

A NEW APPROACH FOR THE COLUMN APPARATUSES MODELING IN CHEMICAL AND POWER ENGINEERING

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The column apparatuses are main devices for solution of technological and ecological problems in chemical and power engineering. A new approach of the column apparatuses modeling on the base of the physical approximations of the mechanics of continua, using two steps models: convection-diffusion type of model (for qualitative analysis) and average concentration model (for quantitative analysis), is presented.

The convection-diffusion type of models describe chemical and mass transfer processes in column apparatuses in the cases of one, two, or three phases systems, where the solid phase is reagent, catalytic, or packed bed. A qualitative analysis of these models, using generalized (dimensionless) variables, where the characteristic (inherent) scales are the maximal or average values of the variables, is presented.

The using of the convection-diffusion type of models for quantitative analysis of the processes in column apparatuses is not possible because the velocity function in the convection-diffusion equation is unknown. The problem can be avoided if the average values of the velocity and concentration over the cross-sectional area of the column are used. The average concentration models permit to analyze the effect of the radial non-uniformities of the velocity and the concentration on the process efficiency in the column and to solve the scale-up problem.

The convection-diffusion type of models are presented as a base for to be created convection and diffusion type of models.

Key words: *column apparatuses modeling, velocity radial non-uniformity, convection-diffusion type of model, convection type of model, diffusion type of model, average concentration model*

Introduction

The chemical and mass transfer processes in column apparatuses are realized in one, two, or three phases systems, where the gas and liquid are moving phases, while the solid phase is catalyst, adsorbent, or packet fixed bed [1]. The main process in the column apparatuses is mass transfer (complicated with volume or interface reaction) of a component of the moving fluid. This component participates in chemical reaction or interphase mass transfer in the column volume.

The column apparatus is possible to be modeled, using a new approach [1-3] on the base of the physical approximations of the mechanics of continua, where the mathematical point is equivalent to a small (elementary) physical volume, which is sufficiently small with

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respect to the apparatus volume, but at the same time sufficiently large with respect to the intermolecular volumes of the medium. As a result a convection-diffusion (or convection) type of model, as a mass balance in this elementary volume, is possible to be obtained in convection-diffusion equation form.

Convection-diffusion type of models

In previous work [3], it was considered a stationary axis-symmetric fluid motion in a cylindrical column apparatus with radius r_0 [m] and active zone height l [m]. In cylindrical co-ordinate system (r, z) , where r and z are radial and axial co-ordinates, the axial and radial velocity components of a no-swirling stream flow are $u(r, z)$ and $v(r, z)$ [ms^{-1}]. One of the fluid components (*reagent*) with concentration $c(t, r, z)$ [kgmolm^{-3}] participates in volume reaction and the reaction rate is $Q(c)$ [$\text{kgmolm}^{-3}\text{s}^{-1}$], where t is the time. The volume reaction leads to different values of the concentration in the column volume and as a result two mass transfer effects exist:

- convective transfer, caused by the fluid laminar or turbulent (as a result of large-scale turbulent pulsations) motion, and
- molecular or turbulent (caused by small-scale turbulent pulsations) diffusion transfer, as a result of the concentration gradient.

The volume reaction leads to creating or disappear of the *reagent* in this volume $\pm Q(c)$. In the case of balance between these three effects in the small (elementary) fluid volume, the mass transfer process is stationary $\partial c/\partial t = 0$. In the opposite case the process is non-stationary $\partial c/\partial t \neq 0$.

Using of convection-diffusion equation, as a mathematical structure of the mass transfer processes model in the column apparatus in the stationary case, leads to:

$$u \frac{\partial c}{\partial z} + v \frac{\partial c}{\partial r} = D \left(\frac{\partial^2 c}{\partial z^2} + \frac{1}{r} \frac{\partial c}{\partial r} + \frac{\partial^2 c}{\partial r^2} \right) \pm Q(c) \quad (1)$$

where the axial and radial velocity components $u(r, z)$ and $v(r, z)$ satisfy the continuity equation:

$$\frac{\partial u}{\partial z} + \frac{\partial v}{\partial r} + \frac{v}{r} = 0, \quad z = 0, \quad u(r, 0) = u_0(r), \quad r = r_0, \quad v(r_0, z) = 0 \quad (2)$$

and $u_0(r)$ is the inlet velocity distribution in the column.

The term $Q(c)$ represents the volume chemical reaction (chemical kinetics model) or interphase mass transfer rate. In the cases of heterogeneous (catalytic) chemical reactions, the model is possible to be used if $Q = aQ_0$, where a [m^2m^{-3}] is the specific reacting (catalytic) interface of the solid phase, and Q_0 [$\text{kgmolm}^{-2}\text{s}^{-1}$] – the heterogeneous (catalytic) chemical reactions rate.

The axial and radial velocity components of a no-swirling stream flow are symmetric with respect to the axial co-ordinate and as a result the concentration distribution is symmetric too.

The model of the mass transfer processes in the column apparatus, eq. (1), includes boundary conditions, which express a symmetric concentration distribution ($r = 0$), impenetrability of the column wall ($r = r_0$), a constant inlet concentration of the *reagent* c_0 [molm^{-3}] and mass balance at the column inlet ($z = 0$):

$$r = 0, \quad \frac{\partial c}{\partial r} = 0, \quad r = r_0, \quad \frac{\partial c}{\partial r} = 0, \quad z = 0, \quad c = c_0, \quad \bar{u}c_0 = u_0(r)c_0 - D \frac{\partial c}{\partial z} \quad (3)$$

where D is the diffusivity of the reagent, and \bar{u} – the average velocity over the cross-sectional area of the column.

For the qualitative analysis of the model, eqs. (1)-(3), is possible to be analyzed the case $u = u(r)$. As a result from continuity eq. (3) we get:

$$\frac{dv}{dr} + \frac{v}{r} = 0, \quad r = r_0, \quad v = 0 \quad (4)$$

and the solution is $v(r, z) \equiv 0$. This leads to a new form of the convection-diffusion type of model [3]:

$$u(r) \frac{\partial c}{\partial z} = D \left(\frac{\partial^2 c}{\partial z^2} + \frac{1}{r} \frac{\partial c}{\partial r} + \frac{\partial^2 c}{\partial r^2} \right) \pm Q(c) \quad (5)$$

$$z = 0, \quad c = c_0, \quad \bar{u}c_0 = u(r)c_0 - D \frac{\partial c}{\partial z}, \quad r = 0, \quad \frac{\partial c}{\partial r} = 0, \quad r = r_0, \quad \frac{\partial c}{\partial r} = 0$$

where the velocity distribution $u(r)$ of a no-swirling stream flow in the column is symmetric with respect to the longitudinal co-ordinate z .

The presented convection-diffusion type model, eq. (5), was used [3] for the qualitative analysis of different processes in the column apparatuses (two components chemical reaction and pseudo-first-order reaction).

Theoretical analysis of the convection-diffusion type of models as a base for convection and diffusion type of models creation will use pseudo-first-order reaction case, *i. e.* in eq. (7) must be replaced $Q(c) = -kc$.

The qualitative analysis of this model will be made, using generalized variables:

$$r = r_0 R, \quad z = lZ, \quad u(r) = u(r_0 R) = \bar{u}U(R),$$

$$c_i(r, z) = c_i(r_0 R, lZ) = c_{i0}C_i(R, Z), \quad (i = 1, 2), \quad \varepsilon = \left(\frac{r_0}{l} \right)^2 \quad (6)$$

where $r_0, l, \bar{u}, c_{0i} (i = 1, 2)$ are the characteristic (inherent) scales (maximal or average values) of the variables.

The introducing the generalized variables from (6) in eqs. (1) and (3) leads to:

$$U(R) \frac{\partial C}{\partial Z} = \text{Fo} \left(\varepsilon \frac{\partial^2 C}{\partial Z^2} + \frac{1}{R} \frac{\partial C}{\partial R} + \frac{\partial^2 C}{\partial R^2} \right) - \text{Da}C, \quad \varepsilon = \text{Fo}^{-1} \text{Pe}^{-1}, \quad (7)$$

$$Z = 0, \quad C = 1, \quad 1 = U - \text{Pe}^{-1} \frac{\partial C}{\partial Z}, \quad R = 0, \quad \frac{\partial C}{\partial R} = 0, \quad R = 1, \quad \frac{\partial C}{\partial R} = 0$$

Diffusion type of models

The effect of the chemical reaction rate is negligible if $0 = \text{Da} \leq 10^{-2}$ and as a result $C \equiv 1$. When a fast chemical reactions take place ($\text{Da} \geq 10^2$), the terms in the model must be divided by Da and the approximation $0 = \text{Da}^{-1} \leq 10^{-2}$ has to be applied. The result is:

$$0 = \frac{Fo}{Da} \left(\frac{1}{R} \frac{dC}{dR} + \frac{d^2C}{dR^2} \right) - C, \quad R = 0, \quad \frac{dC}{dR} = 0, \quad R = 1, \quad \frac{dC}{dR} = 0 \quad (8)$$

i. e. the model, eq. (8), is diffusion type.

Convection type of models

The Fourier number, eq. (7), permits to be made a qualitative analysis of the convective transfer and diffusive transfer effects and in the cases $Fo \sim 1$ these two processes (effects) are comparable.

In many practical cases $0 = Fo \leq 10^{-2}$, $0 = Pe^{-1} = \varepsilon Fo \leq 10^{-2}$, $\varepsilon < 1$, *i. e.* the diffusion transfer is negligible compared to the convective one and the convection-diffusion type of model, eq. (7), has the convective form:

$$U(R) \frac{\partial C}{\partial Z} = -DaC, \quad Z = 0, \quad C = 1 \quad (9)$$

Two phase mass transfer processes

The modeling of two phases (gas-liquid, gas-solid, liquid-solid) interphase mass transfer processes in column apparatuses is used in the case of absorption, adsorption, homogeneous and heterogeneous (catalytic) chemical reactions. For the modeling of two phase processes must be used two model equations and ε_i ($i=1,2$) are the parts the phases in the small (elementary) column volume ($\varepsilon_1 + \varepsilon_2 = 1$).

Chemical absorption

The chemical absorption in a column apparatus will be presented in the case of SO₂ absorption by NaOH solutions. Considering that c_1 (c_2) is the concentration of SO₂ in the gas (liquid) phase and c_3 is the concentration of NaOH in the absorbent, the mass sources (sinks) in the medium elementary volume are equal to the chemical reaction rate, kc_2c_3 and the interphase mass transfer rate across the gas-liquid boundary, $k_0(c_1 - \chi c_2)$, where χ is the Henry's constant, k – the chemical reaction rate constant, k_0 – the interphase mass transfer coefficients. As a result the convection-diffusion equations in a column have the forms:

$$\begin{aligned} \varepsilon_1 u_1 \frac{\partial c_1}{\partial z} &= \varepsilon_1 D_1 \left(\frac{\partial^2 c_1}{\partial z^2} + \frac{1}{r} \frac{\partial c_1}{\partial r} + \frac{\partial^2 c_1}{\partial r^2} \right) - k_0(c_1 - \chi c_2), \\ \varepsilon_2 u_2 \frac{\partial c_2}{\partial z} &= \varepsilon_2 D_2 \left(\frac{\partial^2 c_2}{\partial z^2} + \frac{1}{r} \frac{\partial c_2}{\partial r} + \frac{\partial^2 c_2}{\partial r^2} \right) + k_0(c_1 - \chi c_2) - kc_2c_3, \\ \varepsilon_2 u_2 \frac{\partial c_3}{\partial z} &= \varepsilon_2 D_3 \left(\frac{\partial^2 c_3}{\partial z^2} + \frac{1}{r} \frac{\partial c_3}{\partial r} + \frac{\partial^2 c_3}{\partial r^2} \right) - kc_2c_3 \end{aligned} \quad (10)$$

where $u_1(r)$ and $u_2(r)$ are velocity distributions in the gas and liquid, $c_i(z, r)$ and D_i ($i = 1, 2, 3$) are the concentration distributions and the diffusivities of SO₂ in the gas and liquid and of NaOH in the liquid.

Let us consider a co-current gas-liquid bubble column with a radius r_0 and working zone height l . The boundary conditions of the model equations have the form:

$$\begin{aligned}
 z = 0, \quad c_1(0, r) &\equiv c_1^0, \quad \bar{u}_1 c_1^0 = u_1(r) c_1^0 - D_1 \left(\frac{\partial c_1}{\partial z} \right)_{z=0}, \\
 z = 0, \quad c_2(0, r) &\equiv c_2^0, \quad \bar{u}_2 c_2^0 = u_2(r) c_2^0 - D_2 \left(\frac{\partial c_2}{\partial z} \right)_{z=0}, \\
 z = 0, \quad c_3(0, r) &\equiv c_3^0, \quad \bar{u}_2 c_3^0 = u_2(r) c_3^0 - D_3 \left(\frac{\partial c_3}{\partial z} \right)_{z=0}, \\
 r = 0, \quad \frac{\partial c_1}{\partial r} = \frac{\partial c_2}{\partial r} = \frac{\partial c_3}{\partial r} &= 0, \quad r = r_0, \quad \frac{\partial c_1}{\partial r} = \frac{\partial c_2}{\partial r} = \frac{\partial c_3}{\partial r} = 0
 \end{aligned} \tag{11}$$

where \bar{u}_i and c_i^0 , ($i=1, 2$), are the inlet average velocities and the inlet concentrations in the gas and liquid phases, respectively. Practically $c_2^0 = 0$.

Generalized analysis

A qualitative analysis of the model is possible to be made, using dimensionless (generalized) variables:

$$R = \frac{r}{r_0}, \quad Z = \frac{z}{l}, \quad U_1 = \frac{u_1}{\bar{u}_1}, \quad U_2 = \frac{u_2}{\bar{u}_2}, \quad C_1 = \frac{c_1}{c_1^0}, \quad C_2 = \frac{c_2 \chi}{c_1^0}, \quad C_3 = \frac{c_3}{c_3^0} \tag{12}$$

The model in generalized variables eq. of (12) has the form:

$$\begin{aligned}
 U_1(R) \frac{\partial C_1}{\partial Z} &= \text{Fo}_1 \left(\varepsilon \frac{\partial^2 C_1}{\partial Z^2} + \frac{1}{R} \frac{\partial C_1}{\partial R} + \frac{\partial^2 C_1}{\partial R^2} \right) - K(C_1 - C_2), \\
 U_2(R) \frac{\partial C_2}{\partial Z} &= \text{Fo}_2 \left(\varepsilon \frac{\partial^2 C_2}{\partial Z^2} + \frac{1}{R} \frac{\partial C_2}{\partial R} + \frac{\partial^2 C_2}{\partial R^2} \right) + K \frac{\varepsilon_1 \bar{u}_1 \chi}{\varepsilon_2 \bar{u}_2} (C_1 - C_2) - \text{Da} \frac{c_3^0}{c_1^0} C_2 C_3, \\
 U_2(R) \frac{\partial C_3}{\partial Z} &= \text{Fo}_3 \left(\varepsilon \frac{\partial^2 C_3}{\partial Z^2} + \frac{1}{R} \frac{\partial C_3}{\partial R} + \frac{\partial^2 C_3}{\partial R^2} \right) - \text{Da} C_2 C_3, \\
 Z = 0, \quad C_i(0, R) &\equiv 1, \quad 1 = U_i(R) - \text{Pe}_i^{-1} \left(\frac{\partial C_i}{\partial Z} \right)_{Z=0}, \quad i = 1, 3 \\
 Z = 0, \quad C_2(0, R) &\equiv 0, \quad \left(\frac{\partial C_2}{\partial Z} \right)_{Z=0} \equiv 0, \\
 R = 0, \quad \frac{\partial C_i}{\partial R} &\equiv 0; \quad R = 1, \quad \frac{\partial C_i}{\partial R} \equiv 0; \quad i = 1, 2, 3,
 \end{aligned} \tag{13}$$

where

$$K = \frac{k_0 l}{\varepsilon_1 \bar{u}_1}, \quad \text{Fo}_i = \frac{D_i l}{\bar{u}_i r_0^2}, \quad \text{Da} = \frac{k l c_1^0}{\varepsilon_2 \bar{u}_2 \chi}, \quad \text{Pe}_i = \frac{\bar{u}_i l}{D_i}, \quad \bar{u}_3 = \bar{u}_2, \quad i = 1, 2, 3 \tag{14}$$

The model, eqs. (13), is base for modeling of the physical absorption, chemical adsorption, and catalytic processes.

Physical absorption

From eqs. (13) follows, that the absence of a chemical reaction in liquid phase $k_0 = 0$ (or $c_3^0 = 0$) leads to $Da = 0$, $C_3 \equiv 1$, (or $C_3 \equiv 0$) and as a result the model of the physical absorption has the form:

$$\begin{aligned}
 U_1(R) \frac{\partial C_1}{\partial Z} &= Fo_1 \left(\varepsilon \frac{\partial^2 C_1}{\partial Z^2} + \frac{1}{R} \frac{\partial C_1}{\partial R} + \frac{\partial^2 C_1}{\partial R^2} \right) - K(C_1 - C_2) \\
 U_2(R) \frac{\partial C_2}{\partial Z} &= Fo_2 \left(\varepsilon \frac{\partial^2 C_2}{\partial Z^2} + \frac{1}{R} \frac{\partial C_2}{\partial R} + \frac{\partial^2 C_2}{\partial R^2} \right) + K \frac{\varepsilon_1 \bar{u}_1 \chi}{\varepsilon_2 \bar{u}_2} (C_1 - C_2) \\
 Z = 0, \quad C_1(0, R) &\equiv 1, \quad 1 = U_1(R) - Pe_1^{-1} \left(\frac{\partial C_i}{\partial Z} \right)_{Z=0} \\
 Z = 0, \quad C_2(0, R) &\equiv 0, \quad \left(\frac{\partial C_2}{\partial Z} \right)_{Z=0} \equiv 0, \\
 R = 0, \quad \frac{\partial C_i}{\partial R} &\equiv 0, \quad R = 1, \quad \frac{\partial C_i}{\partial R} \equiv 0, \quad i = 1, 2
 \end{aligned} \tag{15}$$

From eq. (15) is possible to be obtained directly models of the physical absorption in the cases of highly ($\chi \rightarrow 0$, $C_2 \equiv 0$) and slightly ($\chi \rightarrow \infty$, $C_1 \equiv 1$) soluble gases.

Chemical adsorption

The model of the chemical absorption, eq. (10), is possible to be used as a base for the modeling on the chemical adsorption if ε_1 and ε_2 are the parts of the gas phase and sorbent particles phase ($\varepsilon_1 + \varepsilon_2 = 1$) of the medium elementary volume in column apparatus, where the sorbent particles phase is immobile. The concentrations of the active component in the gas phase and in the solid phase (in the capillaries volume of the adsorbent) are c_1 and c_2 [kmolm⁻³]. For the interphase (gas-solid) mass transfer rate is possible to be used $k_0(c_1 - c_2)$, where k_0 is the interphase mass transfer coefficient. The adsorption rate in the solid phase (similar to two components chemical reaction) will be presented as kc_2c_3 , where c_3 [kg-eqm⁻³] is the volume concentration of the active centers (AC) in the solid phase (particles volume), k – chemical reaction rate constant (1 kg-eq AC in the adsorbent combine 1 kg-mol active component in gas phase).

The diffusivity of the active component in the mobile gas phase is D_1 . The diffusion mass transfer of the active component in the solid phase (Knudsen diffusion) can be neglected due to the small value of the Knudsen diffusivity and the inability to transport the free AC between the sorbent particles. The diffusivity of the AC in the adsorbent phase (particles volume) is equal to zero too.

As a result for a non-stationary chemical adsorption from eq. (10) we get:

$$\begin{aligned}
 \varepsilon_1 \frac{\partial c_1}{\partial t} + \varepsilon_1 u \frac{\partial c_1}{\partial z} &= \varepsilon_1 D_1 \left(\frac{\partial^2 c_1}{\partial z^2} + \frac{1}{r} \frac{\partial c_1}{\partial r} + \frac{\partial^2 c_1}{\partial r^2} \right) - k_0(c_1 - c_2) \\
 \varepsilon_2 \frac{\partial c_2}{\partial t} &= k(c_1 - c_2) - kc_2c_3, \quad \varepsilon_2 \frac{\partial c_3}{\partial t} = -kc_2c_3
 \end{aligned} \tag{16}$$

where t is the time. The initial and boundary conditions of eqs. (16) have the form:

$$\begin{aligned}
 t = 0, \quad c_1 &\equiv c_1^0, \quad c_2 \equiv 0, \quad c_3 \equiv c_3^0, \\
 z = 0, \quad c_1(t, 0, r) &\equiv c_1^0, \quad \bar{u}c_1^0 = u(r)c_1^0 - D_1 \left(\frac{\partial c_1}{\partial z} \right)_{z=0}, \\
 r = 0, \quad \frac{\partial c_1}{\partial r} &= 0, \quad r = r_0, \quad \frac{\partial c_1}{\partial r} = 0
 \end{aligned} \quad (17)$$

where \bar{u} and c_1^0 are the inlet average velocity and concentration of the active component in the gas phase, respectively, and c_3^0 is the initial concentration of AC in the solid phase.

The using of dimensionless (generalized) variables:

$$T = \frac{t}{t_0}, \quad R = \frac{r}{r_0}, \quad Z = \frac{z}{l}, \quad U = \frac{u}{\bar{u}}, \quad C_1 = \frac{c_1}{c_1^0}, \quad C_2 = \frac{c_2}{c_1^0}, \quad C_3 = \frac{c_3}{c_3^0} \quad (18)$$

leads to:

$$\begin{aligned}
 \alpha \frac{\partial C_1}{\partial T} + U(R) \frac{\partial C_1}{\partial Z} &= \text{Fo}_1 \left(\varepsilon \frac{\partial^2 C_1}{\partial Z^2} + \frac{1}{R} \frac{\partial C_1}{\partial R} + \frac{\partial^2 C_1}{\partial R^2} \right) - K_0(C_1 - C_2) \\
 \frac{\partial C_2}{\partial T} &= K_1(C_1 - C_2) - K \frac{c_3^0}{c_1^0} C_2 C_3, \quad \frac{\partial C_3}{\partial T} = -K C_2 C_3 \\
 T = 0, \quad C_1 &\equiv 1, \quad C_2 \equiv 0, \quad C_3 \equiv 1, \\
 Z = 0, \quad C_1(T, 0, R) &\equiv 1, \quad 1 = U(R) - \text{Pe}_1^{-1} \left(\frac{\partial C_1}{\partial Z} \right)_{Z=0}, \\
 R = 0, \quad \frac{\partial C_1}{\partial R} &= 0, \quad R = 1, \quad \frac{\partial C_1}{\partial R} = 0
 \end{aligned} \quad (19)$$

where

$$\begin{aligned}
 C_1 = C_1(T, Z, R), \quad C_2 = C_2(T, Z, R), \quad C_3 = C_3(T, Z, R), \\
 \text{Fo}_1 = \frac{D_1 l}{\bar{u} r_0^2}, \quad \text{Pe}_1 = \frac{\bar{u} l}{D_1}, \quad \alpha = \frac{l}{\bar{u} t_0}, \quad \varepsilon = \left(\frac{r_0}{l} \right)^2, \\
 K = \frac{kl}{\varepsilon_1 \bar{u}}, \quad K_0 = \frac{k_0 t_0 c_1^0}{\varepsilon_2}, \quad K_1 = \frac{k_0 t_0}{\varepsilon_2}
 \end{aligned} \quad (20)$$

For long time processes is possible to be used the approximation $0 = \alpha \leq 10^{-2}$.

The convection type of models of the two phase processes is possible to be obtained automatically if put $\text{Fo} = 0$ in eqs. (15)-(25).

Average concentration model

Using the convection-diffusion type of models for a quantitative description of chemical and mass transfer processes in column apparatuses is not possible because the velocity functions in the convection-diffusion equations are unknown. The problem can be avoided if the average values of the velocity and concentration over the cross-sectional area of the column are used, *i. e.* the medium elementary volume (in the physical approximations of the me-

chanics of continua) will be equivalent to a small cylinder with radius r_0 and a height l , which is sufficiently small with respect to the column height and at the same time sufficiently large with respect to the intermolecular distances in the medium.

One phase model

Let's consider a liquid motion in a column reactor with a homogeneous chemical reaction between two liquid components. If the difference between the component concentrations is very large, then the chemical reaction will be first order. If the velocity and concentration distributions in the column are defined:

$$u = u(r, z), \quad c = c(r, z)$$

the convection-diffusion type of model can be expressed:

$$u \frac{\partial c}{\partial z} = D \left(\frac{\partial^2 c}{\partial z^2} + \frac{1}{r} \frac{\partial c}{\partial r} + \frac{\partial^2 c}{\partial r^2} \right) - kc, \quad r = 0, \quad \frac{\partial c}{\partial r} = 0; \quad (21)$$

$$r = r_0, \quad \frac{\partial c}{\partial r} = 0; \quad z = 0, \quad c(r, 0) = c_0, \quad \bar{u}c_0 = uc_0 - D \frac{\partial c}{\partial z}$$

The average velocity and concentration at the column cross-sectional area can be presented:

$$\bar{u}(z) = \frac{2}{r_0^2} \int_0^{r_0} ru(r, z)dr, \quad \bar{c}(t, z) = \frac{2}{r_0^2} \int_0^{r_0} rc(t, r, z)dr \quad (22)$$

The velocities and concentration distributions assume to be presented [1-3] by the average functions, eq. (22):

$$u(r, z) = \bar{u}(z)\tilde{u}(r, z), \quad c(r, z) = \bar{c}(z)\tilde{c}(r, z) \quad (23)$$

where $\tilde{u}(r, z)$ and $\tilde{c}(r, z)$ represent the radial non-uniformity of both the velocity and the concentration distributions, respectively, satisfying the conditions:

$$\frac{2}{r_0^2} \int_0^{r_0} r\tilde{u}(r, z)dr = 1, \quad \frac{2}{r_0^2} \int_0^{r_0} r\tilde{c}(r, z)dr = 1 \quad (24)$$

The average concentration model may be obtained [1-3] if put the expressions, eq. (23), into the model eqs. (21) and then multiply by r and integrate with respect to r over the interval $[0, r_0]$. The result is:

$$\alpha \bar{u} \frac{\partial \bar{c}}{\partial z} + \frac{d\alpha}{dz} \bar{u} \bar{c} = D \frac{\partial^2 \bar{c}}{\partial z^2} - k\bar{c}, \quad z = 0, \quad \bar{c}(0) = c_0, \quad \frac{\partial \bar{c}}{\partial z} = 0 \quad (25)$$

where

$$\alpha = \alpha(r_0, z) = \frac{2}{r_0^2} \int_0^{r_0} r\tilde{u}\tilde{c}dr \quad (26)$$

Using of the generalized variables:

$$Z = \frac{z}{l}, \quad \bar{C} = \frac{\bar{c}}{c_0}, \quad \text{Pe} = \frac{\bar{u}l}{D}, \quad \text{Da} = \frac{kl}{\bar{u}}, \quad \alpha(z) = \alpha(lZ) = A(Z) \quad (27)$$

leads to:

$$A \frac{d\bar{C}}{dZ} + \frac{dA}{dZ} \bar{C} = \text{Pe}^{-1} \frac{d^2\bar{C}}{dZ^2} - \text{Da} \bar{C}, \quad Z = 0, \quad \bar{C} = 1, \quad \frac{d\bar{C}}{dZ} = 0 \quad (28)$$

In the cases $0 = \text{Fo} \leq 10^{-2}$, $0 = \text{Pe}^{-1} = \varepsilon \text{Fo} \leq 10^{-2}$, $\varepsilon < 1$, eq. (9), the model, eq. (28), has the convective form:

$$A \frac{d\bar{C}}{dZ} + \frac{dA}{dZ} \bar{C} = -\text{Da} \bar{C}, \quad Z = 0, \quad \bar{C} = 1 \quad (29)$$

Two phases model

In the cases of two (or three) phase processes, the average concentration model consists of eqs. (28) or (29) for every phase [1-8].

Identification of the function A(Z)

The function $A(Z)$ represents, the effect of the velocity radial non-uniformity on the mass transfer efficiency in the column apparatus, eqs. (26)-(29):

$$A(Z) = \alpha(r_0, z) = \frac{2}{r_0^2} \int_0^{r_0} r \tilde{u} \tilde{c} dr \quad (30)$$

where

$$\tilde{u}(r) = \frac{u(r)}{\bar{u}} = U(R), \quad \tilde{c}(r, z) = \frac{c(r, z)}{\bar{c}(z)} = \frac{C(R, Z)}{\bar{C}(Z)}, \quad \bar{C}(Z) = \frac{\bar{c}(z)}{c_0} = 2 \int_0^1 RC(R, Z) dR \quad (31)$$

and as a result:

$$A(Z) = 2 \int_0^1 RU(R) \frac{C(R, Z)}{\bar{C}(Z)} dR \quad (32)$$

As an example will be used the case of parabolic velocity distribution (Poiseuille flow):

$$u = \bar{u} \left(2 - 2 \frac{r^2}{r_0^2} \right) \quad (33)$$

From eqs. (6), (23), and (33) we get:

$$U(R) = 2 - 2R^2 \quad (34)$$

In the case, for height columns ($0 = \varepsilon \leq 10^{-2}$) and $Fo \leq 1$ ($0 = Pe^{-1} \leq 10^{-2}$ Fo), the models of eqs. (7) and (9) have the forms:

$$(2 - 2R^2) \frac{\partial C}{\partial Z} = Fo \left(\frac{1}{R} \frac{\partial C}{\partial R} + \frac{\partial^2 C}{\partial R^2} \right) - Da C, \quad (35)$$

$$Z = 0, \quad C = 1; \quad R = 0, \quad \frac{\partial C}{\partial R} = 0; \quad R = 1, \quad \frac{\partial C}{\partial R} = 0$$

$$(2 - 2R^2) \frac{\partial C}{\partial Z} = -Da C; \quad Z = 0, \quad C = 1 \quad (36)$$

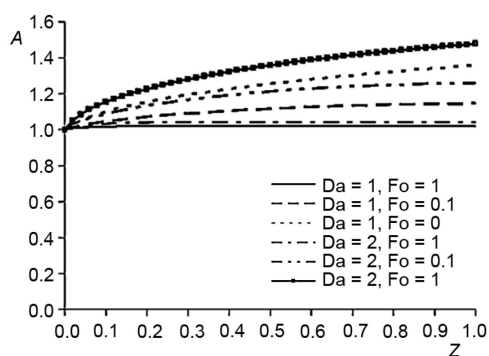


Figure 1. Function $A(Z)$ for different values of Da and Fo

Table 1. Parameter values

	a	a_1	a_0	a_{01}
Da = 1, Fo = 0	0.5511	0.8516		
Da = 1, Fo = 0.1	0.2463	0.3519		
Da = 1, Fo = 1			1.02	0.835
Da = 2, Fo = 0	1.3623	0.7893		
Da = 2, Fo = 0.1	0.4547	0.8068		
Da = 2, Fo = 1			1.04	0.7709

Otherwise ($\varepsilon \sim 10^{-1}$) the mathematical model given by eq. (7) together with boundary conditions was solved by using perturbation method [1, 3].

The solutions of the problems (7) for $Da = 1, 2$ and $Fo = 0, 0.1, 1.0$ permits to be obtained $C(R, Z)$, $\bar{C}(Z)$ and results for $A(Z)$ are presented in fig. 1, where different approximations for $A(Z)$ is possible to be used:

$$Fo = 1, \quad Da = 1, 2,$$

$$A(Z) = a_0, \quad a_0 = \frac{1}{S} \sum_{s=1}^S A(Z_s),$$

$$Fo = 0, 0.1, \quad Da = 1, 2, \quad (37)$$

$$A(Z) = 1 + aZ,$$

$$a = \frac{1}{S} \sum_{s=1}^S \frac{A(Z_s) - 1}{Z_s}, \quad 0 < Z_s < 1$$

The obtained values of a and a_0 in eq. (37) are shown in tab. 1.

The obtained values of the average concentration for $Z = 0.1$:

$$\bar{C}(0.1) = 2 \int_0^1 RC(0.1, R) dR \quad (38)$$

permit to be obtained artificial experimental data:

$$\bar{C}_{\text{exp}}^i(0.1) = (0.95 + 0.1B_i) \bar{C}(0.1), \quad i = 1, \dots, 10 \quad (39)$$

where $0 \leq B_i \leq 1$, $i = 1, \dots, 10$ are obtained by a generator of random numbers. The obtained artificial experimental data of eq. (39) are used for the illustration of the parameter identification in the average concentrations models, eqs. (28) and (29), using the approximations for $A(Z)$ in eq. (37), where $a_0 = a_{01}$, $a = a_1$, $Da = 1, 2$, by the minimization of the least-squares functions for different Z :

$$Q_j(a_{01}^{\min}) = \min_{(a_{01})} \sum_{i=1}^{10} \left[\bar{C}(0.1, a_{01}) - \bar{C}_{\text{exp}}^i(0.1) \right]^2, \quad \text{Fo} = 1, \quad (40)$$

$$Q_j(a_1^{\min}) = \min_{(a_1)} \sum_{i=1}^{10} \left[\bar{C}(0.1, a_1) - \bar{C}_{\text{exp}}^i(0.1) \right]^2, \quad \text{Fo} = 0, 0.1$$

where $\bar{C}(0.1, a_{01})$ and $\bar{C}(0.1, a_1)$ are calculated values which are obtained as solutions of eqs. (28) or (29) and $\bar{C}_{\text{exp}}^i(0.1)$ are ten *experimental data* ($i = 1, \dots, 10$) for $Z = 0.1$. The obtained *experimental values* of a_{01} and a_1 are compared with the *theoretical values* a_0, a in tab. 1.

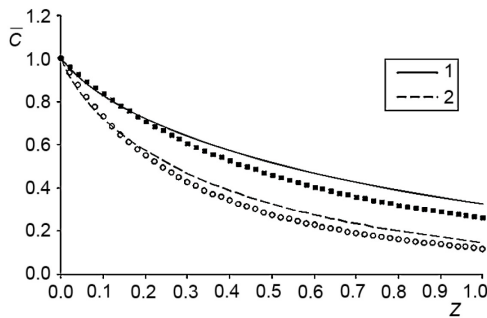


Figure 2(a). Comparison of average concentration distributions Fo = 0
 (1) – Da = 1, $\bar{C}(Z)$ – eq. (37), ‘.’ $\bar{C}(Z = 0.1, a = 0.8516)$ – eq. (38), (2) – Da = 2, $\bar{C}(Z)$ – eq. (37), ‘o’ $\bar{C}(Z = 0.1, a = 1.3622)$ – eq. (38)

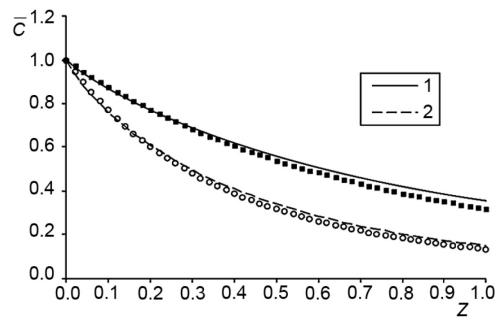


Figure 2(b). Comparison of average concentration distributions Fo = 0.1
 (1) – Da = 1, $\bar{C}(Z)$ – eq. (37), ‘.’ $\bar{C}(Z = 0.1, a = 0.3519)$ – eq. (37), (2) – Da = 2, $\bar{C}(Z)$ – eq. (37), ‘o’ $\bar{C}(Z = 0.1, a = 0.8086)$ – eq. (37)

In figs. 2(a)-(c) are compared average concentration $\bar{C}(Z)$ obtained from eq. (37), using the exact solution $C(Z, R)$ of the models, eqs. (35) or (36) (the lines) and average concentrations $\bar{C}(Z, a_0), \bar{C}(Z, a)$ (the points), obtained in case of parameter identification, using ten *experimental data* values in one point ($Z = 0.1$) only.

As can be seen in figs. 2(a)-(c) in the case $\varepsilon \sim 10^{-1}$, the model parameter in eq. (28) can be calculated using the *experimental data*, obtained from a real column diameter and low column height.

Physical analysis of the convection-diffusion type of model

Using generalized variables, eqs. (6), (12), and (18), in the convection-diffusion type of models, permits to be obtained the relative share of the elementary processes in the complex processes in column apparatuses, on the base of the orders of magnitudes of the dimensionless parameters, eqs. (7), (13).

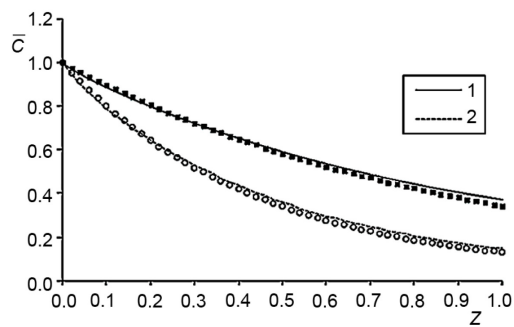


Figure 2(c). Comparison of average concentration distributions Fo = 1
 (1) – Da = 1, $\bar{C}(Z)$ – eq. (37), ‘.’ $\bar{C}(Z = 0.1, a_0 = 0.835)$ – eq. (37), (2) – Da = 2, $\bar{C}(Z)$ – eq. (37), ‘o’ $\bar{C}(Z = 0.1, a_0 = 0.7709)$ – eq. (37)

The parameter $Fo = Dl/\bar{u}r_0^2$, eq. (7), represents the interrelation between diffusion and convection mass transfer and $0 = Fo \leq 10^{-2}$ is the approximation of the convection type of models, eq. (9).

The parameter $Da = (kl/\bar{u})(K = k_0l/\varepsilon\bar{u})$ represents the interrelation between convective mass transfer and chemical reaction rate. The approximation $0 = Da^{-1} \leq 10^{-2}$ represents the diffusion type of models, eq. (8), where Fo/Da shows the interrelation between diffusion mass transfer and chemical reaction rate.

For each concrete process the characteristic velocity (\bar{u}) can be altered over a wide range only, *i. e.* an increase (decrease) of \bar{u} leads to the decrease (increase) of Fo , Da , and K and the effects of the diffusion transfer, chemical reaction, and the interphase mass transfer decrease (increase). As a result the decrease of Fo , Da , and K (*Convective type of model*) leads to an increase of the convective mass transfer and the effect of the velocity radial non-uniformity increase. In the opposite case this effect decrease.

On this base is possible to be explained the results in figs. 2(a)-(c), where the increase of the Fourier number leads to the increase of the radial diffusion transfer and as a result the concentration radial non-uniformity decrease. In these conditions the convection mass transfer and the effect of the velocity radial non-uniformity decrease too.

Conclusions

A new approach, for the column apparatuses modeling of chemical and interphase mass transfer processes, in chemical and power engineering is presented. A physical approximation of the mechanics of continua, where the mathematical point is equivalent to a small (elementary) physical volume, which is sufficiently small with respect to the apparatus volume, but at the same time sufficiently large with respect to the intermolecular volumes of the medium is used. As a result the mathematical model is mass balance in this elementary volume in convection-diffusion equation form.

The presented new approach is based on two steps models – diffusion type of model (for qualitative analysis) and average concentration model (for quantitative analysis). This approach is used for theoretical analysis of the mechanism of gas absorption with two-phase absorbents [5], for modeling of airlift reactors for chemical [6], catalytic [7], and photochemical [8] reaction, for solutions of scale effect and scale-up problems in the column apparatuses (influence of the velocity distribution [9], scale effect modeling [10], and circulation zones modeling [11]).

The theoretical results show the possibility for modeling of the column apparatuses on the base of experimental data, obtained in the columns with real diameter and short height (10% from the real height).

Nomenclature

c – concentration, [kgmolm ⁻³]	r – radial co-ordinate, [m]
c_0 – inlet concentration, [kgmolm ⁻³]	u – axial velocity component, [ms ⁻¹]
D – diffusivity, [m ² s ⁻¹]	v – radial velocity component, [ms ⁻¹]
k – chemical reaction rate constant	z – axial co-ordinate, [m]
k_0 – interphase mass transfer coefficient, [s ⁻¹]	Fo – Fourier number
l – column height, [m]	Da – Damkohler number
r_0 – column radius, [m]	Pe – Peclet number

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