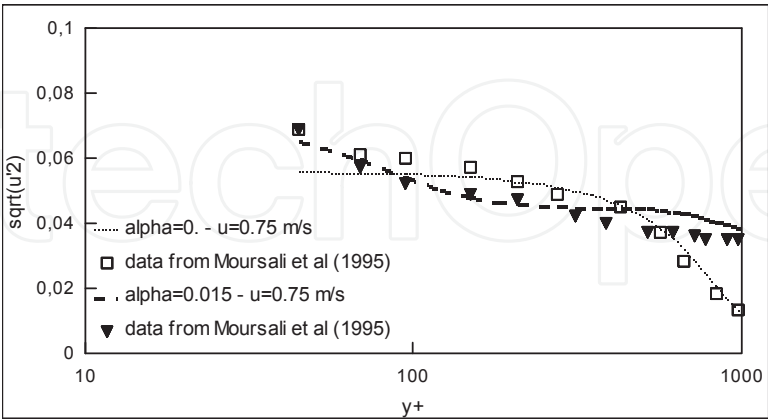

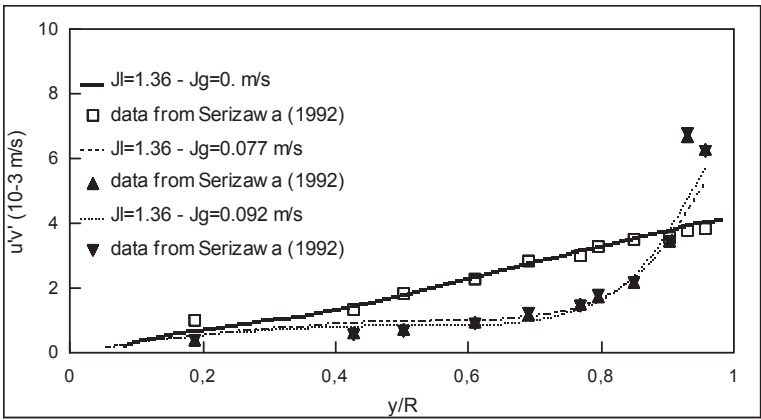Fig. 4. Turbulent intensity in single-phase and bubbly boundary layer.

Fig. 5. Turbulent shear stress in single-phase and bubbly pipe flows.

If from a theoretical point of view, second order is an adequate level for turbulence closure in bubbly flows, the implementation of such turbulence models in two-fluid models clearly improves the predetermination of the turbulence structure in different bubbly flow configurations, (Chahed et al., 2002, 2003). Nevertheless, from a practical point of view, second order modeling is still difficult to use and turbulence models based on turbulent viscosity concept, particularly two-equation models, remain widely used in industrial applications. Several two-equation models were developed for turbulent bubbly flows (Lopez de Bertodano et al., 1994; Lee et al., 1989; Morel, 1995; Troshko & Hassan, 2001). All of these models are founded on an extrapolation of single-phase turbulence models by introducing supplementary terms (source terms) in the transport equations of turbulent energy and dissipation rate. In some models, the turbulent viscosity is split into two contributions according to the model of Sato et al. (1981): a "turbulent" contribution induced by shear and a "pseudo-turbulent" one induced by bubbles displacements. To adjust the turbulence models some modifications of the conventional constants are sometimes proposed (Lee et al., 1989; Morel, 1995).

The reduction of second order turbulence modeling developed for two-phase bubbly flows furnish an interpretation of second order turbulence closure in term of turbulent viscosity

model. On the basis of this turbulent viscosity model, two-equation turbulence models (k-ε model, (Chahed et al., 1999) and k-ω model (Bellakhel et al., 2004) were developed and applied to homogeneous turbulence in bubbly flows (uniform and with a constant shear). The numerical results clearly show that the model reproduces correctly the effect of the bubbles on the turbulence structure.

The turbulent viscosity formulation (18) keeps the essential of the physical mechanisms involved in second order turbulence modeling. It expresses two antagonist interfacial effects due to the presence of the bubbles on the turbulent shear stress of the liquid phase: the bubbles agitation induces in one hand an enhancement of the turbulent viscosity as compared to and on the other hand a modification of the eddies stretching characteristic scale that causes more isotropy of the turbulence with an attenuation of the shear stress. According as the amount of pseudo-turbulence is important or not, we can expect an increase or a decrease of the turbulent viscosity. As a result, the turbulent shear stress in bubbly flow can be more or less important than the corresponding one in the equivalent single-phase flow. In the case where the turbulent shear stress is reduced, the turbulence production by the mean velocity gradient is lower and we can reproduce, under certain conditions, an attenuation of the turbulence as observed in some wall bounded bubbly flows (Liu and Bankoff, 1990; Serizawa et al., 1992).

Void fraction and bubbles size distributions

The distribution of void fraction is governed by the interfacial forces exerted by the continuous phase on the bubbles as they move throughout the liquid. We have to specify the contributions of the average and fluctuating flow fields to this force. Numerical simulations of upward pipe bubbly flow in micro-gravity and in normal gravity conditions show clearly the role of the turbulence and of the interfacial forces on the void fraction distribution, (Chahed et al., 2002). These numerical simulations are compared to the experimental data of Kamp. et al. (1994). An important result of these experiences is to show that the radial void fraction gradient is inverted according as the gravity is active or not (according as the interfacial momentum transfer associated with the average relative velocity is important or not). Figure (5) shows the profile of void fraction in pipe upward and downward bubbly flows in microgravity and in normal gravity conditions. In micro-gravity condition, the average relative velocity between phases is weak; thus the action of the continuous phase on the bubbles is reduced to the pressure gradient effect (Tchen force) and to the turbulent contributions of the interfacial force. The pressure gradient effect provokes a bubble migration toward the wall and can't explain the experimental void fraction profile. When the turbulent terms issued from the added mass force are introduced, the whole action of turbulence is inverted and the phase distribution prediction is in good agreement with the experimental data.

This result indicates that the effect of the continuous phase turbulence on the phase distribution includes, beside the pressure gradient action (Tchen force), the turbulent contributions of the interfacial forces. Consequently, the accuracy in the predetermination of the turbulence of the dispersed phase is also for importance in the computation of the void fraction distribution. The turbulent stress tensor of the dispersed phase can be related to the liquid one through a turbulent dispersion models, (Hinze, 1975; Csanady, 1963). The recent results issued from numerical simulations can be viewed as a prelude to more progress in this direction.

As compared to the void fraction profile in micro-gravity condition, the prediction of the void fraction distribution in upward and downward bubbly flows in normal gravity conditions clearly shows the effect of the lift force. In upward flow, the lift force is

responsible of the near-wall void fraction peaking while in downward flow, the lift force action is inverted and the migration of the bubble toward the centre of the pipe provoked by the global turbulent action is more pronounced than in micro-gravity condition. The adjustment of the coefficients in the expression of the near wall lift force was tested in boundary layer bubbly flow ($\overline{\overline{u}} = 0.75\,m/s$ and $\overline{\overline{u}} = 1\,m/s$) with bubble's diameter between 2.3 and 3.5 mm (the more is the external void fraction the more is the bubble diameter); in these simulations the diameter of the bubbles was adjusted from the experimental data of Moursali et al. (1995). It yields C_L =0.08, y_1^* =1 and y_2^* =1.5. These computations allow us to consider that these coefficients could have a somewhat general character. The value of y_1^* suggests that the position of the void fraction peaking is, for the most part, controlled by lift and wall forces: its value corresponds to the void fraction peaking position observed in the experiences.
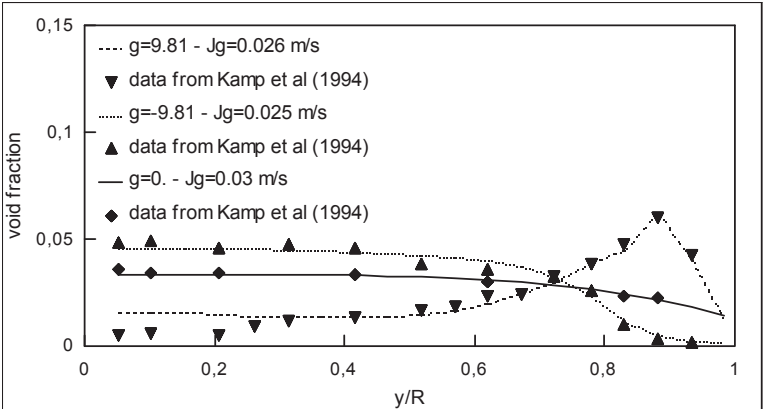

Fig. 5. Void fraction distribution in pipe bubbly flows : upward – downward and in micro-gravity conditions. Data from Kamp et al. (1995)
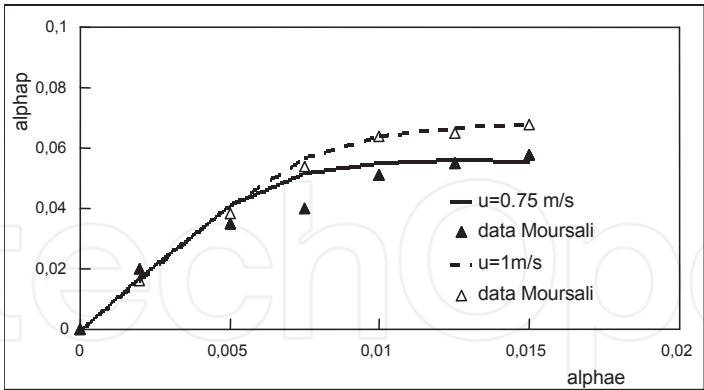

Fig. 6. Amplitude of the near wall void fraction peaking as a function of the external void fraction in boundary layer bubbly flow.

Figure (6) shows that the less is the bubble diameter the more is amplitude of the void fraction peaking near wall. This result is well reproduced by the model for millimetric bubbles: the lift force formulation including the wall effect brings implicitly into account the bubble size. When the bubble's size becomes greater and its shape deviates severely from the sphericity the expression of the force exerted by the liquid should be reviewed. Also on this point, we can expect some progress issued from the numerical simulation. On the other hand.

4. Conclusion

Many industrial processes in chemical, environmental and power engineering employ gas-liquid contacting systems that are often designed to bring about transfer and transformation phenomena in two-phase flows. As for all gas-liquid contacting systems, flotation devices bring into play gas-liquid bubbly flows where the interfacial interactions and exchanges determine not only the dynamics of the system but are, in the same time, the technological reason of the process itself. When applied to flotation, mass transfer approach turns out to be very convenient for representing various behaviors of the flotation kinetics. It allows a more phenomenological approach in the analysis of the interfacial phenomena involved in the flotation process.
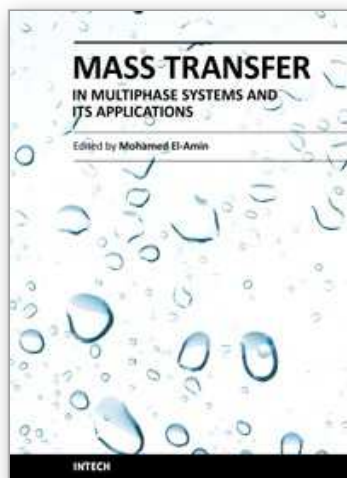
From a practical point of view, the development of general models which are able to predict the fields of certain average kinematic properties of both gas and liquid phases and their presence rates in two-phase flows is of great interest for the design, control and improvement of gas-liquid contacting systems. From the scientific point of view, the modeling and simulation of gas-liquid flows set many important questions; in particular the ability to predict the phase distribution in gas-liquid bubbly flows remains limited by the inadequate modeling of the turbulence and of the interfacial forces. Especially in industrial gas-liquid systems characterized by various additional complexities such as : the geometry of the reactor, the hydrodynamic interactions particularly in dense gas-liquid flows (high void fraction), the chemical reactivity, the interfacial area modulation due to the phenomena of rupture and coalescence... All of these issues require new original experiments in order to sustain the modeling effort that aims at developing more general closures for advanced Computational Fluid Dynamics of complex gas-liquid systems.

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