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Short communication

# Phenomenological simulation model for gas hold-ups and volumetric mass transfer coefficients in external-loop airlift reactors

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**Abstract**

The phenomenological simulation model, proposed previously by the authors for bubble columns, was extended to examine gas hold-ups and volumetric mass transfer coefficients in external-loop airlift reactors. The proposed simulation model is based on bubble break-up and coalescence — both being primary phenomena in airlift reactors. The characteristic liquid velocity in external-loop airlift reactors is assumed to be the superficial liquid velocity in the riser instead of the liquid velocity at the column axis in bubble columns. The predictions of the proposed phenomenological simulation model compare favourably with the present experimental results and the data published in the literature. 

*Keywords:* External-loop airlift; Phenomenological simulation model; Gas hold-up; Volumetric mass transfer coefficient

## 1. Introduction

In our previous work [1], a simulation model for gas hold-up and gas–liquid mass transfer in bubble columns was developed. It is based on a phenomenological model for bubble break-up and coalescence. In order to describe bubble movements in a bubble column, a compartment concept is combined with the population balance model for bubble break-up and coalescence. The bubble column is assumed to consist of a series of discrete compartments in which bubble break-up and coalescence occur and bubbles move from compartment to compartment with different velocities. The model reasonably predicts gas hold-ups and volumetric mass transfer coefficients in bubble columns. In this study, the simulation model developed for bubble columns has been extended to external-loop airlift reactors. The capability of the phenomenological simulation model has been examined using the present experimental data and the results available in the literature. The external-loop airlift reactors have potential applications in various areas such as organic synthesis, biodegradation of polluted air and fermentation [2–5]. The obvious advantages of its design are a well-defined flow path, high gas capacity, low shear levels and good temperature control. The gas entering from the bottom through a sparger and leaving the top induces a circulatory flow of liquid up the riser and down the downcomer. The hydrostatic pressure difference between the riser and the downcomer ensures continued stable liquid circulation. The bubble size determined by bubble break-up and coalescence governs gas hold-up and gas–liquid mass transfer in airlift reactors. Although hydrodynamics and mass transfer in external-loop airlift reactors have been extensively studied and modeled, no correlations for design parameters are based on bubble phenomena, i.e. bubble break-up and coalescence. Computational fluid dynamic (CFD) models have been recognized as ultimate tools to understand hydrodynamics in the bubble column and airlift reactors. In numerical simulations, however, bubble phenomena have not been sufficiently taken into account. Consequently, an establishment of simulation model based on bubble break-up and coalescence phenomena is necessary to provide comprehensive pictures of bubble phenomena in airlift reactors.

## 2. Model

The schematic description of the phenomenological simulation model for an external-loop airlift reactor is illustrated in Fig. 1. The model for external-loop airlift reactor is very

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**Nomenclature**

| | |
|---|---|
| $A_d$ | downcomer cross-sectional area ($m^2$) |
| $A_r$ | riser cross-sectional area ($m^2$) |
| $a$ | specific surface area ($m^{-1}$) |
| $D_r$ | riser diameter (m) |
| $d_{bi}$ | bubble diameter (m) |
| $g$ | gravitational acceleration ($m\,s^{-2}$) |
| $k_l$ | liquid-phase mass transfer coefficient ($m\,s^{-1}$) |
| $U_l$ | characteristic liquid velocity in the bubble column or airlift reactor ($m\,s^{-1}$) |
| $U_{lr}$ | superficial liquid velocity in the riser ($m\,s^{-1}$) |
| $U_{gr}$ | superficial gas velocity in the riser ($m\,s^{-1}$) |
| $u_r$ | bubble rising velocity in a still liquid ($m\,s^{-1}$) |
| $u'_r$ | actual bubble rising velocity ($m\,s^{-1}$) |

*Greek letters*

| | |
|---|---|
| $\phi_{gr}$ | riser gas hold-up |
| $\lambda'$ | parameter in Eq. (1) |
| $\rho_l$ | liquid density ($kg\,m^{-3}$) |
| $\sigma$ | surface tension ($N\,m^{-1}$) |

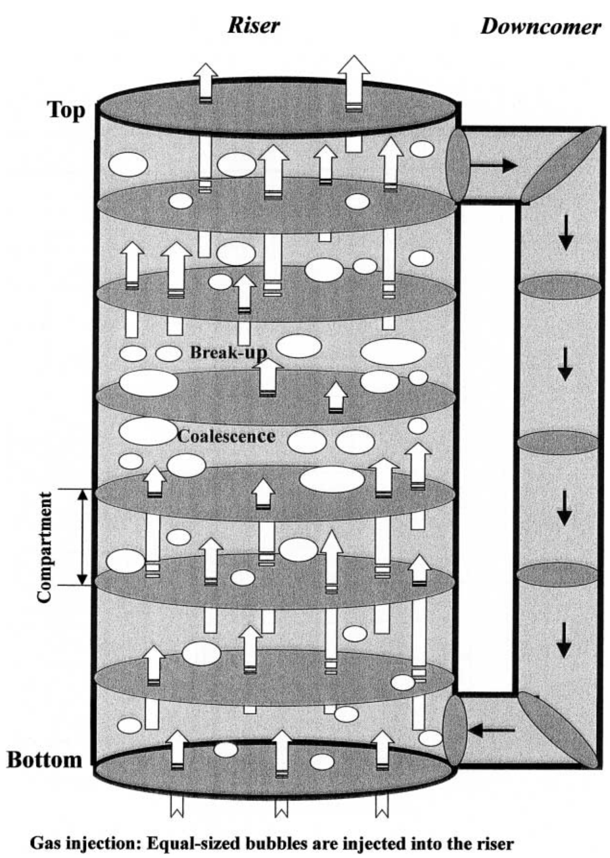


Fig. 1. Schematic description of the phenomenological simulation model for an external-loop airlift reactor.

similar to that for the bubble columns proposed by Shimizu et al. [1] except the characteristic velocity for the estimation of the shear stress and the bubble rising velocity described below. The simulation procedure is the same as used for the simulation of bubble columns [1]. The riser is considered to consist of hypothetical compartments being completely mixed. It is assumed, for simplification, that bubbles rise only in the riser and no bubbles are dragged into the downcomer by liquid circulation. It implies that the downcomer is a conduit connected to the top and the bottom of the riser and it is not necessary to consider bubble phenomena in the downcomer.

Since the liquid in a bubble column flows downwards near the wall and upwards in the center, the characteristic liquid velocity in bubble columns, $U_l$, is assumed to be the liquid velocity at the column axis. In bubble columns operated in a semibatch manner, i.e. with a continuous gas flow into a batch liquid volume, the gulf-stream type of liquid circulation is observed and the average cross-sectional area of the axial liquid velocity is zero. However, in external-loop airlift reactors, liquid flow is uniformly upwards in the riser section and downwards in the downcomer section. In external-loop airlift reactors, therefore, relatively well-ordered liquid flow in the riser may be characterized by the superficial liquid velocity enhanced due to the existence of the downcomer. Kawase [6] proposed a theoretical correlation of superficial liquid velocity in the riser, $U_{lr}$, for external-loop airlift reactors:

$$U_{lr} = 9.81 \times \lambda'(gD_rU_{gr})^{1/3} \tag{1}$$

where $\lambda'$ for non-electrolyte solutions or coalescing systems is given as

$$\lambda' = 0.25\left(\frac{A_d}{A_r}\right) \tag{2}$$

The correlation gives reasonably good predictions for liquid velocity in the riser of external-loop airlift reactor. The superficial liquid velocity in the riser, $U_{lr}$, estimated by Eq. (1), is used as a characteristic velocity, $U_l$, in estimation of the shear stress exerted on the bubble.

In a hypothetical compartment, bubble break-up and coalescence occur simultaneously and the bubble size distribution changes. Bubbles move from lower hypothetical compartment to the upper one according to the bubble rising velocity. The bubble rising velocity in the riser is evaluated by the following equation:

$$u'_r = u_r + U_l = \left\{\left(\frac{2.14\sigma}{\rho_l d_{bi}}\right) + 0.505 g d_{bi}\right\}^{0.5} + U_{lr} \tag{3}$$

The superficial liquid velocity estimated by Eq. (1), $U_{lr}$, is also utilized to compute the bubble rising velocity.

At the start of a simulation, bubbles having a uniform size exist only in the bottom compartment. From the bottom compartment to the top compartment, the new bubble size distribution is calculated by taking account of the rates for bubble break-up and coalescence and then their new locations are evaluated from their rising velocities using Eq. (3). The same simulation procedure for a number of simulation times is repeated till a steady state is attained.

The gas hold-up in the riser, $\phi_{gr}$, was estimated by adding simply the volume of all bubbles in the riser [1]. The volumetric mass transfer coefficient, $k_l a$, was evaluated using the relationship for the specific surface area, $a$, related to gas hold-up and Higbie's penetration theory for $k_l$ as well as our previous work for bubble columns [1].

## 3. Experimental

Experiments were carried out in an external-loop airlift composed of a riser having a diameter of 0.155 m, a downcomer having a diameter of 0.070 m and a bubble column 0.155 m in diameter. They are the same as used in our previous studies [1,7]. Tap water and air were used as the liquid phase and gas phase, respectively. The operation was batchwise with respect to liquid phase. The gas hold-ups were obtained by the volume expansion method and the volumetric mass transfer coefficients were determined by the dynamic method [1,7].

## 4. Results and discussion

In Fig. 2, gas hold-up measurements are shown as a function of the superficial gas velocity in the riser. The riser gas hold-up depended on the riser superficial gas velocity. The simulation model is compared with the present experimental data for the riser gas hold-ups in the external-loop airlift reactor. The model agrees reasonably well with the experimental data. For comparison, the experimental data and the simulation results for the bubble column ($A_d/A_r = 0$) are also plotted in Fig. 2. The gas hold-ups in the external-loop airlift reactors were lower as compared with those in the bubble column. The well-defined liquid circulation induced in the external-loop airlift enhanced the bubble rising velocities and as a result, reduced gas hold-up [8].

Volumetric mass transfer coefficients are shown plotted against superficial gas velocity in the riser in Fig. 3. The $k_l a$ coefficient increased with increasing $U_{gr}$. The $k_l a$ data in the external-loop airlift, presented in Fig. 3, agree reasonably with the predictions of the proposed simulation model. For comparison purposes, the data and predictions of the simulation model for $k_l a$ coefficients in the bubble column ($A_d/A_r = 0$) are also presented. The $k_l a$ coefficient in the airlift reactor was lower than that in the bubble column. As shown in Fig. 3, of course, this coincides with the model prediction. With an increase of liquid velocity resulting in a decrease of gas hold-up, the specific surface area, $a$, decreased and then $k_l a$ decreased.

The predictions of the simulation model are compared with the experimental results for water published in the literature [9–13] in Fig. 4. It is seen that the model agrees satisfactorily with the available data obtained in external-loop airlift reactors with $D_r = 0.1$–$0.23$ m and $A_d/A_r = 0.25$–$1.0$. The average percentage error is about 14.4%.

Fig. 5 depicts a comparison of the proposed model with the available data [9–11,13] for volumetric mass transfer coefficients in external-loop airlift reactors over a range of $D_r = 0.1$–$0.23$ m and $A_d/A_r = 0.25$–$1.0$. The model

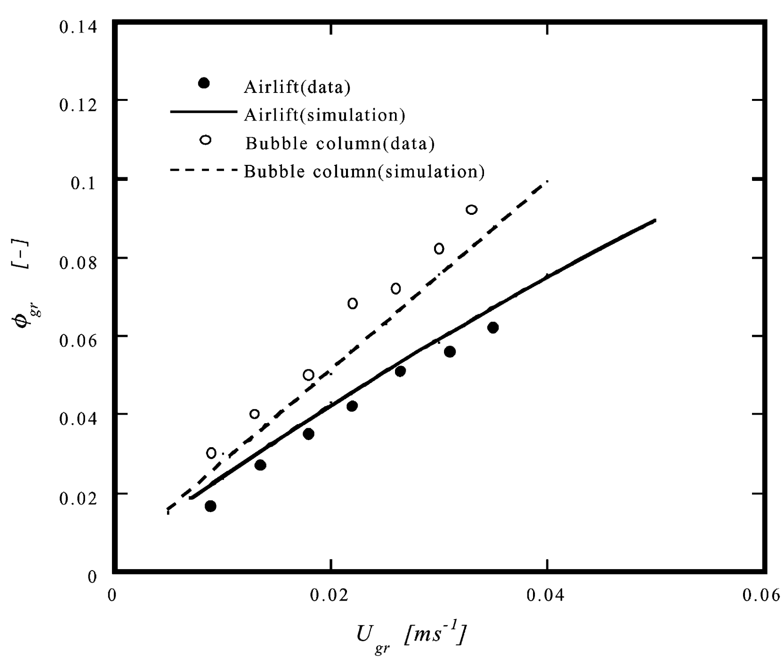


Fig. 2. Gas hold-ups in external-loop airlift reactor and bubble column.

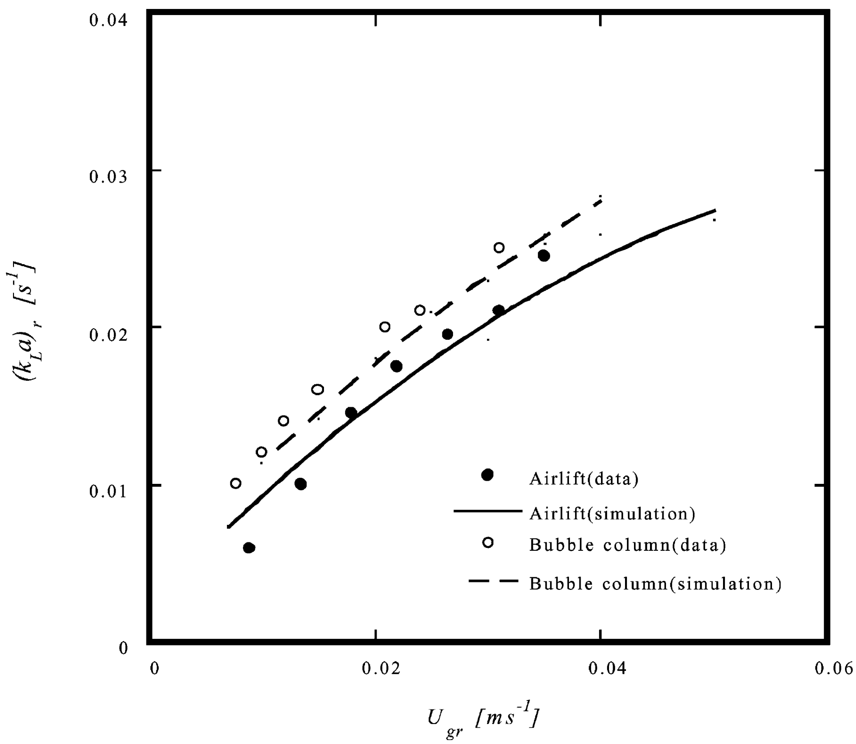


Fig. 3. Volumetric mass transfer coefficients in external-loop airlift reactor and bubble column.

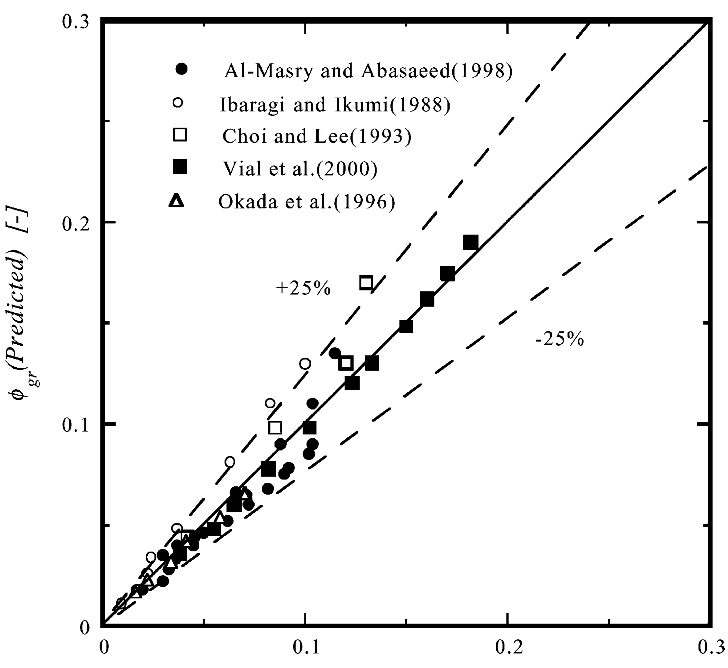


Fig. 4. Comparison between the predicted and experimental results of gas hold-up in external-loop airlift reactors.

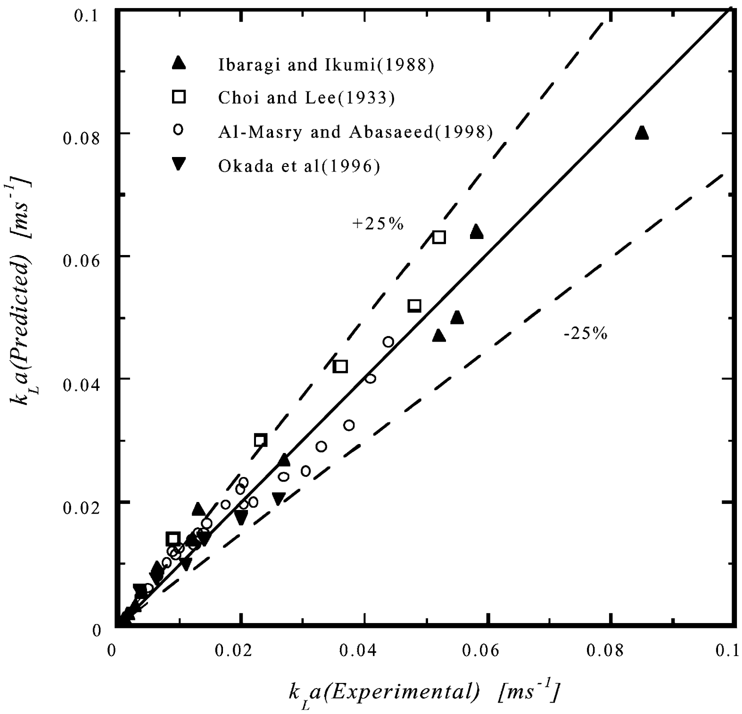


Fig. 5. Comparison between the predicted and experimental results of volumetric mass transfer coefficient in external-loop airlift reactors.

predicts the available data with the average percentage error of about 8.8%.

## 5. Conclusions

A phenomenological simulation model based on bubble phenomena has been developed to describe hydrodynamics and mass transfer in external-loop airlift reactors by extending the model for bubble columns of Shimizu et al. [1]. The proposed simulation model was in good agreement with the present experimental data and the available data in the literature. The experimental data used in this work to examine the validity of the proposed model does not cover those in large diameter reactors. For more discussion of the general applicability of the proposed model, therefore, data on gas hold-ups and volumetric mass transfer coefficients in larger external-loop reactors including commercial-scale reactors are highly desirable.

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