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Short Communication

Modeling of mass-transfer in bubbly flows encompassing different mechanisms

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HIGHLIGHTS

- The relevance of different mechanisms for mass transfer in bubbly flows is assessed.
- Both laminar and turbulent contributions are found important under suitable conditions.
- Comparison with literature data reveals that large eddies dominate the turbulent regime.
- A tentative model covering both regimes and the transition between them is proposed.
- The need for further experiments to reach a final conclusion is emphasized.

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ABSTRACT

Models proposed to describe the liquid side mass transfer coefficient in absorption processes differ widely in such basic questions as on which of the local flow variables they are based. Comparison of different alternatives with experimental data taken from the literature suggests that there are two basic mechanisms, a laminar and a turbulent one, each of which dominates under suitable conditions. A dimensionless number that allows to identify the corresponding regimes is suggested together with a preliminary model encompassing both. New experiments will be needed to come to a final conclusion.

1. Introduction

Mass-transfer from gas bubbles to the surrounding liquid or vice versa is an important consideration in chemical engineering. Models of this process that can be used in full CFD simulations or simplified treatments of industrial equipment have been proposed for a long time. However even quite basic questions apparently have not yet found definitive answers.

This is evidenced for example by looking at some recent works performing Euler–Euler simulations of bubble- and airlift-columns. Talvy et al. (2007), Wiemann and Mewes (2005), and Cockx et al. (2001) use correlations for the mass transfer coefficient involving the mean bubble motion relative to the liquid. Dhanasekharan et al. (2005) use a correlation based on liquid turbulence. Wang and Wang (2007) provide a comparison of models of both types. Krishna and van Baten (2003) simply take the mass-transfer coefficient as constant. Similarly for aerated stirred tanks Fayolle et al. (2007) use a correlation based on bubble size and relative velocity. Gimbun et al. (2009) compare this to a correlation based on liquid turbulence.

Obviously it is not even clear on which parameters the mass transfer coefficient depends, let alone what form the dependence should have. Broadly there are two types of models which assume different mechanisms, namely (i) laminar or mean flow and (ii) turbulent eddies, to govern the mass-transfer. Note that laminar and turbulent flow conditions here refer to the external flow to which the bubbles are subjected. In addition there is a flow disturbance created by the bubbles which in a quiescent flow contains a stationary wake for smaller bubbles while vortex shedding occurs for larger bubbles depending on the material properties (e.g. Clift et al., 1978). Effects of externally imposed flows, in particular turbulent ones, on the wake structure and vortex shedding dynamics are not comprehensively understood yet. Notwithstanding the importance of wake effects on the mass transfer, we here focus on the influence of different external flow conditions.

An attempt to delineate regimes where each of the two mechanisms, i.e. laminar or turbulent external flow, is dominant has been made by Alves et al. (2006) on the basis of data for vertical bubbly pipe flow from Vasconcelos et al. (2002). However, their

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Nomenclature

Notation	Denomination (Unit)
d_B	bulk bubble diameter (m)
D_A	diffusion coefficient of transferred species ($m^2\ s^{-1}$)
D_H	equivalent hydrodynamic diameter of duct (m)
Eo	Eötvös Number (–)
f	Fanning friction factor (–)
J_L	liquid volumetric flux = superficial velocity ($m\ s^{-1}$)
k_L	mass transfer coefficient ($m\ s^{-1}$)
Mo	Morton Number (–)
Re	Reynolds number (–)
Sc	Schmidt number (–)
Sh	Sherwood number (–)
u_{rel}	bubble relative velocity ($m\ s^{-1}$)
ε	turbulent dissipation rate ($m^2\ s^{-3}$)
κ	turbulent kinetic energy ($m^2\ s^{-2}$)
Λ	turbulent integral length scale (m)
ν	kinematic viscosity ($m^2\ s^{-1}$)
τ_c^{-1}	inverse contact time = renewal rate (s^{-1})

main result is not expressed in a way that is applicable as a general estimate as will be explained below. Moreover, the selection of models to obtain quantitative estimates for both mechanisms may not be adequate for the flow configuration considered and no attempt at a unified model comprising both regimes is made.

To this end we here use a simple conceptual model applicable to both external flow situations, namely the penetration model of Higbie (1935) and Danckwerts (1951) (see Kulkarni (2007) for an overview of more recent developments). While this neglects many effects such as bubble deformation and wake, it specifically allows to treat both mechanisms within one and the same framework. While the present contribution still falls short to provide definitive answers, some progress can be made concerning these issues which may be helpful to direct further research on the topic, in particular the acquisition of new high accuracy data covering a large range of flow conditions. Such data may be obtained by using experimental (e.g. Kueck et al., 2009, Jimenez et al., 2013) or direct numerical simulation techniques (e.g. Ganguli and Kenig, 2011, Deising et al., 2016), which have recently been developed to a stage that local concentration fields around a bubble can be mapped with good resolution.

The paper is organized as follows. Some of the available modeling options are summarized in Section 2 and discussed in comparison with a selection of experimental data in Section 3. Following the discussion in Section 4, a proposal for a preliminary unified model is made from which estimates on the transition between both regimes can be drawn.

2. Mass-transfer models

In the following we assume that the resistance to mass-transfer is dominated by the liquid side so that only the liquid mass-transfer coefficient k_L needs to be considered. This assumption applies e.g. during absorption from gas bubbles which are saturated with the transferred species. Predictions of k_L are frequently made based on the penetration model. While this simple conceptual model may not provide a high quantitative accuracy it seems well suited to discuss the general questions posed above.

The penetration model Higbie (1935) considers one-dimensional time-dependent diffusion of the transferred component from the interface with a bulk concentration imposed at infinity. These approximations are suitable for a thin concentration boundary layer at a fluid interface. The mass flux at the interface is evaluated from Fick's law and averaged over a time-interval up to the so-called contact time τ_c. After this time the surface is supposed to be renewed, i.e. to be brought into contact with liquid at the bulk concentration. Depending on the mechanism by which this renewal occurs, different expressions are used for the contact time to be discussed shortly. The expression obtained for the mass-transfer coefficient is

$$k_L \propto \frac{2}{\sqrt{\pi}}\left(D_A \tau_c^{-1}\right)^{1/2} \tag{1}$$

where D_A denotes the diffusion coefficient of the transferred component A in the liquid. There are more refined versions of the model (Dankwerts, 1951) which do not take all elements of the surface to have the same contact time but instead allow a distribution of contact times. A few examples of contact time distributions considered in Danckwerts et al. (1963) give the same functional dependence of k_L on τ_c, the latter now being interpreted as the average contact time. Only the prefactor in Eq. (1) is modified in these examples. Admitting that some adjustment of the prefactor may be necessary in the end to obtain agreement with measured values for k_L we keep the value used in Eq. (1) for the time being and focus on the parameters on which contact time is supposed to depend.

Three expressions are frequently used for τ_c. The first one was proposed by Higbie (1935) assuming laminar flow around the bubble in which fluid elements enter the interface at the front stagnation point and leave it at the rear one. This results in the expression

$$\tau_c^{-1} = \frac{u_{rel}}{d_B} \tag{2}$$

where d_B is the bubble size and u_{rel} its velocity relative to the liquid.

The two other expressions assume homogeneous and isotropic turbulent flow but take eddies of different size to dominate the interface renewal. Fortescue and Pearson (1967) proposed that this process is governed by the largest eddies in the universal turbulent spectrum. This gives the equivalent expressions

$$\tau_c^{-1} \propto \frac{\varepsilon}{\kappa} \propto \frac{\Lambda}{\sqrt{\kappa}} \propto \frac{\sqrt{2}\ \varepsilon^{1/3}}{\Lambda^{2/3}} \tag{3}$$

where κ, ε and Λ denote the turbulent kinetic energy, dissipation and, integral length scale.

In contrast, Lamont and Scott (1970) took the smallest eddies, i.e. those in the dissipation range, as the relevant ones. Then the expression

$$\tau_c^{-1} \propto \left(\frac{\varepsilon}{\nu}\right)^{1/2} \tag{4}$$

is obtained, where ε is again the turbulent dissipation and ν the viscosity of the liquid.

The original works (Fortescue and Pearson, 1967, Lamont and Scott, 1970) contain additional prefactors in Eq. (1) which come from assumptions on the local velocity field within a turbulent eddy. Since this introduces additional hypotheses which are hard to verify we discard them here in line with the consideration above.