

# On the modeling of an airlift reactor

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## Abstract

A model of an airlift reactor in the cases of interphase mass transfer between gas and liquid in the riser and chemical reaction in the liquid phase has been done. The model equations permit to obtain the vertical distribution of the average concentrations of an active gas component in gas and liquid phases and average concentration of the active liquid component, using average velocities and effective diffusivities in the riser and downcomer zones. The proposed model allows scale-up problem solution. An hierarchical approach for model parameter identification on the bases of experimental data has been proposed.

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## 1. Introduction

The hydrodynamic behavior of the gas and liquid flows in airlift reactors is very complicated. In these conditions the convective and diffusive transfer with volume reactions are realized simultaneously. The convective transfer is result of a laminar or turbulent (large-scale pulsations) flows. The diffusive transfer is molecular or turbulent (small-scale pulsations). The volume reactions are mass sources as a result of chemical reaction and interphase mass transfer [1].

The scale-up theory [2] show, that the scale-effect in mathematical modeling is result of the radial nonuniformity of the velocity distribution in the columns. In many papers [3–6] are used diffusion models, where the scale-effect is considered as an increase of the axial mixing.

The creation of the models in these conditions and solving of the scale-up problem [1] require construction of a suitable diffusion model.

## 2. Mathematical model

The investigation of the airlift reactors shows [7–9] that convection–diffusion equation with volume reaction may be use as a mathematical structure of the model.

Let us consider airlift reactor [10–13] with a cross-section area  $F_0$  for the riser zone and  $F_1$  for the downcomer zone. The length of the working zones is  $l$  (Fig. 1). The gas flow rate is  $Q_0$  and the liquid flow rate,  $Q_1$ . The gas and liquid hold-ups in the riser are  $\varepsilon$  and  $(1 - \varepsilon)$ .

The concentrations of the active gas component in the gas phase is  $c(x, r, t)$  and in the liquid phase,  $c_0(x, r, t)$  for the riser and  $c_1(x_1, r, t)$  – for the downcomer, where  $x_1 = l - x$ .

The concentration of active liquid component in the downcomer is  $c_2(x_1, r, t)$  and in the riser –  $c_3(x, r, t)$ .

The average velocities in gas and liquid phases at the inlet (outlet) of the column are

$$\bar{u}_0 = \frac{Q_0}{F_0}, \quad \bar{u}_1 = \frac{Q_1}{F_0}, \quad \bar{u} = \frac{Q_1}{F_1}. \quad (1)$$

The interphase mass transfer rate in the riser is

$$R = k(c - \chi c_0). \quad (2)$$

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### Nomenclature

$c$	active gas component concentration in the gas phase in the riser ( $\text{mol m}^{-3}$ )	$R_1$	chemical reaction rate in the riser ( $\text{mol m}^{-3} \text{s}^{-1}$ )
$c_0$	active gas component concentration in the liquid phase in the riser ( $\text{mol m}^{-3}$ )	$R_2$	chemical reaction rate in the downcomer ( $\text{mol m}^{-3} \text{s}^{-1}$ )
$c_1$	active liquid component concentration in the downcomer ( $\text{mol m}^{-3}$ )	$k_0$	chemical reaction rate constant
$c_2$	active gas component concentration in the downcomer ( $\text{mol m}^{-3}$ )	$k$	mass transfer coefficient ( $\text{s}^{-1}$ )
$c_3$	active liquid component concentration in the riser ( $\text{mol m}^{-3}$ )	$\chi$	Henry's number
		$R$	interphase mass transfer rate ( $\text{mol m}^{-3} \text{s}^{-1}$ )
		$\alpha$	reaction order

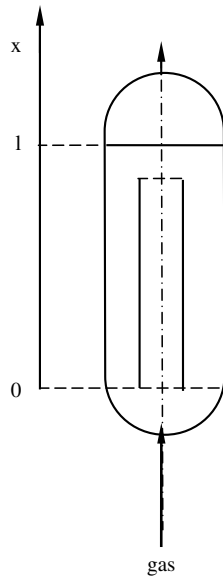


Fig. 1. Airlift reactor.

The chemical reaction rates in the riser and in the downcomer are

$$R_1 = k_0 c_0^{\alpha_1} c_3^{\alpha_2}, \quad R_2 = k_0 c_1^{\alpha_1} c_2^{\alpha_2}. \quad (3)$$

The mathematical model of the chemical processes in airlift reactor will be built on the basis of the differential mass balance in the reactor volume [1]. A convection–diffusion equations with volume reaction will be used.

The equations for the active gas component concentration distributions in the gas and liquid phases in the riser are

$$\varepsilon \frac{\partial c}{\partial t} + \varepsilon u_0 \frac{\partial c}{\partial x} + \varepsilon v_0 \frac{\partial c}{\partial r} = \varepsilon D \left( \frac{\partial^2 c}{\partial x^2} + \frac{1}{r} \frac{\partial c}{\partial r} + \frac{\partial^2 c}{\partial r^2} \right) - k(c - \chi c_0),$$

$$\frac{\partial u_0}{\partial x} + \frac{\partial v_0}{\partial r} + \frac{v_0}{r} = 0, \quad (4)$$

$$(1 - \varepsilon) \frac{\partial c_0}{\partial t} + (1 - \varepsilon) \left( u_1 \frac{\partial c_0}{\partial r} + v_1 \frac{\partial c_0}{\partial x} \right)$$

$$= (1 - \varepsilon) D_0 \left( \frac{\partial^2 c_0}{\partial x^2} + \frac{1}{r} \frac{\partial c_0}{\partial r} + \frac{\partial^2 c_0}{\partial r^2} \right) + k(c - \chi c_0) - k_0 c_0^{\alpha_1} c_3^{\alpha_2},$$

$$\frac{\partial u_1}{\partial x} + \frac{\partial v_1}{\partial r} + \frac{v_1}{r} = 0. \quad (5)$$

It is possible to suppose that  $\varepsilon = \text{const}$ .

The equations for the active liquid and gas concentration distributions in the liquid phase in the downcomer are

$$\frac{\partial c_1}{\partial t} + u \frac{\partial c_1}{\partial x_1} + v \frac{\partial c_1}{\partial r} = D_1 \left( \frac{\partial^2 c_1}{\partial x_1^2} + \frac{1}{r} \frac{\partial c_1}{\partial r} + \frac{\partial^2 c_1}{\partial r^2} \right) - k_0 c_1^{\alpha_1} c_2^{\alpha_2}, \quad (6)$$

$$\frac{\partial c_2}{\partial t} + u \frac{\partial c_2}{\partial x_1} + v \frac{\partial c_2}{\partial r} = D_2 \left( \frac{\partial^2 c_2}{\partial x_1^2} + \frac{1}{r} \frac{\partial c_2}{\partial r} + \frac{\partial^2 c_2}{\partial r^2} \right) - k_0 c_1^{\alpha_1} c_2^{\alpha_2}, \quad (7)$$

where  $x_1 = 1 - x$ .

The equation for the active liquid component concentration distribution in the riser is

$$(1 - \varepsilon) \frac{\partial c_3}{\partial t} + (1 - \varepsilon) \left( u_1 \frac{\partial c_3}{\partial r} + v_1 \frac{\partial c_3}{\partial x} \right)$$

$$= (1 - \varepsilon) D_3 \left( \frac{\partial^2 c_3}{\partial x^2} + \frac{1}{r} \frac{\partial c_3}{\partial r} + \frac{\partial^2 c_3}{\partial r^2} \right) - k_0 c_0^{\alpha_1} c_3^{\alpha_2}. \quad (8)$$

The initial conditions will be formulated for the case, when at  $t = 0$  the process starts with the beginning of gas motion:

$$t = 0, \quad c(x, r, 0) = c^{(0)}, \quad c_0(x, r, 0) = 0,$$

$$c_1(x_1, r, 0) = 0, \quad c_2(x_1, r, 0) = c_2^{(0)}, \quad c_3(x, r, 0) = c_3^{(0)}, \quad (9)$$

where  $c^{(0)}$  and  $c_2^{(0)}$  are initial concentrations of the reagents in two phases.

The boundary conditions are equalities of the concentrations and mass fluxes at the two ends of the working zones –  $x = 0$  ( $x_1 = l$ ) and  $x = l$  ( $x_1 = 0$ ).

The boundary conditions for  $c(x, r, t)$  and  $c_0(x, r, t)$  in Eqs. (4) and (5) are

$$\begin{aligned}
x = 0, \quad \bar{u}_0 c^{(0)} &= u_0 c(0, r, t) - D \left( \frac{\partial c}{\partial x} \right)_{x=0}, \\
x = l, \quad c(l, r, t) &= \chi c_0(l, r, t); \\
x = 0, \quad c_0(0, r, t) &= c_2(l, r, t), \\
\bar{u} \bar{c}_2(l, t) &= u_1 c_0(0, r, t) - D_0 \left( \frac{\partial c_0}{\partial x} \right)_{x=0}; \\
r = 0, \quad \frac{\partial c}{\partial r} &= \frac{\partial c_0}{\partial r} = 0; \\
r = r_0, \quad \frac{\partial c}{\partial r} &= \frac{\partial c_0}{\partial r} = 0.
\end{aligned} \tag{10}$$

The boundary conditions for  $c_1(x_1, r, t)$  and  $c_2(x_1, r, t)$  and  $c_3(x_1, r, t)$  in Eqs. (6)–(8) are

$$\begin{aligned}
x_1 = 0, \quad c_1(0, r, t) &= c_3(l, r, t), \\
\bar{u}_1 \bar{c}_3(l, t) &= u c_1(0, r, t) - D_1 \left( \frac{\partial c_1}{\partial x_1} \right)_{x_1=0}; \\
r = r_0, \quad \frac{\partial c_1}{\partial r} &= 0; \quad r = R_0, \quad \frac{\partial c_1}{\partial r} = 0; \\
x_1 = 0, \quad c_2(0, r, t) &= c_0(l, r, t), \\
\bar{u} \bar{c}_0(l, t) &= u c_2(0, r, t) - D_2 \left( \frac{\partial c_2}{\partial x_1} \right)_{x_1=0}; \\
r = r_0, \quad \frac{\partial c_2}{\partial r} &= 0; \quad r = R_0, \quad \frac{\partial c_2}{\partial r} = 0; \\
x = 0, \quad c_3(0, r, t) &= c_1(l, r, t), \\
\bar{u} \bar{c}_1(l, t) &= u_1 c_3(0, r, t) - D_3 \left( \frac{\partial c_3}{\partial x} \right)_{x=0}; \\
r = 0, \quad \frac{\partial c_3}{\partial r} &= 0; \quad r = r_0, \quad \frac{\partial c_3}{\partial r} = 0.
\end{aligned} \tag{11}$$

The radial nonuniformity of the velocity in the column apparatuses is the cause for the scale effect (decrease of the process efficiency with increase of the column diameter) in the column process scale-up. That is why must be use average velocity and concentration for the cross-section's area. It leads to big priority beside experimental data obtaining for the parameter identification, because measurement the average concentration is very simple in comparison with the local concentration measurement.

### 3. Average concentration models

Let us consider Eq. (4). The velocity  $u_0(x, r)$  and concentration  $c(x, r, t)$  in cylindrical coordinates practical do not depend on the angular coordinate. In this case the average function values are

$$\begin{aligned}
\bar{u}_0(x) &= \frac{2}{r_0^2} \int_0^{r_0} r u_0(x, r) dr, \\
\bar{v}_0(x) &= \frac{2}{r_0^2} \int_0^{r_0} r v_0(x, r) dr, \\
\bar{c}(x, t) &= \frac{2}{r_0^2} \int_0^{r_0} r c(x, r, t) dr, \\
\text{where } \bar{u}_0(0) &= \bar{u}_0.
\end{aligned} \tag{12}$$

The expressions (12) permit to present the velocities and concentration as

$$\begin{aligned}
u_0(x, r) &= \bar{u}_0(x) \tilde{u}_0(r, x), \\
v_0(x, r) &= \bar{v}_0(x) \tilde{v}_0(r, x), \\
c(x, r, t) &= \bar{c}(x, t) \tilde{c}(r, x),
\end{aligned} \tag{13}$$

where  $\tilde{u}_0, \tilde{v}_0$  and  $\tilde{c}$  express radial nonuniformities of the velocities and concentration and

$$\begin{aligned}
\frac{2}{r_0^2} \int_0^{r_0} r \tilde{u}_0(r, x) dr &= 1, \\
\frac{2}{r_0^2} \int_0^{r_0} r \tilde{v}_0(r, x) dr &= 1, \\
\frac{2}{r_0^2} \int_0^{r_0} r \tilde{c}(r, x) dr &= 1.
\end{aligned} \tag{14}$$

If (13) is put in (4), multiply by  $r$  and integrate over  $r$  in the interval  $[0, r_0]$ , the average concentration equation has the form:

$$\begin{aligned}
\frac{\partial \bar{c}}{\partial t} + A(r_0, x) \bar{u}_0 \frac{\partial \bar{c}}{\partial x} + \frac{\partial A}{\partial x} \bar{u}_0 \bar{c} + g(r_0, x) \bar{v}_0 \bar{c} \\
= D \frac{\partial^2 \bar{c}}{\partial x^2} - \frac{k}{\varepsilon} (\bar{c} - \chi \bar{c}_0),
\end{aligned} \tag{15}$$

where

$$\begin{aligned}
A(r_0, x) &= \frac{2}{r_0^2} \int_0^{r_0} r \tilde{u}_0 \tilde{c} dr, \\
g(r_0, x) &= \frac{2}{r_0^2} \int_0^{r_0} r \tilde{v}_0 \frac{\partial \tilde{c}}{\partial r} dr.
\end{aligned} \tag{16}$$

The average radial velocity component  $\bar{v}$  may be obtained if multiply the continuity equation in (4) by  $r^2$  and integrate over  $r$  in the interval  $[0, r_0]$ :

$$\bar{v}_0 = h \frac{\partial \bar{u}_0}{\partial x} + \frac{\partial h}{\partial x} \bar{u}_0, \tag{17}$$

where

$$h(r_0, x) = \frac{2}{r_0^2} \int_0^{r_0} r^2 \tilde{u}_0 dr. \tag{18}$$

If (17) is put in (15), the final form of the diffusion model equation is

$$\begin{aligned}
\frac{\partial \bar{c}}{\partial t} + A(r_0, x) \bar{u}_0 \frac{\partial \bar{c}}{\partial x} + B(r_0, x) \bar{u}_0 \bar{c} + G(r_0, x) \bar{c} \frac{\partial \bar{u}_0}{\partial x} \\
= D \frac{\partial^2 \bar{c}}{\partial x^2} - \frac{k}{\varepsilon} (\bar{c} - \chi \bar{c}_0),
\end{aligned} \tag{19}$$

where for  $B(r_0, x)$  and  $G(r_0, x)$  was obtained [1]:

$$B(r_0, x) = \frac{\partial A}{\partial x} + g \frac{\partial h}{\partial x}, \quad G(r_0, x) = gh. \tag{20}$$

The boundary conditions of (19) have the form:

$$\begin{aligned} t = 0, \quad \bar{c}(x, 0) &= c^{(0)}; \\ x = 0, \quad \bar{u}_0 c^{(0)} &= A(r_0, x) \bar{u}_0(0) \bar{c}(0, t) - D \left( \frac{\partial \bar{c}}{\partial x} \right)_{x=0}; \\ x = l, \quad \bar{c}(l, t) &= \chi \bar{c}_0(l, t). \end{aligned} \quad (21)$$

The parameters in the model (19) and (21) are two tips – specific model parameters ( $D, k, \varepsilon, \chi$ ) and scale model parameters ( $A, B, G$ ). The last ones (scale parameters) are functions of the column radius  $r_0$ . They are result of the radial nonuniformity of the velocity and concentration, and show the influence of the scale-up on the model equations. The parameter  $\chi$  may be obtained beforehand as a result of thermodynamic measurements.

From (19) follow, that the average radial velocity component influence the transfer process in the cases  $\partial \bar{u}_0 / \partial x \neq 0$ , i.e. when the gas hold-up in not constant over the column height. For many practical interesting cases  $\varepsilon = \text{const}$ , i.e.  $\partial \bar{u}_0 / \partial x = 0$  and the radial velocity component did not taken account ( $\bar{v}_0 = 0$ ).

The hold-up  $\varepsilon$  must be obtained using

$$\varepsilon = \frac{(l - l_0)(F_0 + F_1)}{(l - l_0)(F_0 + F_1) + F_0 l_0}, \quad (22)$$

where  $l$  and  $l_0$  are liquid levels in the riser with and without gas motion.

The parameter values  $D, k, A, B, G$  must be obtaining using experimental data for  $\bar{c}(x, t)$  measured on the laboratory column. In the cases of scale-up must be specified  $A, B$  and  $G$  only, using a column with real diameter ( $D$  and  $k$  do not change at scale-up).

The same procedure may be use for Eqs. (5)–(11) and as a result is obtained:

$$\begin{aligned} \frac{\partial \bar{c}_0}{\partial t} + A_0(r_0, x) \bar{u}_1 \frac{\partial \bar{c}_0}{\partial x} + B_0(r_0, x) \bar{u}_1 \bar{c}_0 - G_0(r_0, x) \bar{c}_0 \frac{\partial \bar{u}_1}{\partial x} \\ = D_0 \frac{\partial^2 \bar{c}_0}{\partial x^2} + \frac{k}{1 - \varepsilon} (\bar{c} - \chi \bar{c}_0) - M_0(r_0, x) \frac{k_0}{1 - \varepsilon} \bar{c}_0^{z_1} \bar{c}_3^{z_2}; \\ M_0(r_0, x) = \frac{2}{r_0^2} \int_0^{r_0} r \bar{c}_0^{z_1} \bar{c}_3^{z_2} dr; \\ t = 0, \quad \bar{c}_0(x, 0) = 0; \\ x = 0, \quad \bar{c}_0(0, t) = \bar{c}_1(l, t), \\ \bar{c}_1(l, t) \bar{u} = A_0(r_0, x) \bar{u}_1(0) \bar{c}_0(0, t) - D_0 \left( \frac{\partial \bar{c}_0}{\partial x} \right)_{x=0}, \end{aligned} \quad (23)$$

where  $A_0, B_0$  and  $G_0$  are obtained on the analogy of  $A, B$  and  $G$  (see (16), (18) and (20)). The concrete expressions of  $A, B$  and  $G$  are not interesting because theirs values must be obtained, using experimental data.

The average concentration model for  $\bar{c}_1$  is obtained on the analogy of  $\bar{c}$ :

$$\begin{aligned} \frac{\partial \bar{c}_1}{\partial t} + A_1(r_0, R_0, x_1) \bar{u} \frac{\partial \bar{c}_1}{\partial x_1} + B_1(r_0, R_0, x_1) \bar{u} \bar{c}_1 + G_1(r_0, R_0, x_1) \bar{c}_1 \frac{\partial \bar{u}}{\partial x_1} \\ = D_1 \frac{\partial^2 \bar{c}_1}{\partial x_1^2} - k_0 M(r_0, R_0, x_1) \bar{c}_1^{z_1} \bar{c}_2^{z_2}; \\ t = 0, \quad \bar{c}_1(x_1, 0) = 0; \end{aligned}$$

$$x_1 = 0, \quad \bar{c}_1(0, t) = \bar{c}_3(l, t),$$

$$\bar{c}_3(l, t) \bar{u} = A_1(r_0, R_0, x_1) \bar{u}(0) \bar{c}_1(0, t) - D_1 \left( \frac{\partial \bar{c}_1}{\partial x_1} \right)_{x_1=0}, \quad (24)$$

where

$$\begin{aligned} \bar{u}(x_1) &= \frac{2}{R_0^2 - r_0^2} \int_{r_0}^{R_0} r u(x_1, r) dr, \\ \bar{c}_1(x_1, t) &= \frac{2}{R_0^2 - r_0^2} \int_{r_0}^{R_0} r c_1(x_1, r, t) dr; \\ M(r_0, R_0, x_1) &= \frac{2}{R_0^2 - r_0^2} \int_{r_0}^{R_0} r \bar{c}_1^{z_1} \bar{c}_2^{z_2} dr \end{aligned} \quad (25)$$

and  $A_1, B_1, G_1$  are obtained on the analogy of  $A, B, G$  (see (16), (18), and (20)), but the limits of the integrals are  $[r_0, R_0]$ .

The average concentration model for  $\bar{c}_2$  is

$$\begin{aligned} \frac{\partial \bar{c}_2}{\partial t} + A_2(r_0, R_0, x_1) \bar{u} \frac{\partial \bar{c}_2}{\partial x_1} + B_2(r_0, R_0, x_1) \bar{u} \bar{c}_2 + G_2(r_0, R_0, x_1) \bar{c}_2 \frac{\partial \bar{u}}{\partial x_1} \\ = D_2 \frac{\partial^2 \bar{c}_2}{\partial x_1^2} - M(r_0, R_0, x_1) k_0 \bar{c}_1^{z_1} \bar{c}_2^{z_2}; \end{aligned}$$

$$t = 0, \quad \bar{c}_2 = c_2^{(0)};$$

$$x_1 = 0, \quad \bar{c}_2(0, t) = \bar{c}_0(l, t),$$

$$\bar{u}_1 \bar{c}_3(l, t) = A_2(r_0, R_0, x_1) \bar{u}(0) \bar{c}_2(0, t) - D_2 \left( \frac{\partial \bar{c}_2}{\partial x_1} \right)_{x_1=0}, \quad (26)$$

where

$$\begin{aligned} \bar{c}_2 &= \frac{2}{R_0^2 - r_0^2} \int_{r_0}^{R_0} r c_2(x_1, r, t) dr, \\ \bar{c}_3 &= \frac{2}{r_0^2} \int_0^{r_0} r c_3(x, r, t) dr. \end{aligned} \quad (27)$$

The integration of (8) lead to the equation for  $\bar{c}_3$ :

$$\begin{aligned} \frac{\partial \bar{c}_3}{\partial t} + A_3(r_0, x) \bar{u}_1 \frac{\partial \bar{c}_3}{\partial x} + B_3(r_0, x) \bar{u}_1 \bar{c}_3 + G_3(r_0, x) \bar{c}_3 \frac{\partial \bar{u}_1}{\partial x} \\ = D_3 \frac{\partial^2 \bar{c}_3}{\partial x^2} - M_0(r_0, x) \frac{k_0}{1 - \varepsilon} \bar{c}_0^{z_1} \bar{c}_3^{z_2}; \end{aligned}$$

$$t = 0, \quad \bar{c}_3(x, 0) = c_3^{(0)};$$

$$x = 0, \quad \bar{c}_3(0, t) = \bar{c}_1(l, t),$$

$$\bar{u} \bar{c}_1(l, t) = A_3(r_0, x) \bar{u}_1(0) \bar{c}_3(0, t) - D_3 \left( \frac{\partial \bar{c}_3}{\partial x} \right)_{x=0}, \quad (28)$$

where  $A_3, B_3$  and  $G_3$  are obtained on the analogy of  $A, B$  and  $G$ .

For many practical interesting cases the specific volume ( $\text{m}^3 \text{m}^{-3}$ ) of the catalytic particles or gas hold-up are constant over the column, i.e.

$$\frac{\partial \bar{u}}{\partial x} = \frac{\partial \bar{u}_0}{\partial x} = \frac{\partial \bar{u}_1}{\partial x} = 0, \quad \bar{v} = \bar{v}_0 = \bar{v}_1 = 0 \quad (29)$$

and model parameters number decrease, i.e.  $G = G_0 = G_1 = G_2 = G_3 = 0$ .

#### 4. Hierarchical approach

The problems (19), (21), (23), (24), (26) and (28) are mathematical model of an airlift three phase reactor. The model parameters are five types:

- beforehand known ( $c^{(0)}, c_2^{(0)}, R_0, r_0$ );
- beforehand obtained ( $\varepsilon, \chi, \alpha_1, \alpha_2, k_0$ );
- obtained without chemical reaction ( $k, D, D_0, A, B, A_0, B_0, G, G_0$ );
- obtained with chemical reaction ( $D_1, D_2, D_3, M, M_0$ );
- obtained in the modeling and specified in the scale-up ( $A, A_0, A_1, A_2, A_3, B, B_0, B_1, B_2, B_3, G, G_0, G_1, G_2, G_3, M, M_0$ ).

The problems (19), (21) and (23) permit to obtain ( $k, D, D_0, A, B, A_0, B_0, G, G_0$ ) without chemical reaction if put

$$\bar{c}_1(l, t) = \bar{c}_0(l, t). \quad (30)$$

#### 5. Conclusions

The result obtained shows a possibility to build airlift reactor models, using average velocities and concentrations. This approach permits to solve the scale-up problem as a result to the radial nonuniformity of the velocity and concentration, using radius dependent parameters. The model parameter identification on the bases of average concentration experimental data leads to big priority in comparison with the local concentration measurements.

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