DIFFUSION MODELS AND SCALE-UP

by

Christo BOYADJIEV

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A model for transfer processes in column apparatuses has been done. The model may be modified for different apparatuses as columns with (or without) packet bed, two (or three) phase airlift reactors and fluidized bed reactors. The mass transfer is result of different volume reactions as a chemical, photochemical, biochemical or catalytic reactions, or interphase mass transfer. The using of the average velocities and concentration permit to solve the scale-up problems. A hierarchical approach for model parameter identification has been proposed.

Key words: *diffusion model, scale-up, average velocity, average concentration, scale effect, column, airlift, fluidized bed, volume reaction*

Introduction

Many heat and mass transfer processes in column apparatuses may be described by the convection – diffusion equation with a volume reaction [1]. These are gas absorption in column with (or without) packet bed [2, 3], chemical reactors for homogeneous or heterogeneous reactions [2, 3], airlift or fluidized bed reactors for biochemical, photochemical or catalytic reactions [4-8].

The convective transfer in column apparatuses is result of a laminar or turbulent (large-scale pulsations) flows. The diffusive transfer is molecular or turbulent (small--scale pulsations). The volume reaction is mass sours as a result of chemical, biochemical, photochemical or catalytic reactions or interphase mass transfer [1, 2].

The scale-up theory [1, 2] show that the scale effect in mathematical modeling is result of the radial nonunformity of the velocity distribution in the column. The using of average velocity and concentration permits to solve the scale-up problems.

Column apparatuses

Many heat and mass transfer processes and chemical reactions are realized in column apparatuses. The creation of the models in this condition and solving of the scale-up problem [4, 6] requires construction of a suitable diffusion models.

Diffusion model

Let's consider liquid motion in column apparatus with chemical reaction between two of the liquid components. If the difference between component concentrations is very big, the chemical reaction order will be one. In the case of liquid circulation, the process will be nonstationary. If suppose for velocity and concentration distribution in the column:

$$u = u(r), \quad c = c(t,r,z) \tag{1}$$

the mathematical description has the form:

$$\begin{gathered}
\frac{\partial c}{\partial t} \quad u\frac{\partial c}{\partial z} \quad D \quad \frac{\partial^2 c}{\partial z^2} \quad \frac{1}{r}\frac{\partial c}{\partial r} \quad \frac{\partial^2 c}{\partial r^2} \qquad kc \\
t \quad 0, \quad c \quad c_0; \\
r \quad 0, \quad \frac{\partial c}{\partial r} \quad 0; \quad r \quad R, \quad \frac{\partial c}{\partial r} \quad 0; \\
z \quad 0, \quad \bar{c}(t,0) \quad \bar{c}(t,l), \quad \bar{u}\bar{c} \quad \overline{uc} \quad D\frac{\partial c}{\partial z}
\end{gathered} \tag{2}$$

where u is velocity distribution, c – concentration of the reagent (with small concentration), k – chemical reaction rate constant, t – the time, r and z – radial and axial coordinate, D – diffusivity, c_0 – initial concentration, $\bar{c}$ and $\bar{u}$ – average values of the concentration and the velocity at the inlet (outlet) of the column, R and l – column radius and height.

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

Average function values

Let consider cylinder with $R = R(\varphi)$, where φ is an angle (in cylindrical coordinates z, r, φ). The average values of a function $f(z,r,\ )$ for the cross-section's area is:

$$\overline{f}(z) \quad \frac{\int_{(s)} f(z,r,\varphi)\mathrm{d}S}{S} \tag{3}$$

where

$$S \quad \int_0^{2\pi} \frac{[R(\varphi)]^2}{2}\mathrm{d}\varphi, \qquad \int_{(s)} f(z,r,\varphi)\mathrm{d}S \quad \frac{1}{2}\int_0^{2\pi} R(\varphi) \int_0^{R(\varphi)} f(z,r,\varphi)\mathrm{d}r \ \mathrm{d}\varphi \tag{4}$$

For a circular cylinder R = const and from (3, 4) follow:

$$\overline{f}(z) = \frac{\int_0^{2\pi}\int_0^R f(z,r,\varphi)\mathrm{d}r\,\mathrm{d}\varphi}{2\pi R} \tag{5}$$

Let to present the function $f(z,r,\varphi)$ as a:

$$f(z,r,\varphi) = \overline{f}(z) f_0(z,r,\varphi) \tag{6}$$

where

$$f_0(z,r,\varphi) = \frac{f(z,r,\varphi)}{\overline{f}(z)} \tag{7}$$

If $\overline{f}(z)$ is the average function (5), the integration of eq. (6) over r into interval [0, R] and over φ into interval [0, 2π] lead to:

$$2\pi R\overline{f}(z) = \overline{f}(z)\int_0^{2\pi}\int_0^R f_0(z,r,\varphi)\,\mathrm{d}r\,\mathrm{d}\varphi \tag{8}$$

i. e.

$$\int_0^{2\pi}\int_0^R f_0(z,r,\varphi)\mathrm{d}r\,\mathrm{d}\varphi = 2\pi R \tag{9}$$

and

$$f_0 = f_0(r,\varphi) \tag{10}$$

Let consider column apparatus, where velocity and concentration are:

$$u = u(t,z,r,\varphi), \qquad c = c(t,z,r,\varphi) \tag{11}$$

The results obtained permit to present (11) as a:

$$u(t,z,r,\varphi) = \overline{u}(t,z)\tilde{u}(r,\varphi)$$
and
$$c(t,z,r,\varphi) = \overline{c}(t,z)\tilde{c}(r,\varphi) \tag{12}$$

where

$$\overline{u}(t,z) = \frac{\int_0^{2\pi}\int_0^R u(t,z,r,\varphi)\mathrm{d}r\,\mathrm{d}\varphi}{2\pi \mathrm{R}}, \qquad \overline{c}(t,z) = \frac{\int_0^{2\pi}\int_0^R c(t,z,r,\varphi)\mathrm{d}r\,\mathrm{d}\varphi}{2\pi \mathrm{R}}$$
$$\int_0^{2\pi}\int_0^R \tilde{u}(z,r,\varphi)\mathrm{d}r\,\mathrm{d}\varphi = 2\pi R, \qquad \int_0^{2\pi}\int_0^R \tilde{c}(z,r,\varphi)\,\mathrm{d}r\,\mathrm{d}\varphi = 2\pi R, \tag{13}$$

For the average velocity and concentration in the model (1, 2) follow:

$$
\begin{aligned}
&u(r) \quad \bar{u}u_0(r), \qquad c(t,r,z) \quad \bar{c}(t,z)c_0(r), \\
&\bar{u} \quad \frac{1}{R}\,{}_0^R\, u(r)\mathrm{d}r, \qquad \bar{c}(t,z) \quad \frac{1}{R}\,{}_0^R\, c(t,r,z)\mathrm{d}r, \\
&{}_0^{\mathrm{R}}\, u_0(r)\mathrm{d}r \quad R, \qquad {}_0^{\mathrm{R}}\, c_0(r)\mathrm{d}r \quad R
\end{aligned}
\tag{14}
$$

Average concentration model

The average concentration model may be obtained if put eq. (13) in eq. (2) and to integrate the equations in (2) over r in the interval [0, R]. As a result is obtained:

$$
\begin{aligned}
&\frac{\partial \bar{c}}{\partial t} \quad \alpha(R)\bar{u}\frac{\partial \bar{c}}{\partial z} \quad D\frac{\partial^2 \bar{c}}{\partial z^2} \quad \beta(R)\bar{c} \quad k\bar{c} \\
&t \quad 0, \quad \bar{c} \quad c_0; \\
&z \quad 0, \quad \bar{c}(t,0) \quad \bar{c}(t,l), \quad \bar{u}\bar{c} \quad \alpha(R)\bar{u}\bar{c} \quad D\frac{\partial \bar{c}}{\partial z}
\end{aligned}
\tag{15}
$$

where

$$
\alpha(R) \quad \frac{1}{R}\,{}_0^R\, u_0(r)c_0(r)\mathrm{d}r, \quad \beta(R) \quad \frac{1}{R}\,{}_0^R\, \frac{1}{r}\frac{\partial c_0}{\partial r}\mathrm{d}r \tag{16}
$$

In model (15) $\bar{u}$ is diffusivity or turbulent diffusivity as a result of the small scale pulsation's. The model parameters α and β are related with the radial nonuniformity of the velocity and concentration distributions only. They show the influence of the column radius on the mass transfer kinetics.

The parameters in the model (15) are: α, β, D, and k, where k may be obtained beforehand as a result of the chemical kinetics modeling. The identification of the parameters α, β, and D may be made by using experimental data for $\bar{c}(t, z)$, obtained on the laboratory model. In the cases of scale-up must be obtained $\alpha(R)$ and $\beta(R)$ only (using real column) because the values of D and k are the same.

Qualitative analysis of the model

For the theoretical analysis of the model (15) dimensionless variables must be used:

$$
t \quad t_0 T, \qquad z \quad lZ, \qquad \bar{c} \quad c_0 C \tag{17}
$$

where t_0 is characteristic time of the process.

Dimensionless model will be obtained if put eq. (17) in eq. (15):

$$\frac{\partial C}{\partial T} \quad \bar{\alpha}\frac{\partial C}{\partial Z} \quad \frac{Dt_0}{l^2} \quad \frac{\partial^2 C}{\partial Z^2} \quad \bar{\beta} C \qquad KC$$

$$T \quad 0, \qquad C \quad 1; \tag{18}$$

$$Z \quad 0, \qquad C(T,0) \quad C(T,1), \qquad C \quad \alpha(R)C \quad \frac{D}{\bar{u}l}\frac{\partial C}{\partial Z}$$

where

$$\bar{\alpha} \quad \alpha(R)\frac{\bar{u}t_0}{l}, \quad \bar{\beta} \quad l^2\beta(R), \quad K \quad kt_0 \tag{19}$$

For long time process t_0 is very big and in the cases $\bar{\alpha} > 10^2$ the process is stationary. If chemical reaction rate is very big and K 10^2 the process is stationary too, but if $\bar{\alpha} < 1$ the effect of the convective transport is negligible. Another situations are possible if compare the values of the dimensionless model parameters $\bar{\alpha}$, Dt_0/l^2 and K.

Model with radial velocity component

In the cases $u = u(r, z)$ the velocity has a radial component and the model equation in (2) has the form:

$$\frac{\partial c}{\partial t} \quad u\frac{\partial c}{\partial z} \quad v\frac{\partial c}{\partial r} \quad D \quad \frac{\partial^2 c}{\partial z^2} \quad \frac{1}{r}\frac{\partial c}{\partial r} \quad \frac{\partial^2 c}{\partial r^2} \qquad kc \tag{20}$$

where $v = v(r, z)$ is radial velocity component and satisfy the continuity equation:

$$\frac{\partial u}{\partial z} \quad \frac{\partial v}{\partial r} \quad \frac{v}{r} \quad 0 \tag{21}$$

The boundary conditions of the model equations in (2) and (20) are identical.

Let's present the radial velocity component as a:

$$v(r, z) \quad \bar{v}(z)v_0(r), \quad \bar{v} \quad \frac{1}{R}{}_0^R v(r, z)\mathrm{d}r, \quad {}_0^R v_0(r)\mathrm{d}r \quad R \tag{22}$$

If put eq. (22) in eq. (20) and integrate eq. (20) over r in the interval $[0, R]$, the equation for $\bar{c}$ has the form:

$$\frac{\partial \bar{c}}{\partial t} \quad \alpha(R)\bar{u}\frac{\partial \bar{c}}{\partial z} \quad \gamma_1(R)\bar{v}\bar{c} \quad D\frac{\partial^2 \bar{c}}{\partial z^2} \quad \beta(R)\bar{c} \quad k\bar{c} \tag{23}$$

where

$$\gamma_1(R) \quad \frac{1}{R} \, {}_0^R \, v_0 \frac{\partial c}{\partial r} \mathrm{d}r \tag{24}$$

Let's put eq. (22) into eq. (21) and to integrate eq. (21) over r in the interval [0, R]. As a result eq. (21) has the form:

$$\frac{\partial \bar{u}}{\partial z} \quad \gamma_2(R)\bar{v} \quad 0 \tag{25}$$

where

$$\gamma_2(R) \quad \frac{v_0(R) \quad v_0(0)}{R} \quad \frac{1}{R} \, {}_0^R \, \frac{v_0}{r} \mathrm{d}r \tag{26}$$

In eq. (26) on the solid interphase v_o (R) = 0 and as a result:

$$\gamma_2(R) \quad \frac{v_0(0)}{R} \quad \frac{1}{R} \, {}_0^R \, \frac{v_0}{r} \mathrm{d}r \tag{27}$$

The solution of eq. (27) is:

$$v_0(r) \quad \gamma_2(R) \quad \frac{v_0(0)}{R} \quad \frac{2 \quad 2a_0}{R} r^2 \quad ar \tag{28}$$

i. e. v_0 (0) = 0.

In eq. (28) the constant a may be obtained using the boundary condition v_0 (R) = 0 and as a result $a_0 = 2$, *i. e.*

$$v_0(R) \quad \gamma_2(R) \; 2r \quad \frac{2}{R} r^2 \tag{29}$$

The constant $\gamma_2(R)$ may be obtained, using eq. (22), and as a result

$$\gamma_2(R) \quad \frac{3}{R}, \quad v_0(r) \quad \frac{3}{R} \quad 2r \quad \frac{2}{R} r^2 \tag{30}$$

If put eq. (30) in eq. (25) for the average radial velocity component is obtained:

$$\bar{v} \quad \frac{R}{3} \frac{\partial \bar{u}}{\partial z} \tag{31}$$

and eq. (23) has the form:

$$\frac{\partial \bar{c}}{\partial t} \quad \alpha(R)\bar{u} \frac{\partial \bar{c}}{\partial z} \quad \gamma(R)\bar{c} \frac{\partial \bar{u}}{\partial z} \quad D \frac{\partial^2 \bar{c}}{\partial z^2} \quad \beta(R)\bar{c} \quad k\bar{c} \tag{32}$$

where

$$\gamma(R) \quad \frac{R}{3}\gamma_1(R) \tag{33}$$

The parameters $\alpha, \beta, \gamma, \gamma_1$, and γ_2 in eqs. (15)-(33) are functions of the column radius R and may be obtained, using experimental data only.

The model eq. (32) has an additional parameter $\gamma(R)$ in comparison with eq. (15) and identical boundary conditions. The theoretical analysis of the model (15) is valid for the model (32) too. From eq. (31) follow, that the average radial velocity component influence the transfer process in the cases $\partial \bar{u}/\partial z \quad 0$, *i. e.* when the specific volume (m^3/m^3) of the solid phase in column (packed by catalyst particles) or the gas hold-up is not constant over the column height. For many practical interesting cases $\bar{v} \quad 0$.

Interphase mass transfer model

In the cases of interphase mass transfer between gas-liquid or liquid-liquid phases in the models (2) or (20) may be replace convection-diffusion equations for the two phases and the chemical reaction rate must be replaced with interphase mass transfer rate:

$$k(c_1 \quad \chi c_2) \tag{34}$$

where k is interphase mass transfer coefficient, c_1 – concentration of the transferred substance in the gas (liquid) phase, c_2 – the concentration of the transferred substance in the liquid phase, χ – Henry's number (liquid-liquid distribution coefficient).

As a result the diffusion model for interphase mass transfer in the column apparatuses has the form:

$$\varepsilon_i \frac{\partial c_i}{\partial t} \quad \varepsilon_i u_i \frac{\partial c_i}{\partial z} \quad \varepsilon_i D_i \quad \frac{\partial^2 c_i}{\partial z^2} \quad \frac{1}{r}\frac{\partial c_i}{\partial r} \quad \frac{\partial^2 c_i}{\partial r^2} \qquad (\ \ 1)^{i \ \ 1} k(c_1 \quad \chi c_2) \tag{35}$$

where ε_i ($i = 1, 2$) are hold-up coefficients ($\varepsilon_1 + \varepsilon_2 = 1$). The boundary conditions for eq. (35) are similar to the boundary conditions in eq. (2), but a difference is possible depending on the conditions for contact between two phases.

A similar equation may be obtained for the cases of two velocity component (20). All theoretical analysis of eq. (15) may be repeated for the model (35).

Stationary processes

In the cases of stationary processes $\bar{u} \quad$ const, $\bar{c} \quad \bar{c}(z)$ and from eq. (15) follow:

$$\bar{u}\frac{\partial \bar{c}}{\partial z} \quad D_{\text{eff}}\frac{\partial^2 \bar{c}}{\partial z^2} \quad k_{\text{eff}}\bar{c} \tag{36}$$

where

$$D_{\mathrm{eff}} \quad D_{\mathrm{eff}}(R) \quad \frac{D}{\alpha}, \quad k_{\mathrm{eff}} \quad k_{\mathrm{eff}}(R) \quad \frac{D\beta}{\alpha} \quad \frac{k}{\alpha} \tag{37}$$

The boundary conditions of eq. (36) are:

$$z \quad 0, \quad \bar{c} \quad c_0, \quad c_0\bar{u} \quad \alpha\bar{u}\bar{c} \quad D\frac{\partial \bar{c}}{\partial z} \tag{38}$$

In the cases of radial velocity component $\bar{u} \quad \bar{u}(z)$, $\bar{c} \quad \bar{c}(z)$ and from eq. (32) follow:

$$\bar{u}\frac{\partial \bar{c}}{\partial z} \quad \frac{\gamma}{\alpha}\bar{c}\frac{\partial \bar{u}}{\partial z} \quad D_{\mathrm{eff}}\frac{\partial^2 \bar{c}}{\partial z^2} \quad k_{\mathrm{eff}}\bar{c} \tag{39}$$

The results obtained show that stationary model eqs. (15) and (23) are equivalent to convection – diffusion models with chemical reaction (36) and (39), where diffusivity and chemical reaction rate constant are functions of the column radius.

From eq. (37) follow, that effective diffusivity D_{eff} and chemical reaction rate k_{eff} decrease with the increasing of the velocity and concentration distributions nonuniformities.

Airlift photobioreactors

Photobioprocesses represent dissolution of an active gas component (CO_2, O_2) in liquid and its reaction with a photoactive substance (cells). These two processes may to realize in one volume (tubular photobioreactors) or in different volumes (airlift photobioreactor) [10-12].

The comparison analyses between these two tipes reactors shows, that airlift reactor give an opportunity for more intensive photoprocesses in the downcomer zone of the reactor [13-16].

The hydrodynamic behavior of the gas and liquid flows in airlift reactors is very complicated, but in all cases the process is result of convective transport, diffusion transport and volume reactions. That is why convection-diffusion equation with volume reaction may be use as a mathematical structure of the model.

Mathematical model

Let consider airlift reactor (fig. 1) with a cross-section's area F_0 for the riser zone and F_1 for the downcomer zone. The length of the working zones is l. The gas flow rate is Q_0 and the liquid flow rate (water) Q_1.The gas and liquid hold-up in the riser are ε and $(1 - \varepsilon)$. The concentrations of the active gas component (CO_2) 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 $x_1 = 1 - x$. The concentration of the photoactive substance in the downcomer is $c_2(x_1,r,t)$ and in the riser $c_3(x_1, r, t)$.

The average velocities in gas and liquid phases are:

$$\bar{\bar{u}}_0 \quad \frac{Q_0}{F_0}, \quad \bar{\bar{u}}_1 \quad \frac{Q_1}{F_1}, \quad \bar{\bar{u}} \quad \frac{Q_1}{F_1}, \tag{40}$$

The interphase mass transfer rate in the riser is:

$$I_0 = k(c - \chi c_0) \tag{41}$$

The photoreaction rates in the downcomer and the riser are:

$$I \quad k_0 c_1 c_2 J, \quad I_1 \quad k_0 c_0 c_3 J_1 \tag{42}$$

where photon flux densities $J(R)$ and $J_1(R)$ are a function of the radial coordinate r, because they increase with the radius decreasing and decrease as a result of the light absorption from the photoactive substance.

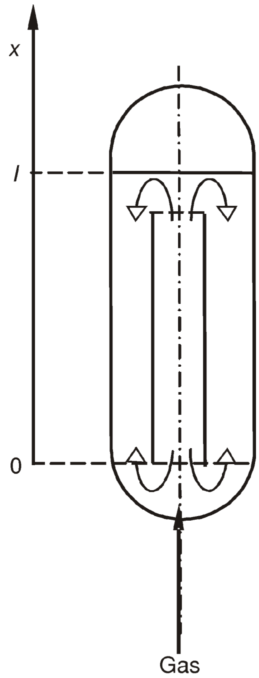

Figure 1.

Let consider (fig. 2) cylindrical surface with radius R_0 and length 1 m, which is regular irradiate with a photon flux density J_0. The photon flux density over cylindrical surface with radiuses $r \quad R_0$ is:

$$i(r) \quad \frac{R_0 J_0}{r} \tag{43}$$

The increasing of the photon flux density between r and $r - \quad r$ (as a result of the radius decreasing) is:

$$\Delta J_1 \quad \frac{J_0 R_0}{r \quad \Delta r} \quad \frac{J_0 R_0}{r} \quad \frac{J_0 R_0 \Delta r}{r(r \quad \Delta r)} \tag{44}$$

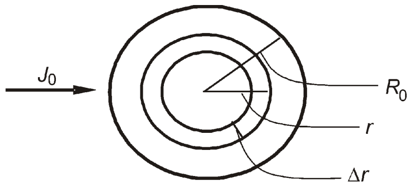

Figure 2.

The volume between cylindrical surfaces with radiuses r and $r - \quad r$ is:

$$V \quad \Delta r \;\; 1 \quad \frac{\Delta r}{2r} \tag{45}$$

The decreasing of the photon density between r and $r - \quad r$ (as a result of the light absorption from the photoactive substance) is:

$$\Delta J_2 \quad J(x_1, r, t)\delta c_2 \Delta r \;\; 1 \quad \frac{\Delta r}{2r} \tag{46}$$

where $c_2 = c_2(x_1, r, t)$ is the concentration of the fotoactive substance in the downcomer.

The difference between photon flux densities for r and $r -\quad r$ is:

$$\Delta J \quad \Delta J_1 \quad \Delta J_2 \quad \frac{J_0 R_0 \Delta r}{r(r \quad \Delta r)} \quad J\delta c_2 \Delta r \;\; 1 \quad \frac{\Delta r}{2r} \tag{47}$$

As a result

$$\lim_{\Delta r \quad 0} \frac{\Delta J}{\Delta r} \quad \frac{\partial J}{\partial r} \quad \frac{R_0 J_0}{r^2} \quad \delta c_2 J \tag{48}$$

where $J(R_0) = J_0$. The solution of eq. (48) for $c_2 = c_2(x_1, r, t)$ is:

$$J(x_1, r, t) \quad \exp \;\; \delta \overset{R_0}{\underset{r}{}} c_2(x_1, \rho, t) \mathrm{d}\rho \quad J_0 \quad R_0 J_0 \overset{R_0}{\underset{r}{}} \frac{1}{\rho^2} \exp \;\; \delta \overset{R_0}{\underset{\rho}{}} c_2(x_1, \eta, t) \mathrm{d}\eta \;\; \mathrm{d}\rho \tag{49}$$

The mathematical model of the photoprocesses in airlift photobioreactor will be built on the basis of the differential mass balance in the reactor volume [17-19]. A convection-diffusion equation with volume reaction will be used, where convective transfer will be results of the laminar flow or large scale turbulent pulsations, the diffusivities are molecular or turbulent (as a result of the small scale turbulent pulsations) and the volume reactions are interphase mass transfer or photochemical reaction.

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

$$\begin{gathered} \varepsilon \frac{\partial c}{\partial t} \quad \varepsilon u_0 \frac{\partial c}{\partial x} \quad \varepsilon v_0 \frac{\partial c}{\partial r} \quad \varepsilon D \;\; \frac{\partial^2 c}{\partial x^2} \quad \frac{1}{r} \frac{\partial^2 c}{\partial r^2} \quad k(c \quad \chi c_0) \\ \frac{\partial u_0}{\partial x} \quad \frac{\partial v_0}{\partial r} \quad \frac{v_0}{r} \quad 0 \end{gathered} \tag{50}$$

$$\begin{gathered} (1 \quad \varepsilon) \frac{\partial c_0}{\partial t} \quad (1 \quad \varepsilon) \;\; u_1 \frac{\partial c_0}{\partial r} \quad v_1 \frac{\partial c_0}{\partial x} \quad (1 \quad \varepsilon) D_0 \;\; \frac{\partial^2 c_0}{\partial x^2} \quad \frac{1}{r} \frac{\partial c_0}{\partial r} \quad \frac{\partial^2 c_0}{\partial r^2} \quad k(c \quad \chi c_0) \\ a k_0 c_0 c_3 J_1, \qquad \frac{\partial u_1}{\partial x} \quad \frac{\partial v_1}{\partial r} \quad \frac{v_1}{r} \quad 0 \end{gathered} \tag{51}$$

It is possible to suppose that ε = const.

The equations for the active gas component and photoactive substance concentration distribution in the liquid phase in the downcomer are:

$$\frac{\partial c_1}{\partial t} \quad u \frac{\partial c_1}{\partial x_1} \quad v \frac{\partial c_1}{\partial r} \quad D_1 \;\; \frac{\partial^2 c_1}{\partial x^2} \quad \frac{1}{r} \frac{\partial c_1}{\partial r} \quad \frac{\partial^2 c_1}{\partial r^2} \quad a k_0 c_1 c_2 J \tag{52}$$

$$\frac{\partial c_2}{\partial t} \quad u\frac{\partial c_2}{\partial x_1} \quad v\frac{\partial c_2}{\partial r} \quad D_2 \quad \frac{\partial^2 c_2}{\partial x^2} \quad \frac{1}{r}\frac{\partial c_2}{\partial r} \quad \frac{\partial^2 c_2}{\partial r^2} \quad k_0 c_1 c_2 J$$

$$\frac{\partial u}{\partial x_1} \quad \frac{\partial v}{\partial r} \quad \frac{v}{r} \quad 0 \qquad (53)$$

where $x_1 = 1 - x$.

Photochemical reaction in riser is possible too and equation for the photoactive substance concentration is:

$$(1 \quad \varepsilon)\frac{\partial c_3}{\partial t} \quad (1 \quad \varepsilon)\ u_1 \frac{\partial c_3}{\partial r} \quad v_1 \frac{\partial c_3}{\partial x} \quad (1 \quad \varepsilon)D_3 \quad \frac{\partial^2 c_3}{\partial x^2} \quad \frac{1}{r}\frac{\partial c_3}{\partial r} \quad \frac{\partial^2 c_3}{\partial r^2} \quad k_0 c_0 c_3 J_1 \qquad (54)$$

where $J_1 = J_1\ (x,r,t)$ is photon flux density in the riser:

$$\frac{\partial J_1}{\partial r} \quad \frac{r_0 J(x_1, r_0, t)}{r^2} \quad \delta c_3 J_1$$

$$r \quad r_0, \quad J_1 \quad J(x_1, r_0, t), \quad x_1 \quad l \quad x \qquad (55)$$

and $c_3 = c_3\ (x,r,t)$ is concentration of the photoactive substance in the riser.

The initial conditions will be formulated for the case, when it have thermodynamic equilibrium between gas and liquid phases, *i. e*. a full liquid saturation with the active gas component and the process starts with the starting of the illumination of the downcomer zone:

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

$$c_1(x_1 r,0) \quad \frac{c^{(0)}}{\chi}, \quad c_2(x_1,r,0) \quad c_2^{(0)} \qquad (56)$$

where $c^{(0)}$ and $c_2^{(0)}$ are initial concentrations of the active gas component in gas phase and the photoactive substance in the liquid phase.

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. (50) and (51) are:

$$x \quad 0, \quad \overline{\overline{u}}_0 c^{(0)} \quad u_0 c(0,r,t) \quad D \quad \frac{\partial c}{\partial x}_{\ x \quad 0}$$

$$x \quad l, \quad c(l,r,t) \quad \chi c_0(l,r,t);$$

$$x \quad 0, \quad c_0(0,r,t) \quad c_1(l,r,t)$$

$$\overline{c}_1(l,t)\overline{\overline{u}} \quad c_0(0,r,t)u_1 \quad D_0 \quad \frac{\partial c_0}{\partial x}_{\ x \quad 0}; \qquad (57)$$

$$r \quad 0, \quad \frac{\partial c}{\partial r} \quad \frac{\partial c_0}{\partial r} \quad 0,$$

$$r \quad r_0, \quad \frac{\partial c}{\partial r} \quad \frac{\partial c_0}{\partial r} \quad 0$$

The boundary conditions for $c_1(x_1,r,t)$, $c_2(x_1,r,t)$ and $c_3(x,r,t)$ are:

$$
\begin{array}{c}
x_1 \quad 0, \quad c_1(0,r,t) \quad c_0(l,r,t) \\
\bar{c}_0(l,t)\bar{\bar{u}}_1 \quad c_1(0,r,t)u \quad D_1 \left.\dfrac{\partial c_1}{\partial x_1}\right|_{x_1 \quad 0} \\
r \quad r_0, \quad \dfrac{\partial c_1}{\partial r} \quad 0; \quad r \quad R_0, \quad \dfrac{\partial c_1}{\partial r} \quad 0 \\
x_1 \quad 0, \quad c_2(0,r,t) \quad c_3(l,r,t) \\
\bar{c}_3(l,t)\bar{\bar{u}} \quad c_2(0,r,t)u \quad D_2 \left.\dfrac{\partial c_2}{\partial x_1}\right|_{x_1 \quad 0} \\
r \quad r_0, \quad \dfrac{\partial c_2}{\partial r} \quad 0; \quad r \quad R_0, \dfrac{\partial c_2}{\partial r} \quad 0 \\
x \quad 0, \quad c_3(0,r,t) \quad c_2(l,r,t) \\
\bar{c}_2(l,t)\bar{u}_1 \quad c_3(0,r,t)u_1 \quad D_3 \left.\dfrac{\partial c_3}{\partial x}\right|_{x \quad 0} \\
r \quad 0, \quad \dfrac{\partial c_3}{\partial r} \quad 0; \quad r \quad r_0, \quad \dfrac{\partial c_3}{\partial r} \quad 0
\end{array}
\qquad (58)
$$

The radial nonuniformity of the velocity in the airlift is the cause for the scale effect. That is why must be use average velocity and concentration for the cross-section area.

Average concentration models

Let's consider eq. (50). 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 equivalent to the integral average values over radial coordinate:

$$
\bar{u}_0(x) \quad \frac{1}{r_0}\int_0^{r_0} u_0(x,r)\mathrm{d}r, \quad \bar{v}_0(x) \quad \frac{1}{r_0}\int_0^{r_0} v_0(x,r)\mathrm{d}r, \quad \bar{c}(x,t) \quad \frac{1}{r_0}\int_0^{r_0} c(x,r,t)\mathrm{d}r \qquad (59)
$$

where $\bar{u}_0(0) \quad \bar{\bar{u}}_0$.

For the introducing of eq. (59) in eq. (50) must be integrated eq. (50) over r in the interval $[0, r_0]$. For this aim will be used a property of the average function values:

$$
u_0(x,r) \quad \bar{u}_0(x)\tilde{u}_0(r), \quad v_0(x,r) \quad \bar{v}_0(x)\tilde{v}_0(r), \quad c(x,r,t) \quad \bar{c}(x,t)\tilde{c}(r) \qquad (60)
$$

where

$$\int_0^{r_0} \tilde{u}_0(r)\,\mathrm{d}r \quad r_0, \quad \int_0^{r_0} \tilde{v}_0(r)\,\mathrm{d}r \quad r_0, \quad \int_0^{r_0} \tilde{c}(r)\,\mathrm{d}r \quad r_0 \tag{61}$$

As a result is obtained:

$$\frac{\partial \bar{c}}{\partial t} \quad A(r_0)\bar{u}_0 \frac{\partial \bar{c}}{\partial x} \quad G_1(r_0)\bar{v}_0\bar{c} \quad D\frac{\partial^2 \bar{c}}{\partial x^2} \quad B(r_0)\bar{c} \quad \frac{k}{\varepsilon}(\bar{c} \quad \bar{c}_0) \tag{62}$$

where

$$A(r_0) \quad \frac{1}{r_0}\int_0^{r_0} \tilde{u}_0(r)\tilde{c}(r)\,\mathrm{d}r, \quad B(r_0) \quad \frac{1}{r_0}\int_0^{r_0} \frac{1}{r}\frac{\partial \tilde{c}}{\partial r}\mathrm{d}r, \quad G_1(r_0) \quad \frac{1}{r_0}\int_0^{r_0} \tilde{v}_0 \frac{\partial \tilde{c}}{\partial r}\mathrm{d}r \tag{63}$$

If put eq. (61) into second equation in eq. (50) and integrated over r in the interval $[0, r_0]$, the continuity equation has the form:

$$\frac{\partial \bar{u}_0}{\partial x} \quad G_2(r_0)\bar{v}_0 \quad 0 \tag{64}$$

where

$$G_2(r_0) \quad \frac{\tilde{v}_0(r_0) \quad \tilde{v}_0(0)}{r_0} \quad \frac{1}{r_0}\int_0^{r_0} \frac{\tilde{v}_0}{r}\,\mathrm{d}r \tag{65}$$

If put eq. (64) in eq. (62), the final form of the model equation is:

$$\frac{\partial \bar{c}}{\partial t} \quad A(r_0)\bar{u}_0 \frac{\partial \bar{c}}{\partial x} \quad G(r_0)\bar{c}\frac{\partial \bar{u}_0}{\partial x} \quad D\frac{\partial^2 \bar{c}}{\partial x^2} \quad B(r_0)\bar{c} \quad \frac{k}{\varepsilon}(\bar{c} \quad \chi\bar{c}_0) \tag{66}$$

where for $G(r_0)$ was obtained – see eq. (63):

$$G(r_0) \quad \frac{r_0}{3}G_1(r_0) \tag{67}$$

The boundary condition of eq. (66) has the form:

$$\begin{gathered} t \quad 0, \quad \bar{c}(x,0) \quad c^{(0)} \\ x \quad 0, \quad \bar{\bar{u}}_0 c^{(0)} \quad A(r_0)\bar{u}_0(0)\bar{c}(0,t) \quad D\left.\frac{\partial \bar{c}}{\partial z}\right|_{x \quad 0} \\ x \quad 1, \quad \bar{c}(l,t) \quad \chi c_0(l,t) \end{gathered} \tag{68}$$

The parameters in the model (66) and (68) are two tips: specific model parameters (D, k, ε, χ) 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 distributions and show the influence of the scale-up on the model equations. The parameter χ may be obtained beforehand as a result of thermodynamic measurements.

From eq. (66) follow, that the average radial velocity component influence the transfer process in the cases $\partial \bar{u}_0/\partial x \quad 0$, *i. e.* when the gas hold-up in not constant over the column height. For many practical interesting cases $\bar{v}_0 \quad 0$ and the radial velocity component did not taken account in the model.

The hold-up ε must be obtained using:

$$\varepsilon \quad \frac{(l \quad l_0)(F_0 \quad F_1)}{(l \quad l_0)(F_0 \quad F_1) \quad F_0 l_0} \tag{69}$$

where l and l_0 are liquid level in the riser without gas motion.

The parameter values *D, k, A, B,* and *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 but with small height (*D* and *k* do not change at scale-up).

The same procedure may be use for eqs. (51) and (57) and as a result is obtained:

$$\begin{gathered}
\frac{\partial \bar{c}_0}{\partial t} \quad A_0(r_0)\bar{u}_1 \frac{\partial \bar{c}_0}{\partial x} \quad G_0(r_0)\bar{c}_0 \frac{\partial \bar{u}_1}{\partial x} \quad D_0 \frac{\partial^2 \bar{c}_0}{\partial x^2} \quad B_0(r_0)\bar{c}_0 \quad \frac{k}{1 \quad \varepsilon}(\bar{c} \quad \chi \bar{c}_0) \\
a \frac{k_0}{(1 \quad \varepsilon)} M_3(r_0)\bar{c}_0 \bar{c}_3 \bar{J}_1, \\
t \quad 0, \quad \bar{c}_0(x,0) \quad \frac{c^{(0)}}{\chi}, \\
x \quad 0, \quad \bar{c}_0(0,t) \quad \bar{c}_1(l,t), \\
\bar{c}_1(l,t)\bar{u} \quad A(r_0)\bar{u}_1(0)\bar{c}_0(0,t) \quad D \left. \frac{\partial \bar{c}_0}{\partial x} \right|_{x \quad 0}
\end{gathered} \tag{70}$$

where A_0, B_0, and G_0 are obtained on the analogy of *A, B,* and *G* – see eqs. (63), (65) and (67). The concrete expressions of *A, B,* and *G* are not interesting because its values must be obtained, using experimental data.

In the eqs. (52) and (53) with boundary conditions (58) must put the average velocity, concentrations and photon flux density:

$$\begin{gathered}
u(x,r) \quad \bar{u}(x)\tilde{u}(r), \quad c_1(x,r,t) \quad \bar{c}_1(x,t)\tilde{c}_1(r) \\
c_2(x,r,t) \quad \bar{c}_2(x,t), \quad J(x,r,t) \quad \bar{J}(x,t)\tilde{J}(r)
\end{gathered} \tag{71}$$

where

$$\begin{gathered}
\bar{u}(x) \quad \frac{1}{R_0 \quad r_0} \int_{r_0}^{R_0} u(x,r)\mathrm{d}r, \quad \bar{c}_1(x,t) \quad \frac{1}{R_0 \quad r_0} \int_{r_0}^{R_0} c_1(x,r,t)\mathrm{d}r \\
\bar{c}_2(x,t) \quad \frac{1}{R_0 \quad r_0} \int_{r_0}^{R_0} c_2(x,r,t)\mathrm{d}r, \quad \bar{J}(x,t) \quad \frac{1}{R_0 \quad r_0} \int_{r_0}^{R_0} J(x,r,t)\mathrm{d}r
\end{gathered} \tag{72}$$

After integration of eqs. (52) and (53) over r in the interval $[r_0, R_0]$ the problem has the form:

$$\frac{\partial \bar{c}_1}{\partial t} \quad A_1(r_0,R_0)\bar{u}\frac{\partial \bar{c}_1}{\partial x} \quad G_1(r_0,R_0)\bar{c}_1\frac{\partial \bar{u}}{\partial x}$$
$$D_1 \frac{\partial^2 \bar{c}_1}{\partial x^2} \quad B_1(r_0,R_0)\bar{c}_1 \quad ak_0 M(r_0,R_0)\bar{c}_1\bar{c}_2, \bar{J}$$
$$t \quad 0, \quad \bar{c}_1(x_1,0) \quad \frac{c^{(0)}}{\chi} \tag{73}$$
$$x_1 \quad 0, \quad \bar{c}_1(0,t) \quad \bar{c}_0(l,t)$$
$$\bar{c}_0(l,t)\bar{\bar{u}}_1 \quad A_1(r_0,R_0)\bar{u}(0)\bar{c}_1(0,t) \quad D_1 \left.\frac{\partial \bar{c}_1}{\partial x_1}\right|_{x_1 \; 0}$$

$$\frac{\partial \bar{c}_2}{\partial t} \quad A_2(r_0,R_0)\bar{u}\frac{\partial \bar{c}_2}{\partial x} \quad G_2(r_0,R_0)\bar{c}_2\frac{\partial \bar{u}}{\partial x}$$
$$D_2 \frac{\partial^2 \bar{c}_2}{\partial x^2} \quad B_2(r_0,R_0)\bar{c}_2 \quad k_0 M(r_0,R_0)\bar{c}_1\bar{c}_2, \bar{J}$$
$$t \quad 0, \quad \bar{c}_2 \quad c_2^{(0)} \tag{74}$$
$$x_1 \quad 0, \quad \bar{c}_2(0,t) \quad \bar{c}_3(l,t)$$
$$\bar{c}_3(l,t)\bar{\bar{u}}_1 \quad A_2(r_0,R_0)\bar{u}(0)\bar{c}_2(0,t) \quad D_2 \left.\frac{\partial \bar{c}_2}{\partial x_1}\right|_{x_1 \; 0}$$

where

$$M(r_0,R_0) \quad \frac{1}{R_0 \quad r_0}\int_{r_0}^{R_0} \tilde{c}_1\tilde{c}_2\tilde{J}\,\mathrm{d}r \tag{75}$$

and are obtained an the analogy – see eqs. (24), (26), and (28), but limits of the integrals are $[r_0, R_0]$.

$\bar{J}$ in eqs. (73) and (74) may be obtained from eq. (48) if put eq. (71) and to integrate over r in the interval $[r_0, R_0]$. As a result:

$$\bar{J} \quad \frac{1}{N_1 \quad \delta N_2 \bar{c}_2} \tag{76}$$

where

$$N_1(r_0,R_0) \quad \frac{1}{R_0 J_0(R_0 \quad r_0)}\int_{r_0}^{R_0} r^2 \frac{\partial \tilde{J}}{\partial r}\mathrm{d}r$$
$$N_2(r_0,R_0) \quad \frac{1}{R_0 J_0(R_0 \quad r_0)}\int_{r_0}^{R_0} r^2 \tilde{c}_2\tilde{J}\,\mathrm{d}r \tag{77}$$

The integration of eqs. (54), and (58) lead to the equation for $\bar{c}_3$:

$$\frac{\partial \bar{c}_3}{\partial t} + A_3(r_0)\bar{u}_1\bar{c}_3 + G_3(r_0)\bar{c}_3\frac{\partial \bar{u}_1}{\partial x} = D_3\frac{\partial^2 \bar{c}_3}{\partial x^2} + B_3(r_0)\bar{c}_3 - \frac{k_0}{(1-\varepsilon)}M_3(r_0)c_0\bar{c}_3\bar{J}_1;$$
$$t = 0, \quad \bar{c}_3(x,0) = c_2^{(0)};$$
$$x = 0, \quad \bar{c}_3(0,t) = \bar{c}_2(l,t),$$
$$\bar{c}_2(l,t)\bar{\bar{u}} = A_3(r_0)\bar{u}_1(0)\bar{c}_3(0,t) - D_3\left(\frac{\partial \bar{c}_3}{\partial x}\right)_{x=0} \tag{78}$$

where

$$\bar{c}_3 = \frac{1}{r_0}\int_{r_0}^{R_0} c_3(x,r,t)\,\mathrm{d}r, \quad M_3(r_0) = \frac{1}{r_0}\int_0^{r_0}\tilde{c}_0\tilde{c}_3\tilde{J}_1\,\mathrm{d}r \tag{79}$$

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

$\bar{J}_1$ in eq. (76) may be obtained from eq. (55) after integration:

$$\bar{J}_1(x,t) = \frac{\bar{J}(x,t)}{P_1 + \delta P_2\bar{c}_3} \tag{80}$$

where

$$P_1(r_0) = \frac{1}{r_0^2\tilde{J}(r_0)}\int_0^{r_0} r^2\tilde{J}_1\,\mathrm{d}r$$
$$P_2(r_0) = \frac{1}{r_0^2\tilde{J}(r_0)}\int_0^{r_0} r^2\tilde{c}_3\tilde{J}_1\,\mathrm{d}r \tag{81}$$

For many practical interesting cases:

$$\frac{\partial \bar{u}}{\partial x} = \frac{\partial \bar{u}_0}{\partial x} = \frac{\partial \bar{u}_1}{\partial x} = 0 \tag{82}$$

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

Hierarchical approach

The problems (66), (68), (70), (73), (74), and (78) are mathematical model of an airlift photobioreactor. The model parameters are five tipes:

– beforehand known ($c^{(0)}, c_2^{(0)}, R_0, J_0, r_0$),
– beforehand obtained (ε, χ, a, δ, k_0),
– obtained without photobioreaction (k, D, D_0, A, B, A_0, B_0),
– obtained with photobioreaction (D_1, D_2, D_3), and

– 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, M, M_3, P_1, P_2).

The problems eq. (66), (68), and (70) permit to obtain (k, D, D_0, A, B, A_0, B_0) without photobioreaction if put:

$$\bar{c}_1(l,t) \quad \bar{c}_0(l,t) \tag{83}$$

The result obtained show a possibility to build airlift photobioreactor models using average velocities and concentrations. These models has different type parameters related with the process and with the apparatus (scale-up). This approach permit to solve the scale-up problem as a result to the radial nonuniformity of the velocity and concentration cross-section distributions, using radius dependent parameters.

Airlift three phase catalytic reactors

The hydrodynamic behavior of the gas and liquid flows in airlift three phase catalytic reactors is very complicated. In these conditions the convective and diffusive transfer with heterogeneous catalytic reactions are realized simultaneously [4, 20, 21].

The creation of the models in these conditions and solving of the scale - up problem [1, 2] require construction of a suitable diffusion models.

Mathematical model

Let consider airlift reactor for alcohol oxidation [22-25] 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-up in the riser are ε and $1-\varepsilon$.

The concentrations of the active gas component (O_2) 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 $x_1 = 1 - x$.

The concentration of the alcohol in the downcomer is $c_2\,(x_1,r,t)$ and in the riser section $c_3\,(x,r,t)$.

If the active sites concentration of the catalyst particles is sufficiently big it may be put equal to constant.

The average velocities in gas and liquid phases are:

$$\bar{\bar{u}}_0 \quad \frac{Q_0}{F_0}, \quad \bar{\bar{u}}_1 \quad \frac{Q_1}{F_0}, \quad \bar{\bar{u}} \quad \frac{Q_1}{F_1} \tag{84}$$

The interphase mass transfer rate in the riser is:

$$R \quad k(c \quad \chi c_0) \tag{85}$$

The alcohol oxydation rates in the downcomer and the riser are:

$$R_1 \quad k_0 c_0^{\mu_1} c_0^{\mu_2}, \quad R_2 \quad k_0 c_1^{\mu_1} c_2^{\mu_2} \tag{86}$$

The mathematical model of the chemical processes in airlift reactor will be built on the basis of the differential mass balance. A convection-diffusion equation with volume reaction will be used, where convective transfer will be results of the laminar flow or large scale turbulent pulsations, the diffusion transfer is molecular or turbulent (as a result of the small scale turbulent pulsations) and the volume reactions are interphase mass transfer and chemical reaction.

The equations for oxygen concentration distributions in the gas and liquid phases in the riser are:

$$\varepsilon \frac{\partial c}{\partial t} \quad \varepsilon u_0 \frac{\partial c}{\partial x} \quad \varepsilon v_0 \frac{\partial c}{\partial r} \quad \varepsilon D \quad \frac{\partial^2 c}{\partial x^2} \quad \frac{1}{r}\frac{\partial c}{\partial r} \quad \frac{\partial^2 c}{\partial r^2} \quad k(c \quad \chi c_0)$$
$$\frac{\partial u_0}{\partial x} \quad \frac{\partial v_0}{\partial r} \quad \frac{v_0}{r} \quad 0 \tag{87}$$

$$(1 \quad \varepsilon)\frac{\partial c_0}{\partial t} \quad (1 \quad \varepsilon) \ u_1 \frac{\partial c_0}{\partial r} \quad v_1 \frac{\partial c_0}{\partial x}$$
$$(1 \quad \varepsilon) D_0 \quad \frac{\partial^2 c_0}{\partial x^2} \quad \frac{1}{r}\frac{\partial c_0}{\partial r} \quad \frac{\partial^2 c_0}{\partial r^2} \quad k(c \quad \chi c_0) \quad k_0 c_0^{\mu_1} c_3^{\mu_2} \tag{88}$$
$$\frac{\partial u_1}{\partial x} \quad \frac{\partial v_1}{\partial r} \quad \frac{v_1}{r} \quad 0$$

It is possible to suppose that ε = const.

The equations for the alcohol and oxygen concentration distributions in the liquid phase in the downcomer are:

$$\frac{\partial c_1}{\partial t} \quad u \frac{\partial c_1}{\partial x_1} \quad v \frac{\partial c_1}{\partial r} \quad D_1 \quad \frac{\partial^2 c_1}{\partial x^2} \quad \frac{1}{r}\frac{\partial c_1}{\partial r} \quad \frac{\partial^2 c_1}{\partial r^2} \quad k_0 c_1^{\mu_1} c_2^{\mu_2} \tag{89}$$

$$\frac{\partial c_2}{\partial t} \quad u \frac{\partial c_2}{\partial x_1} \quad v \frac{\partial c_2}{\partial r} \quad D_2 \quad \frac{\partial^2 c_2}{\partial x^2} \quad \frac{1}{r}\frac{\partial c_2}{\partial r} \quad \frac{\partial^2 c_2}{\partial r^2} \quad k_0 c_1^{\mu_1} c_2^{\mu_2} \tag{90}$$

where $x_1 = l - x$.

The equation for alcohol concentration distribution in the riser is:

$$(1 \quad \varepsilon)\frac{\partial c_3}{\partial t} \quad (1 \quad \varepsilon) \ u_1 \frac{\partial c_3}{\partial r} \quad v_1 \frac{\partial c_3}{\partial x} \quad (1 \quad \varepsilon) D_3 \quad \frac{\partial^2 c_3}{\partial x^2} \quad \frac{1}{r}\frac{\partial c_3}{\partial r} \quad \frac{\partial^2 c_3}{\partial r^2} \quad k_0 c_0^{\mu_1} c_3^{\mu_2} \tag{91}$$

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

$$
\begin{gathered}
t = 0, \quad c(x,r,0) = c^{(0)}, \quad c_0(x,r,0) = 0 \\
c_1(x_1,r,0) = 0, \quad c_2(x_1,r,0) = c_2^{(0)}, \quad c_3(x,r,0) = c_2^{(0)}
\end{gathered} \tag{92}
$$

where $c^{(0)}$ and $c_2^{(0)}$ are initial concentrations of the oxygen in the gas phase and of the alcohol in the liquid phase.

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. (87) and (88) are:

$$
\begin{gathered}
x = 0, \quad \bar{\bar{u}}_0 c^{(0)} = u_0 c(0,r,t) - D \left(\frac{\partial c}{\partial x} \right)_{x=0} \\
x = l, \quad c(l,r,t) = \chi c_0(l,r,t) \\
x = 0, \quad c_0(0,r,t) = c_2(l,r,t) \\
\bar{c}_2(l,t)\bar{\bar{u}} = c_0(0,r,t)u_1 - D_0 \left(\frac{\partial c_0}{\partial x} \right)_{x=0} \\
r = 0, \quad \frac{\partial c}{\partial r} = \frac{\partial c_0}{\partial r} = 0 \\
r = r_0, \quad \frac{\partial c}{\partial r} = \frac{\partial c_0}{\partial r} = 0
\end{gathered} \tag{93}
$$

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. (89)-(91) are:

$$
\begin{gathered}
x_1 = 0, \quad c_1(0,r,t) = c_3(l,r,t) \\
\bar{c}_3(l,t)\bar{\bar{u}}_1 = c_1(0,r,t)u - D_1 \left(\frac{\partial c_1}{\partial x_1} \right)_{x=0} \\
r = r_0, \quad \frac{\partial c_1}{\partial r} = 0; \quad r = R_0, \quad \frac{\partial c_1}{\partial r} = 0 \\
x_1 = 0, \quad c_2(0,r,t) = c_0(l,r,t) \\
\bar{c}_0(l,t)\bar{\bar{u}} = c_2(0,r,t)u - D_2 \left(\frac{\partial c_2}{\partial x_1} \right)_{x=0} \\
r = r_0, \quad \frac{\partial c_2}{\partial r} = 0; \quad r = R_0, \quad \frac{\partial c_2}{\partial r} = 0 \\
x = 0, \quad c_3(0,r,t) = c_1(l,r,t) \\
\bar{c}_1(l,t)\bar{\bar{u}} = c_3(0,r,t)u_1 - D_3 \left(\frac{\partial c_3}{\partial x} \right)_{x=0} \\
r = 0, \quad \frac{\partial c_3}{\partial r} = 0; \quad r = r_0, \quad \frac{\partial c_3}{\partial r} = 0
\end{gathered} \tag{94}
$$

The radial nonuniformity of the velocity in the column apparatuses is the cause for the scale effect (decreasing of the process efficiency with increasing of the column diameter) in the column process scale-up. That is why must be use average velocity and concentration for the cross-section area.

Average concentration models

Let's consider eq. (87). 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 equivalent to the integral average values over radial coordinate:

$$\bar{u}_0(x) \quad \frac{1}{r_0}\,{}_0^{r_0} u_0(x,r)\,\mathrm{d}r, \quad \bar{v}_0(x) \quad \frac{1}{r_0}\,{}_0^{r_0} v_0(x,r)\,\mathrm{d}r, \quad \bar{c}(x,t) \quad \frac{1}{r_0}\,{}_0^{r_0} c(x,r,t)\,\mathrm{d}r \tag{95}$$

where $\bar{u}_0(0) \quad \bar{\bar{u}}_0$.

For the introducing of eq. (95) in eq. (87) must be integrated eq. (87) over r in the interval $[0, r_0]$. For this aim will be used a property of the average function values:

$$u_0(x,r) \quad \bar{u}_0(x)\tilde{u}_0(r), \quad v_0(x,r) \quad \bar{v}_0(x)\tilde{v}_0(r), \quad c(x,r,t) \quad \bar{c}(x,t)\tilde{c}(r) \tag{96}$$

where

$$ {}_0^{r_0}\tilde{u}_0(r)\,\mathrm{d}r \quad r_0, \quad {}_0^{r_0}\tilde{v}_0(r)\,\mathrm{d}r \quad r_0, \quad {}_0^{r_0}\tilde{c}_0(r)\,\mathrm{d}r \quad r_0 \tag{97}$$

As a result is obtained:

$$\frac{\partial \bar{c}}{\partial t} \quad A(r_0)\bar{u}_0 \frac{\partial \bar{c}}{\partial x} \quad G_1(r_0)\bar{v}_0\bar{c}_0 \quad D\frac{\partial^2 \bar{c}}{\partial x^2} \quad B(r_0)\bar{c} \quad \frac{k}{\varepsilon}(\bar{c} \quad \chi\bar{c}_0) \tag{98}$$

where

$$A(r_0) \quad \frac{1}{r_0}\,{}_0^{r_0}\tilde{u}_0(r)\tilde{c}(r)\,\mathrm{d}r, \quad B(r_0) \quad \frac{1}{r_0}\,{}_0^{r_0}\frac{1}{r}\frac{\partial \tilde{c}}{\partial r}\,\mathrm{d}r, \quad G_1(r_0) \quad \frac{1}{r_0}\,{}_0^{r_0}\tilde{v}_0\frac{\partial \tilde{c}}{\partial r}\,\mathrm{d}r \tag{99}$$

If put eq. (97) into second equation in eqs. (87) and integrated over r in the interval $[0, R]$, the continuity equation has the form:

$$\frac{\partial \bar{u}_0}{\partial x} \quad G_2(r_0)\bar{v}_0 \quad 0 \tag{100}$$

where

$$G_2(r_0) \quad \frac{\tilde{v}_0(r_0) \quad \tilde{v}_0(0)}{r_0} \quad \frac{1}{r_0}\,{}_0^{r_0}\frac{\tilde{v}_0}{r}\,\mathrm{d}r \tag{101}$$

If put eq. (100) in eq. (98), the final form of the model equation is:

$$\frac{\partial \bar{c}}{\partial t} + A(r_0)\bar{u}_0 \frac{\partial \bar{c}}{\partial x} + G(r_0)\bar{c}\frac{\partial \bar{u}_0}{\partial x} = D\frac{\partial^2 \bar{c}}{\partial x^2} + B(r_0)\bar{c} - \frac{k}{\varepsilon}(\bar{c} - \chi \bar{c}_0) \qquad (102)$$

where for G(r_0) was obtained:

$$G(r_0) = \frac{r_0}{3} G_1(r_0) \qquad (103)$$

The boundary conditions of eq. (102) has the form:

$$t = 0, \quad \bar{c}(x,0) = c^{(0)}$$
$$x = 0, \quad \bar{\bar{u}}_0 c^{(0)} = A(r_0)\bar{u}_0(0)\bar{c}(0,t) - D\left(\frac{\partial \bar{c}}{\partial x}\right)_{x=0} \qquad (104)$$
$$x = l, \quad \bar{c}(l,t) = \chi c_0(l,t)$$

The parameters in the model (102)-(104) are two tips: specific model parameters (*D, k, ε,* χ) 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 χ may be obtained beforehand as a result of thermodynamic measurements.

From eq. (102) 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 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 but with small height (*D* and *k* do not change at scale-up).

The same procedure may be use for eqs. (88)-(94), and as a result is obtained:

$$\frac{\partial \bar{c}_0}{\partial t} + A_0(r_0)\bar{u}_1\frac{\partial \bar{c}_0}{\partial x} + G_0(r_0)\bar{c}_0\frac{\partial \bar{u}_1}{\partial x} =$$
$$D_0\frac{\partial^2 \bar{c}_0}{\partial x^2} + B_0(r_0)\bar{c}_0 - \frac{k}{1-\varepsilon}(\bar{c} - \chi\bar{c}_0) - M_0(r_0)\frac{k_0}{1-\varepsilon}\bar{c}_0^{\mu_1}\bar{c}_3^{\mu_2}$$
$$M_0(r_0) = \frac{1}{r_0}\int_0^{r_0}\tilde{c}_0^{\mu_1}\tilde{c}_3^{\mu_2}\,\mathrm{d}r \qquad (105)$$
$$t = 0, \quad \bar{c}_0(x,0) = 0$$
$$x = 0, \quad \bar{c}_0(0,t) = \bar{c}_1(l,t)$$
$$\bar{c}_1(l,t)\bar{\bar{u}} = A(r_0)\bar{u}_1(0)\bar{c}_0(0,t) - D_0\left(\frac{\partial \bar{c}_0}{\partial x}\right)_{x=0}$$

where A_0, B_0, and G_0 are obtained on the analogy of *A, B,* and *G* – see (99), (101), and (105). The concrete expressions of *A, B,* and *G* are not interesting because its values must be obtained, using experimental data.

The integration of eq. (89) over *r* in the interval $[r_0, R_0]$ lead to the equations for $\bar{c}_1$:

$$\frac{\partial \bar{c}_1}{\partial t} \quad A_l(r_0, R_0)\, \bar{u}\, \frac{\partial \bar{c}_1}{\partial x} \quad G_1(r_0, R_0)\, \bar{c}_1 \frac{\partial \bar{u}}{\partial x}$$
$$D_1 \frac{\partial^2 \bar{c}_1}{\partial x^2} \quad B_1(r_0, R_0) \bar{c}_1 \qquad k_0 M(r_0, R_0)\, c_1^{\mu_1} \bar{c}_2^{\mu_2}$$
$$t \quad 0, \quad \bar{c}_1(x_1, 0) \quad 0 \tag{106}$$
$$x_1 \quad 0, \quad \bar{c}_1(0, t) \quad \bar{c}_3(l, t)$$
$$\bar{c}_3(l, t)\, \bar{\bar{u}}_1 \quad A_1(r_0, R_0)\, \bar{u}\,(0)\, \bar{c}_1(0, t) \quad D_1 \frac{\partial \bar{c}_1}{\partial x_1}\Big|_{x \; 0}$$

where

$$\bar{u}(x) \quad \frac{1}{R_0 \quad r_0} \int_{r_0}^{R_0} u(x, r)\, \mathrm{d}r, \quad \bar{c}_1(x, t) \quad \frac{1}{R_0 \quad r_0} \int_{r_0}^{R_0} c_1(x, r, t)\, \mathrm{d}r;$$
$$M(r_0, R_0) \quad \frac{1}{R_0 \quad r_0} \int_{r_0}^{R_0} \tilde{c}_1^{\mu_1} \tilde{c}_2^{\mu_2} \mathrm{d}r \tag{107}$$

and $A_1(r_0,R_0)$, $B_1(r_0,R_0)$, and $G_1(r_0,R_0)$, are obtained an the analogy of *A, B,* and *G* – see eqs. (99), (101), and (103), but limits of the integrals are $[r_0, \mathrm{R}_0]$.

The integration of eq. (90) over *r* in interval $[r_0, R_0]$ lead to the equations for $\bar{c}_2$:

$$\frac{\partial \bar{c}_2}{\partial t} \quad A_2(r_0, R_0) \bar{u} \frac{\partial \bar{c}_2}{\partial x} \quad G_2(r_0, R_0)\, \bar{c}_2 \frac{\partial \bar{u}}{\partial x}$$
$$D_2 \frac{\partial^2 \bar{c}_2}{\partial x^2} \quad B_2(r_0, R_0)\, \bar{c}_2 \qquad M(r_0, R_0)\, k_0 \bar{c}_1^{\mu_1} \bar{c}_2^{\mu_2}$$
$$t \quad 0, \quad \bar{c}_2 \quad c_2^{(0)} \tag{108}$$
$$x_1 \quad 0, \quad \bar{c}_2(0, t) \quad \bar{c}_0(l, t)$$
$$\bar{c}_3(l, t) \bar{\bar{u}}_1 \quad A_2(r_0, R_0)\, \bar{u}(0) \bar{c}_2(0, t) \quad D_2 \frac{\partial \bar{c}_2}{\partial x_1}\Big|_{x_1 \; 0}$$

where

$$\bar{c}_2 \quad \frac{1}{R_0 \quad r_0} \int_{r_0}^{R_0} c_2(x, r, t)\, \mathrm{d}r, \quad \bar{c}_3 \quad \frac{1}{r_0} \int_0^{r_0} c_3(x, r, t)\, \mathrm{d}r \tag{109}$$

The integration of eq. (91) lead to the equation for $\bar{c}_3$:

$$\frac{\partial \bar{c}_3}{\partial t} \quad A_3(r_0)\, \bar{u}_1 \frac{\partial \bar{c}_3}{\partial x} \quad G_3(r_0)\, \bar{c}_3 \frac{\partial \bar{u}_1}{\partial x} \quad D_3 \frac{\partial^2 \bar{c}_3}{\partial x^2} \quad B_3(r_0)\, \bar{c}_3 \qquad M_0(r_0) \frac{k_0}{1 \quad \varepsilon} \bar{c}_0^{\mu_1} \bar{c}_3^{\mu_2}$$

$$
\begin{aligned}
&t \quad 0, \quad \bar{c}_3(x,0) \quad c_2^{(0)} \\
&x \quad 0, \quad \bar{c}_3(0,t) \quad \bar{c}_1(l,t) \\
&\bar{c}_1(l,t)\,\bar{\bar{u}} \quad A_3(r_0)\,\bar{u}_1(0)\,\bar{c}_3(0,t) \quad D_3 \; \frac{\partial \bar{c}_3}{\partial x}_{x \; 0}
\end{aligned}
\qquad (110)
$$

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 (m^3/m^{-3}) of the catalytic particles or gas hold-up are constant over the column, *i. e.*:

$$
\frac{\partial \bar{u}}{\partial x} \quad \frac{\partial \bar{u}_0}{\partial x} \quad \frac{\partial \bar{u}_1}{\partial x} \quad 0, \quad \bar{v} \quad \bar{v}_0 \quad \bar{v}_1 \quad 0 \qquad (111)
$$

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

Hierarchical approach

The problems (102), (104), (105), (106), (108), and (110) are mathematical model of an airlift three phase catalytic reactor. The model parameters are five tipes:

- beforehand known ($c^{(0)}, c_2^{(0)}, R_0, r_0$),
- beforehand obtained ($\varepsilon, \chi, \mu_1, \mu_2, k_0$),
- obtained without chemical reaction (k, D, D_0, A, B, A_0, B_0),
- obtained with chemical reaction (D_1, D_2, D_3, M, M_0), and
- 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, M, M_0).

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

$$
\bar{c}_1(l,t) \quad \bar{c}_0(l,t) \qquad (112)
$$

The result obtained show a possibility to build three phase catalytic airlift reactor models, using average velocities and concentrations. This approach permit to solve the scale-up problem as a result to the radial nonuniformity of the velocity and concentration, using radius dependent parameters.

Fluidized bed reactors

Many technological processes, as a catalytic chemical reactions, burning, heating, drying, *etc.*, are realized in column apparatuses with fluidized bed [9]. The hydrodynamic behavior of the fluidized bed like to the motion in counter-current flows. A cylindrical surface, where velocity is equal to zero, is the border between the rising and the downcomer flows. In this sens the fluidized bed reactors are similar to the airlift reactors, where the solid phase plays the role of the liquid phase. On this base is possible to use the methods for modeling of the airlift apparatuses for fluidized bed modeling.

Hydrodynamic model

Let's consider a fluidized bed column with a horizontal cross-sections area *f,* for the riser zone and $(F - f)$ for the downcomer zone, where F is the horizontal cross-section's area of the column.

The average velocities of the solid particle in the riser and downcomer are $\bar{v}$ and $\bar{v}_0$, where $\bar{v}_0$ is the average sedimentation velocity of the solid particles.

Let's assume that velocities of the solid phase $\bar{v}$ and $\bar{v}_0$ are known beforehand as a result of experimental or computing methods.

From the mass balance of the solid phase is obtained:

$$\bar{v}f \quad (F \quad f)\bar{v}_0 \tag{113}$$

i. e.

$$f \quad \frac{\bar{v}_0}{\bar{v} \quad \bar{v}_0} F \tag{114}$$

Let's assume that gas flow in the riser carry away the solid phase, while in the downcomer solid flow carry away the gas phase. If average gas velocities in the riser and downcomer are $\bar{u}$ and $\bar{v}_0$, a circulation gas flow exist.

The gas flow rate in the riser zone Q is result of the inlet gas flow Q_0 and circulation gas flow Q_1:

$$Q \quad Q_0 \quad Q_1 \quad \bar{u}_0 f \tag{115}$$

where

$$Q_1 \quad \bar{v}_0(F \quad f) \tag{116}$$

As a result was obtained:

$$\bar{u}_0 \quad \bar{v} \quad \frac{\bar{v}_0 \quad \bar{v}}{\bar{v}_0} \frac{Q_0}{F} \tag{117}$$

If accept a cylindrical form of the riser and downcomer zone, the radii may be obtained from:

$$f \quad \pi r_0^2, \quad F \quad f \quad \pi(R^2 \quad r_0^2) \tag{118}$$

Convection-diffusion model

Let's consider fluidized bed column with catalytic chemical reaction on the solid interface. The axial and radial gas velocity components in the riser are *u* and *w*:

$$u \quad u(r,z), \quad w \quad w(r,z), \quad 0 \quad r \quad r_0, \quad 0 \quad z \quad l \tag{119}$$

where *l* is fluidized bad height.

A component of the gas phase react on the catalyst particles interface and its concentration has radial and axial non-uniformity:

$$c \quad c(r,z), \quad 0 \quad r \quad t_0, \quad 0 \quad z \quad l \tag{120}$$

The convection-diffusion equation for this case is:

$$u\frac{\partial c}{\partial z} \quad w\frac{\partial c}{\partial r} \quad D \quad \frac{\partial^2 c}{\partial z_1^2} \quad \frac{1}{r}\frac{\partial c}{\partial r} \quad \frac{\partial^2 c}{\partial r^2} \qquad kc \tag{121}$$

where the velocity components satisfy the continuity equation:

$$\frac{\partial u}{\partial z} \quad \frac{\partial w}{\partial r} \quad \frac{w}{r} \quad 0 \tag{122}$$

The convective transfer is result of a laminar or turbulent (large-scale pulsations) flow, the diffusive transfer is molecular or turbulent (small-scale pulsations) and the order of the catalytic chemical reaction is one.

In the downcomer the convection-diffusion equation has the form:

$$u_1\frac{\partial c_1}{\partial z_1} \quad w_1\frac{\partial c_1}{\partial r} \quad D \quad \frac{\partial^2 c_1}{\partial z_1^2} \quad \frac{1}{r}\frac{\partial c_1}{\partial r} \quad \frac{\partial^2 c_1}{\partial r^2} \qquad kc_1 \tag{123}$$

$$\frac{\partial u_1}{\partial z_1} \quad \frac{\partial w_1}{\partial r} \quad \frac{w_1}{r} \quad 0 \tag{124}$$

where $z_1 = l - z$, $u_1 = u_1(r, z_1)$, $w_1 = w_1(r, z_1)$, $c_1 = c_1(r, z_1)$ are axial coordinate, velocity components and concentration in the downcomer.

The boundary conditions of eqs. (121)-(124) are obtained on the base of the assumption for an ideal mixing in the two ends of the column:

$$\begin{gathered} z \quad 0, \quad c \quad \bar{c}_0, \quad \frac{Q_0}{f}c_0 \quad \frac{Q_1}{f}c_1(r,l) \quad uc \quad D\frac{\partial c}{\partial z} \\ z_1 \quad 0, \quad c_1(r,0) \quad \bar{c}(l), \quad \bar{v}_0 c_1(r,0) \quad u_1 c_1 \quad D_1\frac{\partial c_1}{\partial z_1} \\ r \quad 0, \quad \frac{\partial c}{\partial r} \quad 0, \quad r \quad r_0, \quad \frac{\partial c}{\partial r} \quad \frac{\partial c_1}{\partial r} \quad 0; \quad r \quad R, \quad \frac{\partial c_1}{\partial r} \quad 0 \end{gathered} \tag{125}$$

where c_0 is initial gas concentration, and $\bar{c}_0, \bar{c}$ – are average gas concentrations:

$$\bar{c}(z) = \frac{1}{r_0}\int_0^{r_0} c(r,z)\,\mathrm{d}r$$
$$\bar{c}_0 = \frac{Q_0}{fQ}c_0 + \frac{Q_1}{fQ}c_1(r,l) \tag{126}$$

The radial non-uniformity of the velocity is the cause for the scale effect (decreasing of the process efficiency with increasing of the column diameter). That is why an average velocity and concentration for the horizontal cross-section's area are used.

Average function values

For the average velocity and concentration in the riser zone may be obtained:

$$\bar{u}(z) = \frac{1}{r_0}\int_0^{r_0} u(r,z)\,\mathrm{d}r, \quad \bar{w}(z) = \frac{1}{r_0}\int_0^{r_0} w(r,z)\,\mathrm{d}r, \quad \bar{c}(z) = \frac{1}{r_0}\int_0^{r_0} c(r,z)\,\mathrm{d}r \tag{127}$$

If use a property of the average functions, the velocity and concentration may to present as a:

$$u(r,z) = \bar{u}(z)\tilde{u}(r), \quad w(r,z) = \bar{w}(z)\tilde{w}(r), \quad c(r,z) = \bar{c}(z)\tilde{c}(r) \tag{128}$$

where

$$\frac{1}{r_0}\int_0^{r_0} \tilde{u}(r)\,\mathrm{d}r = 1, \quad \frac{1}{r_0}\int_0^{r_0} \tilde{w}(r)\,\mathrm{d}r = 1, \quad \frac{1}{r_0}\int_0^{r_0} \tilde{c}(r)\,\mathrm{d}r = 1, \tag{129}$$

The same results for the average velocity and concentration is obtained in the downcomer zone:

$$u_1(r,z) = \bar{u}_1(z)\tilde{u}_1(r), \quad w_1(r,z) = \bar{w}_1(z)\tilde{w}_1(r)$$
$$c_1(r,z) = \bar{c}_1(z)\tilde{c}_1(r), \quad \frac{1}{R - r_0}\int_{r_0}^{R} \tilde{u}_1(r)\,\mathrm{d}r = 1$$
$$\frac{1}{R - r_0}\int_{r_0}^{R} \tilde{w}_1(r)\,\mathrm{d}r = 1, \quad \frac{1}{R - r_0}\int_{r_0}^{R} \tilde{c}_1(r)\,\mathrm{d}r = 1 \tag{130}$$

Average concentration model

The average concentration model may be obtained if put eqs. (128)-(130) in eqs. (121)-(125) and to integrated the eqs. (121), (122), and(125) over r in the interval $[0, r_o]$ and eqs. (123)-(125) in the interval $[r_0, R]$. As a result was obtained:

$$\alpha(r_0)\bar{u}\frac{\partial \bar{c}}{\partial z} \quad \gamma(r_0)\bar{c}\frac{\partial \bar{u}}{\partial z} \quad D\frac{\partial^2 \bar{c}}{\partial z^2} \quad \beta(r_0)\bar{c} \quad k\bar{c}$$

$$z \quad 0, \quad \bar{c} \quad \bar{c}_0, \quad \bar{u}_0\bar{c}_0 \quad \alpha(r_0)\bar{u}\bar{c} \quad D\frac{\partial \bar{c}}{\partial z} \tag{131}$$

$$\frac{\partial \bar{u}}{\partial z} \quad \gamma_0(r_0)\bar{w}$$

$$\alpha(r_0) \quad \frac{1}{r_0}\int_0^{r_0}\tilde{u}(r)\tilde{c}(r)\,\mathrm{d}r, \quad \beta(r_0) \quad \frac{1}{r_0}\int_0^{r_0}\frac{1}{r}\frac{\partial \tilde{c}}{\partial r}\,\mathrm{d}r,$$

$$\gamma(r_0) \quad \frac{1}{3}\int_0^{r_0}\tilde{w}(r)\frac{\partial \bar{c}}{\partial r}\,\mathrm{d}r, \quad \gamma_0 \quad \frac{\tilde{w}(r_0) \quad \tilde{w}(0)}{r_0} \quad \frac{1}{r_0}\int_0^{r_0}\frac{\tilde{w}}{r}\,\mathrm{d}r \tag{132}$$

$$\alpha_1(r_0,R)\bar{u}_1\frac{\partial \bar{c}_1}{\partial z_1} \quad \gamma_1(r_0,R)\bar{c}_1\frac{\partial \bar{u}_1}{\partial z_1}$$

$$D_1\frac{\partial^2 \bar{c}_1}{\partial z_1^2} \quad \beta_1(r_0,R)\bar{c}_1 \quad k\bar{c}_1, \tag{133}$$

$$z_1 \quad 0, \quad \bar{c}_1(0) \quad \bar{c}(l), \quad \bar{v}_0\bar{c}_1(0) \quad \alpha_1(r_0,R)\bar{u}_1\bar{c}_1 \quad D_1\frac{\partial \bar{c}_1}{\partial z_1}$$

$$\frac{\partial \bar{u}_1}{\partial z} \quad \gamma_1^{(0)}(r_0,R)\bar{w}_1$$

$$\alpha_1(r_0,R) \quad \frac{1}{R \quad r_0}\int_{r_0}^{R}\tilde{u}_1(r)\tilde{c}_1(r)\,\mathrm{d}r, \quad \beta_1(r_0,R) \quad \frac{1}{R \quad r_0}\int_{r_0}^{R}\frac{1}{r}\frac{\partial \bar{c}_1(r)}{\partial r}\,\mathrm{d}r \tag{134}$$

$$\gamma_1(r_0,R) \quad \frac{1}{3}\int_{r_0}^{R}\tilde{w}_1(r)\frac{\partial \bar{c}_1(r)}{\partial r}\,\mathrm{d}r, \quad \gamma_1^{(0)}(r_0,R) \quad \frac{\tilde{w}_1(R) \quad \tilde{w}_1(r_0)}{R \quad r_0} \quad \frac{1}{R \quad r_0}\int_{r_0}^{R}\frac{\tilde{w}_1(r)}{r}\,\mathrm{d}r$$

where $\alpha, \alpha_1, \beta, \beta_1, \gamma$, and γ_1 are obtained on the analogy for α, β, and γ in eq. (32).

In many cases the concentration of the solid phase is constant, *i. e.* $\partial \bar{u}/\partial z \quad 0$ and $\partial \bar{u}_1/\partial z_1 \quad 0$, *i. e.* $\gamma = \gamma_1 = 0$.

A similar models may be obtained for burning or heat and mass transfer processes in fluidized bed (heating or drying of the solid phase), but must be used two-phase models.

Hierarchical approach

The problems (131) and (133) are mathematical model of a fluidized bed catalytic reactor. The model parameters are different types:

– beforehand known – F, R, Q_0, c_0,
– beforehand obtained – f, r_0, $\bar{v}_0$, $\bar{v}$, l, $\bar{u}_0$, $\bar{c}_0$, k,
– obtained with chemical reaction – D, D_1, $\alpha, \beta, \alpha_1, \beta_1$, and
– specified in the scale-up – $\alpha, \beta, \alpha_1, \beta_1$.

As a result a hierarchical approach in mathematical modeling (model parameters identification) is possible to be used. The parameters D, D_1, α, β, α_1, and β_1 may be obtained using experimental data for $\bar{c}$ and $\bar{c}_1$ after solution of the inverse identification problems.

Conclusion

The result obtained show a possibility to construct diffusion models of column apparatuses for heat and mass transfer, complicated with chemical, photochemical, biochemical, or catalytic reactions. Models of a column with (or without) packed bed, two (or three) phase airlift reactor, and fluidized bed reactors are presented. Average velocities and concentrations are used. These models have different type parameters related with the process and with the apparatus (scale-up). This approach permit to solve the scale-up problem as a result to the radial nonuniformity of the velocity and concentration cross-section distributions, 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. In many cases the diffusivities in the convection-diffusions equations are small parameters and inverse problems for parameter identifications are incorrect (ill-posed) [26, 27].

Nomenclature

a – photoreaction equivalent (kg active gas component / kg photoactive substance (cells)),
c – concentration, [kg/m^3]
D – diffusivity, [m^2/s]
F – horizontal section's area of the fluidized bed column, [m^2]
F_0 – horizontal section's area for the riser zone, [m^2]
F_1 – horizontal section's area for the downcomer zone, [m^2]
f – horizontal section's area of the riser zone in fluidized bed column, [m^2]
J – photon flux density in the downcomerzone, [erg m^{-2} s^{-1}]
J_1 – photon flux density in the riser zone, [erg m^{-2} s^{-1}]
k – chemical reaction (interphase mass transfer) rate coefficient, [s^{-1}]
l – apparatus height, working zone length, [m]
Q_0 – gas flow rate, [m^{3}s^{-1}]
Q_1 – liquid flow rate, [m^{3}s^{-1}]
r – radial coordinate, [m]
r_0 – riser radius, [m]
R – downcomer radius, [m]
R_0 – column radius, [m]
t – time, [s]

u – axial velocity component, [m/s]
v – radial velocity component, [m/s]
w – radial velocity component in fluidized bed column, [m/s]
x – longitudinal coordinate, [m]
z – axial coordinate of airlift column, [m]

Greek letters

δ – light absorption coefficient
ε – hold-up
μ – reaction order
φ – angle coordinate, [rad]
χ – Henry's number

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Author's address:

Chr. Boyadjiev
Institute of Chemical Engineering
Bulgarian Academy of Sciences
"Acad. G. Bonchev"-street, bl. 103
1113 Sofia, Bulgaria

E-mail: chboyadj@bas.bg

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