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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.

Keywords: Diffusion model; Airlift; Chemical reactor; Average concentration model; Scale-up

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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 ε 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

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

The interphase mass transfer rate in the riser is

$$R = k(c - \chi c_0). \tag{2}$$

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Nomenclature

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

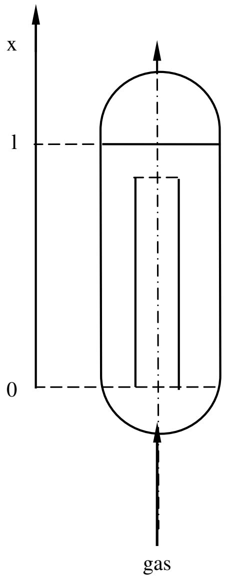

Fig. 1. Airlift reactor.

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

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

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

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

$$\frac{\partial u_o}{\partial x}+\frac{\partial v_0}{\partial r}+\frac{v_o}{r}=0, \tag{4}$$

$$(1-\varepsilon)\frac{\partial c_0}{\partial t}+(1-\varepsilon)\left(u_1\frac{\partial c_0}{\partial r}+v_1\frac{\partial c_0}{\partial x}\right)$$
$$=(1-\varepsilon)D_0\left(\frac{\partial^2 c_0}{\partial x^2}+\frac{1}{r}\frac{\partial c_0}{\partial r}+\frac{\partial^2 c_0}{\partial r^2}\right)+k(c-\chi c_0)-k_0 c_0^{\alpha_1} c_3^{\alpha_2},$$

$$\frac{\partial u_1}{\partial x}+\frac{\partial v_1}{\partial r}+\frac{v_1}{r}=0. \tag{5}$$

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

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

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

where $x_1 = 1 - x$.

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

$$(1-\varepsilon)\frac{\partial c_3}{\partial t}+(1-\varepsilon)\left(u_1\frac{\partial c_3}{\partial r}+v_1\frac{\partial c_3}{\partial x}\right)$$
$$=(1-\varepsilon)D_3\left(\frac{\partial^2 c_3}{\partial x^2}+\frac{1}{r}\frac{\partial c_3}{\partial r}+\frac{\partial^2 c_3}{\partial r^2}\right)-k_0 c_0^{\alpha_1} c_3^{\alpha_2}. \tag{8}$$

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

$$t=0, \quad c(x,r,0)=c^{(0)}, \quad c_0(x,r,0)=0,$$
$$c_1(x_1,r,0)=0, \quad c_2(x_1,r,0)=c_2^{(0)}, \quad c_3(x,r,0)=c_2^{(0)}, \tag{9}$$

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