

## New approach to modelling and simulation of chemical and mass transfer processes in column apparatuses

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The classical mass transfer theory is not applicable for the modeling the mass transfer of chemical, absorption, adsorption and catalytic processes in column apparatuses, where the velocity distributions and interphase boundaries are unknown. The modeling of these processes is related with the creation of new type of convection-diffusion models (for qualitative analysis) and average-concentration models (for quantitative analysis), where the surface reactions are replaced by equivalent volume reaction, while the velocity and concentration distributions are replaced by average velocity and concentrations. The effect of the radial non-uniformity of the velocity in the average-concentration models is introduced by model parameters, which must be obtained experimentally. The new convection-diffusion and average-concentration models are obtained in the cases of different processes in column apparatuses: simple and complicated chemical reactions, physical and chemical absorption, physical and chemical adsorption, heterogeneous catalytic processes (physical and chemical adsorption mechanism). These models are presented in the monograph Chr. Boyadjiev, M. Doichinova, B. Boyadjiev, P. Popova-Krumova, "Modelling of Column Apparatus Processes" (Second edition), Springer-Verlag, Berlin Heidelberg, 2018. Two hydrodynamic situations are considered, when the radial velocity component is equal to zero, in the cases of an axial modification of the radial non-uniformity of the axial velocity component and when the radial velocity component is not equal to zero. The use of experimental data, for the average concentrations at the column end, for a concrete process and column, permits to be obtained the model parameters, related with the radial non-uniformity of the velocity. These parameter values permit to be used the average-concentration models for modeling of different processes.

**Keywords:** industrial mass transfer processes, convection-diffusion model, average-concentration model, velocity radial non-uniformity, parameters identification.

### INTRODUCTION

The classical mass transfer theory is not applicable for the modeling the mass transfer of chemical, absorption, adsorption and catalytic processes in column apparatuses, where the velocity distributions and interphase boundaries are unknown. The modeling of these processes is related with the creation of new type of convection-diffusion and average-concentration models, where the surface reactions are replaced by equivalent volume reactions, while the velocity and concentration distributions are replaced by average velocity and concentrations.

In the general case a multicomponent ( $i=1,2,\dots,i_0$ ) and multiphase ( $j=1,2,3$  for gas, liquid and solid phases) flow, in a cylindrical column with radius  $r_0$  [m] and active zone height  $l$  [m], will be considered. If  $F_0$  is the fluid flow rate in the column and  $F_j$ ,  $j=1,2,3$  are the phase flow rates [ $\text{m}^3\cdot\text{s}^{-1}$ ], the parts of the column volume occupied by the gas, liquid and solid phase are respectively:

$$\varepsilon_j = \frac{F_j}{F_0}, \quad j=1,2,3, \quad \sum_j \varepsilon_j = 1, \quad (1)$$

i.e., the phase volumes [ $\text{m}^3$ ] in  $1 \text{ m}^3$  of the column volume (hold-up coefficients of the phases).

The input velocities of the phases in the column  $u_j^0$  [ $\text{m}\cdot\text{s}^{-1}$ ],  $j=1,2,3$  may be defined as:

$$u_j^0 = \frac{F_j}{\varepsilon_j \pi r_0^2}, \quad j=1,2,3; \quad F_0 = \sum_{j=1}^3 F_j. \quad (2)$$

The column apparatuses are possible to be modelled using a new approach [1-3] on the basis of the physical approximations of the mechanics of continua, where the mathematical point (in the phase volume or on the surface between the phases) 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 in the medium. On this base convection-diffusion models for qualitative analysis of the processes are proposed [1, 2].

### Convection-diffusion models

The physical elementary column volumes contain the elementary phase volumes and will be

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presented as mathematical points  $M$  in a cylindrical coordinate system  $(r, z)$ , where  $r$  and  $z$  [m] are radial and axial coordinates. As a result, the mathematical point  $M(r, z)$  is equivalent to the elementary phase volumes, too.

The concentrations [kg-mol.m<sup>-3</sup>] of the reagents (components of the phases) are  $c_{ij}, i=1,2,\dots,i_0, j=1,2,3$ , i.e. the quantities of the reagents (kg-mol) in 1 m<sup>3</sup> of the phase volumes in the column.

In the cases of a stationary motion of fluids in cylindrical column apparatus  $u_j(r, z), v_j(r, z), j=1,2,3$  [m.s<sup>-1</sup>] are the axial and radial velocity components of the phases in the elementary phase volumes.

In the column apparatuses the phase boundaries are unknown, and therefore the heterogeneous reactions (absorption, adsorption, catalytic reactions) are introduced as a volume sources (sinks) in the elementary phase volumes.

The volume reactions [kg-mol.m<sup>-3</sup>.s<sup>-1</sup>] in the phases (homogeneous chemical reaction and interphase mass transfer, as a volume source or sink in the phase volume in the column) are  $Q_{ij}(c_{ij}), j=1,2,3, i=1,2,\dots,i_0$ . The reagent (substance) concentrations in the elementary phase volumes can be created or disappear and the reaction rates  $Q_{ij}$  are determined by these concentrations  $c_{ij}(t, r, z)$  [kg-mol.m<sup>-3</sup>], where  $t$  (s) is the time.

The volume reactions lead to different values of the reagent (substance) concentrations in the elementary phase volumes and as a result, two mass transfer effects exist - convective transfer (caused by the fluid motion) and diffusion transfer (caused by the concentration gradient).

The convective transfer in column apparatus is caused by a laminar or turbulent (as a result of large-scale turbulent pulsations) flow. In a small (elementary) phase volume around the point  $M(r, z)$  in the column, the mass transfer in this volume, as a result of the convection, is  $u_j \frac{\partial c_{ij}}{\partial z} + v_j \frac{\partial c_{ij}}{\partial r}$  [kg-mol.m<sup>-3</sup>.s<sup>-1</sup>],  $j=1,2,3, i=1,2,\dots,i_0$ , i.e. convective transfer rate (kg-mol.s<sup>-1</sup>) in 1 m<sup>3</sup> of the phase volume.

The molecular (or turbulent, caused by small-scale turbulent pulsations) diffusive mass transfer is

$$D_{ij} \left( \frac{\partial^2 c_{ij}}{\partial z^2} + \frac{1}{r} \frac{\partial c_{ij}}{\partial r} + \frac{\partial^2 c_{ij}}{\partial r^2} \right) \text{ [kg-mol.m}^{-3}\text{.s}^{-1}\text{]}, \text{ i.e.}$$

diffusive transfer rate (kg-mol.s<sup>-1</sup>) in 1 m<sup>3</sup> of the phase volume and  $D_{ij}$  [m<sup>2</sup>.s<sup>-1</sup>] are the diffusivities of the reagents ( $i=1,2,\dots,i_0$ ) in the phases ( $j=1,2,3$ ).

The mathematical models of the processes in the column apparatuses, in the physical approximations of the mechanics of continua, represent the mass balances in the phase volumes (phase parts in the elementary column volume) between the convective transfer, the diffusive transfer and the volume mass sources (sinks) (as a result of the chemical reactions and interphase mass transfer). The sum total of these three effects is equal to  $\partial c_{ij} / \partial t, j=1,2,3, i=1,2,\dots,i_0$ . In the case of balance between these three effects, the mass transfer process is stationary ( $\partial c_{ij} / \partial t = 0$ ).

In the stationary case, the convection-diffusion equations in the phases (as a mathematical structures of the mass transfer process models in the column apparatuses) are:

$$u_j \frac{\partial c_{ij}}{\partial z} + v_j \frac{\partial c_{ij}}{\partial r} = D_{ij} \left( \frac{\partial^2 c_{ij}}{\partial z^2} + \frac{1}{r} \frac{\partial c_{ij}}{\partial r} + \frac{\partial^2 c_{ij}}{\partial r^2} \right) + Q_{ij}(c_{ij}), \quad j=1,2,3, \quad i=1,2,\dots,i_0. \quad (3)$$

The axial and radial velocity components  $u_j(r, z)$  and  $v_j(r, z), j=1,2,3$  satisfy the continuity equations in the phases:

$$\begin{aligned} \frac{\partial u_j}{\partial z} + \frac{\partial v_j}{\partial r} + \frac{v_j}{r} &= 0; \\ z=0, \quad u_j &\equiv u_j(r, 0), \quad j=1,2,3; \\ r=r_0, \quad v_j(r_0, z) &\equiv 0, \quad j=1,2,3. \end{aligned} \quad (4)$$

The models of the mass transfer processes in the column apparatuses (3) include boundary conditions, which express symmetric concentration distributions ( $r=0$ ), impenetrability of the column wall ( $r=r_0$ ), constant input concentrations  $c_{ij}^0$  and mass balances at the column input ( $z=0$ ) of the phases:

$$\begin{aligned} r=0, \quad \frac{\partial c_{ij}}{\partial r} &\equiv 0; \quad r=r_0, \quad \frac{\partial c_{ij}}{\partial r} \equiv 0; \\ z=0, \quad c_{ij} &\equiv c_{ij}^0, \quad u_j^0 c_{ij}^0 \equiv u_j c_{ij}^0 - D_{ij} \left( \frac{\partial c_{ij}}{\partial z} \right)_{z=0}; \\ j=1,2,3, \quad i &= 1,2,\dots,i_0. \end{aligned} \quad (5)$$

In this paper two hydrodynamic situations will be considered, when the radial velocity component is equal to zero, in the cases of an axial modification of the radial non-uniformity of the

axial velocity component and when the radial velocity component is not equal to zero.

### RADIAL VELOCITY COMPONENT IS EQUAL TO ZERO

Chemical reaction in column apparatus

#### Convection-diffusion model

Let's consider one-component chemical reaction in one-phase column, where  $u_j = u(r)$ ,  $v_j = v = 0$ ,  $c_{ij} = c(r, z)$ ,  $D_{ij} = D$ ,  $Q_{ij} = kc$ . In this case the model (3, 5) has the form:

$$\begin{aligned} u(r) \frac{\partial c}{\partial z} &= D \left( \frac{\partial^2 c}{\partial z^2} + \frac{1}{r} \frac{\partial c}{\partial r} + \frac{\partial^2 c}{\partial r^2} \right) + kc; \\ r=0, \quad \frac{\partial c}{\partial r} &\equiv 0; \quad r=r_0, \quad \frac{\partial c}{\partial r} \equiv 0; \\ z=0, \quad c &\equiv c^0, \quad u^0 c^0 \equiv uc^0 - D \left( \frac{\partial c}{\partial z} \right)_{z=0}. \end{aligned} \quad (6)$$

The qualitative analysis of the model (6) will be made, using generalized variables [1]:

$$\begin{aligned} r=r_0 R, \quad z=lZ, \quad u(r) &= u(r_0 R) = u^0 U(R), \\ c(r, z) &= c(r_0 R, lZ) = c^0 C(R, Z), \quad \varepsilon = \left( \frac{r_0}{l} \right)^2, \end{aligned} \quad (7)$$

where  $r_0, l, u^0, c^0$  are the characteristic (inherent) scales (maximal or average values) of the variables. The introduction of the generalized variables (7) in (6) leads to:

$$\begin{aligned} U(R) \frac{\partial C}{\partial Z} &= \text{Fo} \left( \varepsilon \frac{\partial^2 C}{\partial Z^2} + \frac{1}{R} \frac{\partial C}{\partial R} + \frac{\partial^2 C}{\partial R^2} \right) - \text{Da} C; \\ R=0, \quad \frac{\partial C}{\partial R} &\equiv 0; \quad R=1, \quad \frac{\partial C}{\partial R} \equiv 0; \\ Z=0, \quad C &\equiv 1, \quad 1 \equiv U - \text{Pe}^{-1} \frac{\partial C}{\partial Z}; \\ \text{Fo} &= \frac{Dl}{u_0 r_0^2}, \quad \text{Da} = \frac{kl}{u_0}, \quad \text{Pe} = \frac{u_0 l}{D}, \end{aligned} \quad (8)$$

where Fo, Da and Pe are the Fourier, Damkohler and Peclet numbers, respectively.

In industrial conditions the parameters  $\text{Fo} < 10^{-2}$ ,  $\text{Pe}^{-1} < 10^{-2}$  are small and model (8) has a convective form:

$$U(R) \frac{\partial C}{\partial Z} = -\text{Da} C; \quad Z=0, \quad C \equiv 1. \quad (9)$$

#### Average-concentration model

Let us consider the model of the stationary simple chemical reaction case (6). The average values of the velocity and concentration at the column cross-sectional area are:

$$\bar{u} = \frac{2}{r_0^2} \int_0^{r_0} ru(r) dr, \quad \bar{c}(z) = \frac{2}{r_0^2} \int_0^{r_0} rc(r, z) dr. \quad (10)$$

The functions  $u(r)$ ,  $c(r, z)$  in (6) can be presented with the average functions (10):

$$u(r) = \bar{u} \tilde{u}(r), \quad c(r, z) = \bar{c}(z) \tilde{c}(r, z), \quad (11)$$

where  $\tilde{u}(r)$  and  $\tilde{c}(r, z)$  represent the radial non-uniformity of the velocity and concentration.

The average concentration model may be obtained if (11) is put into (6), multiplied by  $r$  and integrated over  $r$  in the interval  $[0, r_0]$ . As a result, the average-concentration model has the form:

$$\begin{aligned} \alpha \bar{u} \frac{d\bar{c}}{dz} + \frac{d\alpha}{dz} \bar{u} \bar{c} &= D \frac{d^2 \bar{c}}{dz^2} - k\bar{c}; \\ z=0, \quad \bar{c}(0) &= c^0, \quad \frac{d\bar{c}}{dz} = 0, \end{aligned} \quad (12)$$

where

$$\alpha(z) = \frac{2}{r_0^2} \int_0^{r_0} r \tilde{u}(r) \tilde{c}(r, z) dr; \quad (13)$$

represents effect of the radial non-uniformity of the velocity.

The use of the generalized variables

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

$$\tilde{u}(r) = \frac{u(r)}{\bar{u}} = U(R), \quad c(r, z) = c^0 C(R, Z),$$

$$\bar{c}(z) = c^0 \bar{C}(Z), \quad \tilde{c}(r, z) = \frac{c(r, z)}{\bar{c}(z)} = \frac{C(R, Z)}{\bar{C}(Z)},$$

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

$$\alpha(z) = A(Z) = 2 \int_0^1 RU(R) \frac{C(R, Z)}{\bar{C}(Z)} dR, \quad (14)$$

leads to:

$$\begin{aligned} A(Z) \frac{d\bar{C}}{dZ} + \frac{dA}{dZ} \bar{C} &= \text{Pe}^{-1} \frac{d^2 \bar{C}}{dZ^2} - \text{Da} \bar{C}; \\ Z=0, \quad \bar{C} &= 1, \quad \frac{d\bar{C}}{dZ} = 0. \end{aligned} \quad (15)$$

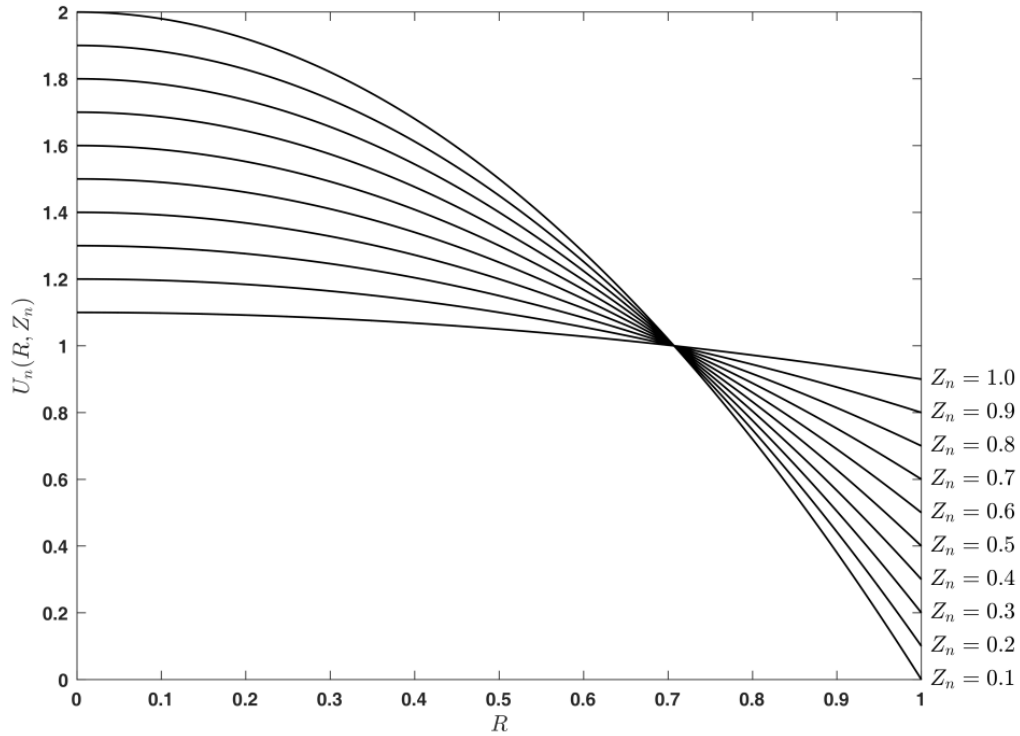
In industrial conditions the parameter  $\text{Pe}^{-1} < 10^{-2}$  is small and model (15) has a convective form:

$$A(Z)\frac{d\bar{C}}{dZ} + \frac{dA}{dZ}\bar{C} = -Da\bar{C}; \quad Z=0, \quad \bar{C}=1. \quad (16)$$

*Axial modification of the radial non-uniformity of the axial velocity component*

Very often in the industrial conditions an axial modification of the radial non-uniformity of the velocity is realized. This radial non-uniformity is caused by the fluid hydrodynamics at the column inlet, where it has as maximum and decreases along the column height as a result of the fluid viscosity.

The theoretical determination of the change in the radial non-uniformity of the axial velocity component in a column is difficult in one-phase processes and practical impossible in two-phase and three-phase processes. For a theoretical analysis of the effect of the axial modification of the radial non-uniformity of the velocity, this difficulty can be circumvented by appropriate hydrodynamic model, where the average velocity at the cross section of the column is a constant, while the maximal velocity (and as a result the radial non-uniformity of the axial velocity component too) decreases along the column height.



**Fig. 1.** Velocity distributions  $U_n(R, Z_n)$ ,  $Z_n = 0.1(n+1)$ ,  $n = 0, 1, \dots, 9$ .

Let's consider [4] the velocity distribution:

$$u_n(r, z_n) = u^0 U_n(R, Z_n), \quad n = 0, 1, \dots, 9, \quad (17)$$

where  $u^0 = const$  is the inlet velocity, and an axial step change of the radial non-uniformity of the axial velocity component in a column (Fig. 1):

$$\begin{aligned} U_n(R, Z_n) &= a_n - b_n R^2, \\ a_n &= 2 - 0.1n, \quad b_n = 2(1 - 0.1n), \\ 0.1n &\leq Z_n \leq 0.1(n+1), \quad n = 0, 1, \dots, 9, \quad 0 \leq R \leq 1. \end{aligned} \quad (18)$$

If we put (17, 18) in (9), the model has the form:

$$\begin{aligned} U_n \frac{\partial C_n}{\partial Z_n} &= -Da C_n; \\ 0.1n &\leq Z_n \leq 0.1(n+1); \\ Z_n &= 0.1n, \quad C_n(R, Z_n) = C_{n-1}(R, Z_n); \\ n &= 0, 1, \dots, 9; \quad Z_0 = 0, \quad C_0(R, Z_0) \equiv 1. \end{aligned} \quad (19)$$

The solution of (19)  $C(R, Z) = C_n(R, Z_n)$ ,  $Z_n = 0.1(n+1)$ ,  $n = 0, 1, \dots, 9$  in the case  $Da = 1$  is presented on the Fig. 2. This solution  $C(R, Z)$  permits to be obtained in (14) the average ("theoretical") concentration distribution  $\bar{C}(Z) = \bar{C}_n(Z_n)$ ,  $Z_n = 0.1(n+1)$ , in the column (the points on the Fig. 3) and function  $A(Z) = A_n(Z_n)$ ,

(the points on the Fig. 4) on every step  $n=0,1,\dots,9$

$$A(Z) = a_0 + a_1 Z + a_2 Z^2 \quad (20)$$

From Fig. 4 is seen, that the function  $A(Z)$  is possible to be presented as a quadratic approximation:

As a result, in the case of axial modification of the radial non-uniformity of the velocity, the model (16) has the form:

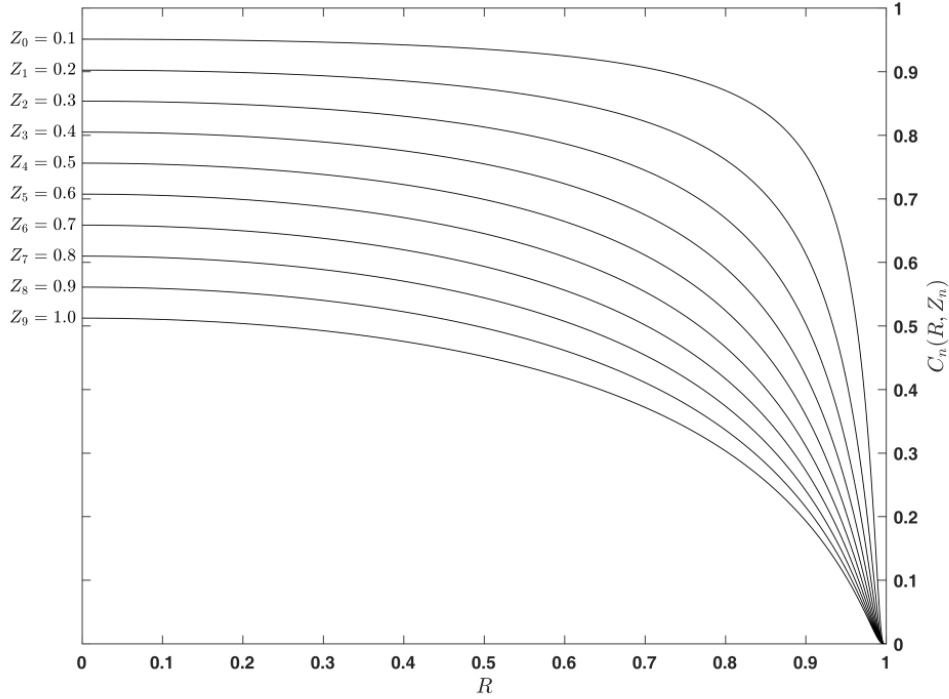


Fig. 2 Concentration distributions  $C(Z) = C(Z_n), Z_n = 0.1(n+1), n=0,1,\dots,9$

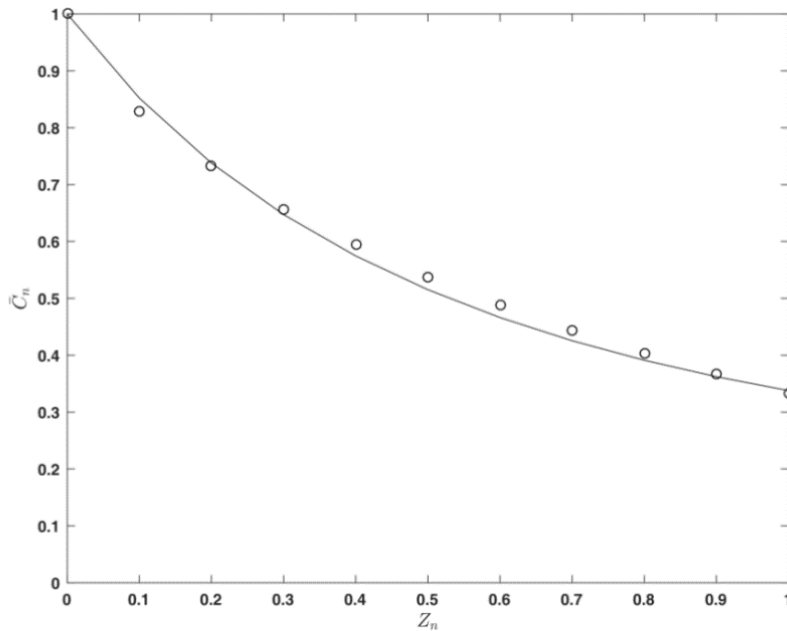


Fig. 3. Average concentration distribution: “theoretical” values (as solution of(10.1.4) and (10.1.5))  $\bar{C}(Z) = \bar{C}_n(Z_n), Z_n = 0.1(n+1), n=0,1,\dots,9$  (points);  $\bar{C}(Z)$  as a solution of (10.1.7) for “experimental” values of  $a_0, a_1, a_2$  (line).

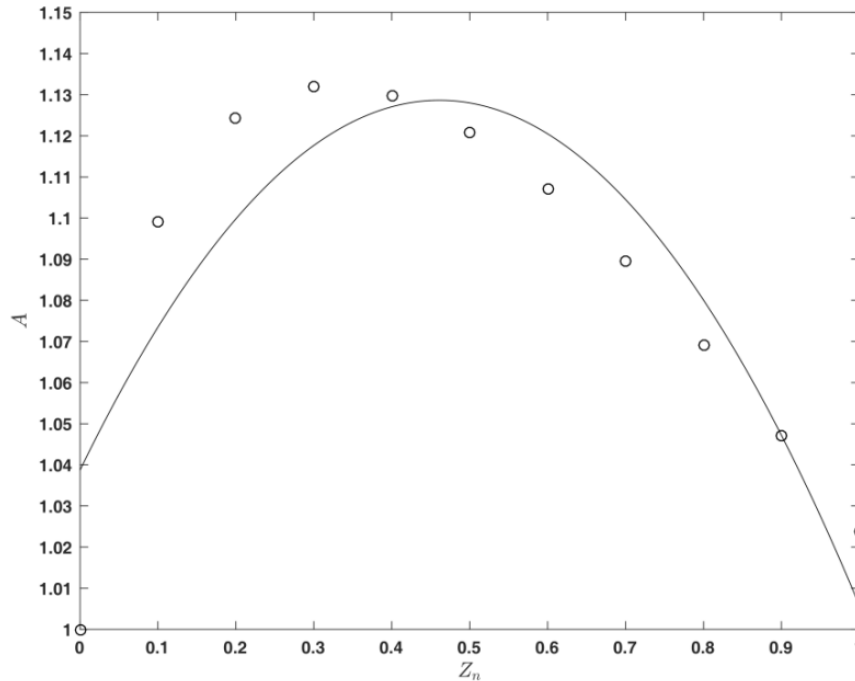


Fig. 4. Function  $A(Z) = A_n(Z_n)$ ,  $Z_n = 0.1(n+1)$ ,  $n = 0, 1, \dots, 9$  (14) (points);

$A(Z)$  as a quadratic approximation (20) (line)

$$(a_0 + a_1 Z + a_2 Z^2) \frac{d\bar{C}}{dZ} + (a_1 + 2a_2 Z) \bar{C} = -Da \bar{C};$$

$$Z = 0, \quad \bar{C} = 1,$$

(21)

where the parameters  $a_0, a_1, a_2$  must be obtained, using experimental data.

The obtained value of the function  $\bar{C}(1)$  (Fig. 3) permit to be obtained the artificial experimental data  $\bar{C}_{\text{exp}}^m(1)$  for the column end ( $Z = 1$ ):

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

(22)

where  $0 \leq B_m \leq 1$ ,  $m = 0, 1, \dots, 10$  are obtained by a generator of random numbers. The obtained artificial experimental data (22) are used for the illustration of the parameters  $(a_0, a_1, a_2)$  identification in the average concentrations model (21) by the minimization of the least-squares function:

$$Q(a_0, a_1, a_2) = \sum_{m=1}^{10} [\bar{C}(1, a_0, a_1, a_2) - \bar{C}_{\text{exp}}^m(1)]^2,$$

(23)

where the value of  $\bar{C}(1, a_0, a_1, a_2)$  is obtained after the solution of (21) for  $Z = 1$ . The parameters  $(a_0, a_1, a_2)$  are used for the solution of (21) and the result (the line) is compared with the average

(“theoretical”) concentration values  $\bar{C}(Z) = \bar{C}_n(Z_n)$ ,  $Z_n = 0.1(n+1)$ ,  $n = 0, 1, \dots, 9$ . (points) (as solution of (19) and (14)) on the Fig. 3.

Gas absorption in column apparatus

#### Convection-diffusion and average-concentration models

The new approach for the modelling of the processes in column apparatuses [1-3] will be used in the cases of the physical absorption processes in a co-current column [5], where the convection-diffusion and average-concentration models have the forms:

$$u_1 \frac{\partial c_1}{\partial z} = D_1 \left( \frac{\partial^2 c_1}{\partial z^2} + \frac{1}{r} \frac{\partial c_1}{\partial r} + \frac{\partial^2 c_1}{\partial r^2} \right) - k(c_1 - \chi c_2);$$

$$u_2 \frac{\partial c_2}{\partial z} = D_2 \left( \frac{\partial^2 c_2}{\partial z^2} + \frac{1}{r} \frac{\partial c_2}{\partial r} + \frac{\partial^2 c_2}{\partial r^2} \right) + k(c_1 - \chi c_2);$$

$$r = 0, \quad \frac{\partial c_j}{\partial r} \equiv 0;$$

$$r = r_0, \quad \frac{\partial c_j}{\partial r} \equiv 0; \quad j = 1, 2;$$

$$z = 0, \quad c_1 \equiv c_1^0, \quad c_2 \equiv 0,$$

$$u_1^0 c_1^0 \equiv u_1 c_1^0 - D_1 \left( \frac{\partial c_1}{\partial z} \right)_{z=0}, \quad \left( \frac{\partial c_2}{\partial z} \right)_{z=0} = 0.$$

(24)

$$\begin{aligned}
 \alpha_1(z)\bar{u}_1 \frac{d\bar{c}_1}{dz} + \frac{d\alpha_1}{dz}\bar{u}_1\bar{c}_1 &= D_1 \frac{d^2\bar{c}_1}{dz^2} - k(\bar{c}_1 - \chi\bar{c}_2); \\
 \alpha_2(z)\bar{u}_2 \frac{d\bar{c}_2}{dz} + \frac{d\alpha_2}{dz}\bar{u}_2\bar{c}_2 &= D_2 \frac{d^2\bar{c}_2}{dz^2} + k(\bar{c}_1 - \chi\bar{c}_2); \\
 z=0, \quad \bar{c}_1(0) &\equiv c_1^0, \quad \bar{c}_2(0) \equiv 0, \\
 \frac{d\bar{c}_1}{dz} &\equiv 0, \quad \frac{d\bar{c}_2}{dz} \equiv 0; \\
 \alpha_j(z) &= \frac{2}{r_0^2} \int_0^{r_0} r \tilde{u}_j \tilde{c}_j dr, \quad \tilde{u}_j(r) = \frac{u_j(r)}{\bar{u}_j}, \\
 \tilde{c}_j(r, z) &= \frac{c_j(r, z)}{\bar{c}_j(z)}, \quad j=1,2.
 \end{aligned} \tag{25}$$

In (24, 25)  $\chi$  is the Henry's number,  $k$  - volume interphase mass transfer coefficient [ $s^{-1}$ ],  $k_0$  - chemical reaction rate constant [ $s^{-1}$ ],  $u_j^0, c_j^0, j=1,2$  - input ( $z=0$ ) velocities and concentrations,  $\bar{u}_j, \bar{c}_j(z), j=1,2$  - the average velocities and concentrations at the column cross-sectional area,  $\tilde{u}_j(r), \tilde{c}_j(r, z), j=1,2$  - the radial non-uniformities of the velocities and concentrations.

In (24, 25) the generalized variables can be introduced:

$$\begin{aligned}
 r &= r_0 R, \quad z = lZ, \quad u_j(r) = \bar{u}_j U_j(R), \quad j=1,2, \\
 c_1(r, z) &= c_1^0 C_1(R, Z), \quad c_2(r, z) = \frac{c_1^0}{\chi} C_2(R, Z), \\
 \bar{c}_1(z) &= c_1^0 \bar{C}_1(Z), \quad \bar{c}_2(z) = \frac{c_1^0}{\chi} \bar{C}_2(Z),
 \end{aligned} \tag{26}$$

and as a result is obtained:

$$\begin{aligned}
 U_1 \frac{\partial C_1}{\partial Z} &= \text{Fo}_1 \left( \varepsilon^2 \frac{\partial^2 C_1}{\partial Z^2} + \frac{1}{R} \frac{\partial C_1}{\partial R} + \frac{\partial^2 C_1}{\partial R^2} \right) - \\
 &- K_1 (C_1 - C_2); \\
 U_2 \frac{\partial C_2}{\partial Z} &= \text{Fo}_2 \left( \varepsilon^2 \frac{\partial^2 C_2}{\partial Z^2} + \frac{1}{R} \frac{\partial C_2}{\partial R} + \frac{\partial^2 C_2}{\partial R^2} \right) + \\
 &+ K_2 (C_1 - C_2); \\
 R=0, \quad \frac{\partial C_j}{\partial R} &\equiv 0; \quad R=1, \quad \frac{\partial C_j}{\partial R} \equiv 0; \quad j=1,2; \\
 Z=0, \quad C_1 &\equiv 1, \quad C_2=0,
 \end{aligned} \tag{27}$$

$$1 \equiv U_1 - \text{Pe}_1^{-1} \frac{\partial C_1}{\partial Z}, \quad \frac{\partial C_2}{\partial Z} \equiv 0.$$

$$\begin{aligned}
 A_1(Z) \frac{d\bar{C}_1}{dZ} + \frac{dA_1}{dZ} \bar{C}_1 &= \text{Pe}_1^{-1} \frac{d^2\bar{C}_1}{dZ^2} - K_1 (\bar{C}_1 - \bar{C}_2); \\
 A_2(Z) \frac{d\bar{C}_2}{dZ} + \frac{dA_2}{dZ} \bar{C}_2 &= \text{Pe}_2^{-1} \frac{d^2\bar{C}_2}{dZ^2} + K_2 (\bar{C}_1 - \bar{C}_2); \\
 Z=0, \quad \bar{C}_1 &= 1, \quad \bar{C}_2=0, \quad \frac{d\bar{C}_1}{dZ} = 0, \quad \frac{d\bar{C}_2}{dZ} = 0.
 \end{aligned}$$

In (27) are used the expressions:

$$\begin{aligned}
 \bar{C}_j(Z) &= 2 \int_0^1 R C_j(R, Z) dR, \\
 \tilde{c}_j(r, z) &= \frac{c_j(r, z)}{\bar{c}_j(z)} = \frac{C_j(R, Z)}{\bar{C}_j(Z)}, \\
 \alpha_j(z) = A_j(Z) &= 2 \int_0^1 R U_j(R) \frac{C_j(R, Z)}{\bar{C}_j(Z)} dR, \\
 j &= 1,2.
 \end{aligned} \tag{28}$$

In practical conditions the models (26, 27) have convective forms:

$$\begin{aligned}
 U_1 \frac{dC_1}{dZ} &= -K_1 (C_1 - C_2); \\
 U_2 \frac{dC_2}{dZ} &= \omega K_1 (C_1 - C_2); \\
 Z=0, \quad C_1 &\equiv 1, \quad C_2=0.
 \end{aligned} \tag{29}$$

$$\begin{aligned}
 A_1(Z) \frac{d\bar{C}_1}{dZ} + \frac{dA_1}{dZ} \bar{C}_1 &= -K_1 (\bar{C}_1 - \bar{C}_2); \\
 A_2(Z) \frac{d\bar{C}_2}{dZ} + \frac{dA_2}{dZ} \bar{C}_2 &= \omega K_1 (\bar{C}_1 - \bar{C}_2); \\
 Z=0, \quad \bar{C}_1 &= 1, \quad \bar{C}_2=0.
 \end{aligned} \tag{30}$$

*Effect of the axial modification of the radial non-uniformity of the axial velocity components*

Let's consider [5] the velocity distributions:

$$u_{jn}(r, z_n) = u_j^0 U_{jn}(R, Z_n), \quad j=1,2, \quad n=0,1,\dots,9, \tag{31}$$

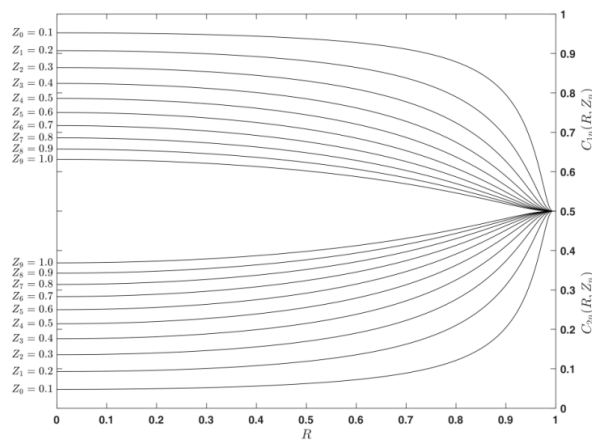
where

$$\begin{aligned}
 U_{j_n}(R, Z_n) &= a_{j_n} - b_{j_n} R^2, \quad a_{j_n} = 2 - 0.1n, \\
 b_{j_n} &= 2(1 - 0.1n), \quad 0.1n \leq Z_n \leq 0.1(n+1), \\
 n &= 0, 1, \dots, 9, \quad j = 1, 2.
 \end{aligned}
 \tag{32}$$

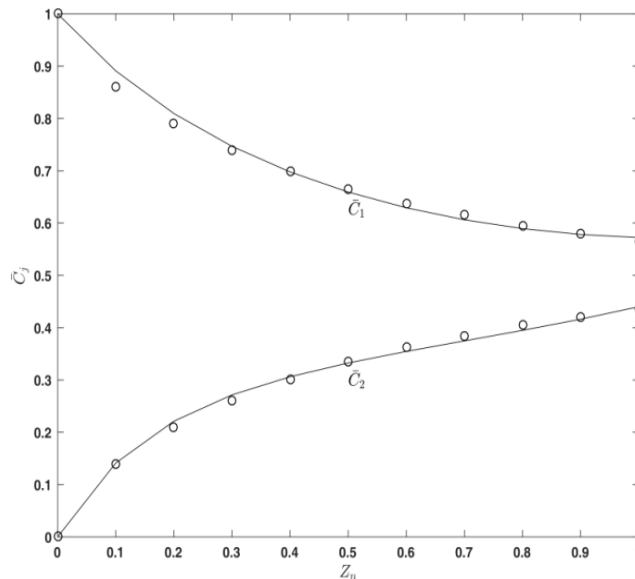
If we put (32) in (29), the model has the form:

$$\begin{aligned}
 U_{1n} \frac{dC_{1n}}{dZ_n} &= -K_1(C_{1n} - C_{2n}), \\
 U_{2n} \frac{dC_{2n}}{dZ_n} &= \omega K_1(C_{1n} - C_{2n}); \\
 Z_n &= 0.1n, \quad C_{j_n}(R, Z_n) = C_{j(n-1)}(R, Z_n), \\
 n &= 0, 1, \dots, 9, \quad j = 1, 2; \\
 Z_0 &= 0, \quad C_{10}(R, Z_0) \equiv 1, \quad C_{20}(R, Z_0) = 0.
 \end{aligned}
 \tag{33}$$

The parameter  $\omega$  in (33) is known beforehand. The solution of (33), for a concrete absorption process ( $\omega=1$ ) of an average soluble gas and “theoretical” value of  $K_1=1$ , permits to be obtained the concentration distributions  $C_{j_n}(R, Z_n)$ ,  $j=1, 2$  for different  $Z_n=0.1(n+1)$ ,  $n=0, 1, \dots, 9$  (Fig. 5). The solution of (33) (Fig. 5) and (28) permit to obtain the “theoretical” average concentration distributions



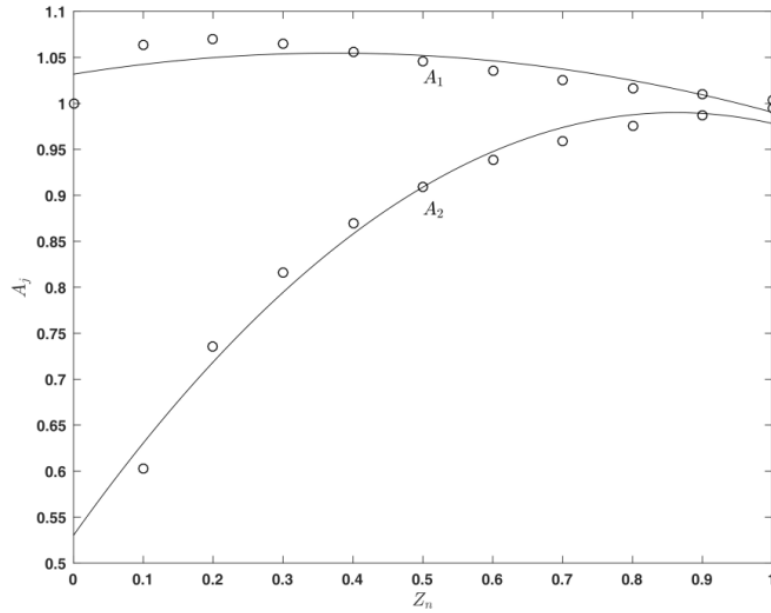
**Fig. 5.** Concentration distributions  $C_{j_n}(R, Z_n)$ ,  $j=1, 2$  in the case  $\omega = K_1 = 1$  for different  $Z_n = 0.1(n+1)$ ,  $n=0, 1, \dots, 9$ .



**Fig. 6.** Average concentration  $\bar{C}_j(Z)$ ,  $j=1, 2$  in the case  $\omega = K_1 = 1$ : “theoretical” values

$\bar{C}_j(Z) = \bar{C}_{j_n}(Z_n)$ ,  $j=1, 2$  as solutions of (33) and (28) for different  $Z_n = 0.1(n+1)$ ,  $n=0, 1, \dots, 9$  (points);  $\bar{C}_j(Z)$ ,  $j=1, 2$  as a solution of (35), using the “experimental” parameter values  $a_{j_0}, a_{j_1}, a_{j_2}$ ,  $j=1, 2, K_1$  (lines)





**Fig. 7.** Function  $A_{jn}(Z_n)$ ,  $j=1,2$  in the case  $\omega = K_1 = 1$ : as a solution of (29) and (28) for different  $Z_n = 0.1(n+1)$ ,  $n=0,1,\dots,9$  (points);  $A_j(Z)$ ,  $j=1,2$  as a quadratic approximation (34) (line).

$\bar{C}_{jn}(Z_n)$ ,  $j=1,2$  (the points in Fig. 6) and the functions  $A_{jn}(Z_n)$ ,  $j=1,2$  (the points in Fig. 7) for different  $Z_n = 0.1(n+1)$ ,  $n=0,1,\dots,9$ .

From Fig. 7 it is seen that the functions  $A_{jn}(Z_n)$ ,  $n=0,1,\dots,4$ ,  $j=1,2$  may be presented as quadratic approximations:

$$\begin{aligned} A_1(Z) &= a_{10} + a_{11}Z + a_{12}Z^2, \\ A_2(Z) &= a_{20} + a_{21}Z + a_{22}Z^2. \end{aligned} \quad (34)$$

As a result, in the case of axial modification of the radial non-uniformity of the velocity, the model (30) has the form:

$$\begin{aligned} (a_{10} + a_{11}Z + a_{12}Z^2) \frac{d\bar{C}_1}{dZ} + (a_{11} + 2a_{12}Z)\bar{C}_1 &= \\ = -K_1(\bar{C}_1 - \bar{C}_2); \\ (a_{20} + a_{21}Z + a_{22}Z^2) \frac{d\bar{C}_2}{dZ} + (a_{21} + 2a_{22}Z)\bar{C}_2 &= \\ = \omega K_1(\bar{C}_1 - \bar{C}_2); \\ Z=0, \quad \bar{C}_1=1, \quad \bar{C}_2=0, \end{aligned} \quad (35)$$

where (at unknown velocity distributions in the two phases)  $\omega$  is known beforehand for a concrete process, while the parameters  $a_{j0}, a_{j1}, a_{j2}$ ,  $j=1,2$ ,  $K_1$  must be obtained using experimental data.

The obtained values of the functions  $\bar{C}_{jn}(Z_n)$ ,  $j=1,2$ , for a concrete process ( $\omega=1$ ),

“theoretical” value of  $K_1=1$  and different  $Z_n = 0.1(n+1)$ ,  $n=0,1,\dots,9$  (Fig. 6), permit to be obtained the values of  $\bar{C}_j(1)$ ,  $j=1,2$  and the artificial experimental data:

$$\begin{aligned} \bar{C}_{j\text{exp}}^m(1) &= (0.95 + 0.1B_m)\bar{C}_j(1), \quad j=1,2, \\ m &= 1, \dots, 10, \end{aligned} \quad (36)$$

where  $0 \leq B_m \leq 1$ ,  $m=1,\dots,10$  are obtained by a generator of random numbers. The obtained artificial experimental data (36) are used for the illustration of the parameters  $P = (a_{j0}, a_{j1}, a_{j2}, j=1,2, K_1)$  identification in the average concentrations model (35) by the minimization of the least-squares function with respect to  $P = (a_{j0}, a_{j1}, a_{j2}, j=1,2, K_1)$ :

$$\begin{aligned} Q(P) &= \sum_{m=1}^{10} [\bar{C}_1(1, P) - \bar{C}_{1\text{exp}}^m(1)]^2 + \\ &+ \sum_{m=1}^{10} [\bar{C}_2(1, P) - \bar{C}_{2\text{exp}}^m(1)]^2, \end{aligned} \quad (37)$$

where the values of  $\bar{C}_j(1, P)$ ,  $j=1,2$  are obtained as solutions of (35). The obtained (“experimental”) parameter values  $a_{j0}, a_{j1}, a_{j2}$ ,  $j=1,2$ ,  $K_1$  are used for the solution of (35) and the results (the lines) are compared with the “theoretical” average concentration values on Fig.6.

RADIAL VELOCITY COMPONENT IS NOT EQUAL TO ZERO

Chemical reaction in column apparatus

Convection-diffusion model

A theoretical analysis of the effect of the radial velocity components in the industrial column chemical reactors will be presented in the case, when the radial velocity component is not equal to zero for pseudo-first order chemical reactions. In the stationary case, the convection-diffusion model (3-5) has the form:

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

$$r = 0, \quad \frac{\partial c}{\partial r} \equiv 0; \quad r = r_0, \quad \frac{\partial c}{\partial r} \equiv 0;$$

$$z = 0, \quad c \equiv c^0, \quad u^0 c^0 \equiv uc^0 - D \frac{\partial c}{\partial z}. \quad (38)$$

$$\frac{\partial u}{\partial z} + \frac{\partial v}{\partial r} + \frac{v}{r} = 0;$$

$$r = r_0, \quad v(r_0, z) \equiv 0; \quad z = 0, \quad u = u(r, 0). \quad (39)$$

The theoretical analysis of the model (38, 39) will be made, using generalized variables (7) and

$$v(r, z) = v(r_0 R, lZ) = u^0 \varepsilon V(R, Z). \quad (40)$$

As a result from (7, 38-40) the following may be obtained:

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

$$R = 0, \quad \frac{\partial C}{\partial R} \equiv 0; \quad R = 1, \quad \frac{\partial C}{\partial R} \equiv 0; \quad (41)$$

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

$$\frac{\partial U}{\partial Z} + \frac{\partial V}{\partial R} + \frac{V}{R} = 0;$$

$$R = 1, \quad V(1, Z) \equiv 0; \quad Z = 0, \quad U = U(R, 0). \quad (42)$$

In industrial conditions the parameters  $\text{Fo} < 10^{-2}$ ,  $\text{Pe}^{-1} < 10^{-2}$  are small and the model (41) has a convective form:

$$U \frac{\partial C}{\partial Z} + V \frac{\partial C}{\partial R} = -\text{Da} C;$$

$$R = 1, \quad C \equiv 0; \quad Z = 0, \quad C \equiv 1. \quad (43)$$

Average-concentration model

The functions  $u(r, z), v(r, z), c(r, z)$  in (38) can be presented with the help of the average functions (10):

$$u(r, z) = \bar{u} U(R, Z), \quad v(r, z) = \varepsilon \bar{u} V(R),$$

$$c(r, z) = \bar{c}(z) \tilde{c}(r, z). \quad (44)$$

As a result, the following is obtained:

$$\alpha(z) \bar{u} \frac{d\bar{c}}{dz} + [\beta(z) + \gamma(z)] \bar{u} \bar{c}_i = D \frac{d^2 \bar{c}}{dz^2} - k \bar{c};$$

$$z = 0, \quad \bar{c} \equiv c^0, \quad \frac{d\bar{c}}{dz} \equiv 0, \quad (45)$$

where

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

$$\gamma(z) = \frac{2}{r_0^2} \int_0^{r_0} r V \frac{\partial \tilde{c}}{\partial r} dr, \quad \tilde{c}(r, z) = \tilde{C}(R, Z),$$

$$U = U(R, Z), \quad V = V(R). \quad (46)$$

The theoretical analysis of the model (45) will be made, using the next generalized variables and functions:

$$z = lZ, \quad r = r_0 R, \quad \bar{c}(z) = c^0 \bar{C}(Z),$$

$$\bar{C}(Z) = 2 \int_0^1 R C(R, Z) dR,$$

$$\tilde{c}(r, z) = \frac{c(r, z)}{\bar{c}(z)} = \frac{C(R, Z)}{\bar{C}(Z)} = \tilde{C}(R, Z),$$

$$\alpha(z) = A(Z) = 2 \int_0^1 R U(R, Z) \tilde{C}(R, Z) dR,$$

$$\beta(z) = \beta(lZ) = B(Z) = 2 \int_0^1 R U(R, Z) \frac{\partial \tilde{C}}{\partial Z} dR,$$

$$\gamma(z) = \gamma(lZ) = G(Z) = 2 \int_0^1 R V(R) \frac{\partial \tilde{C}}{\partial R} dR, \quad (47)$$

and as a result:

$$A(Z) \frac{d\bar{C}}{dZ} + [B(Z) + G(Z)] \bar{C} = \text{Pe}^{-1} \frac{d^2 \bar{C}}{dZ^2} - \text{Da} \bar{C};$$

$$Z = 0, \quad \bar{C} = 1, \quad \frac{d\bar{C}}{dZ} = 0. \quad (48)$$

In industrial conditions  $\text{Pe} > 10^2$  and the model (48) has the convective form:

$$A(Z)\frac{d\bar{C}}{dZ} + [B(Z) + G(Z)]\bar{C} = -Da\bar{C};$$

$$Z = 0, \quad \bar{C} = 1. \tag{49}$$

*Axial and radial velocity components*

The theoretical analysis of the change in the radial non-uniformity of the axial velocity

component (effect of the radial velocity component) in a column can be made by an appropriate hydrodynamic model, where the average velocity at the cross section of the column is a constant (inlet average axial velocity component), while the radial non-uniformity of the axial velocity component decreases along the column height and as a result a radial velocity

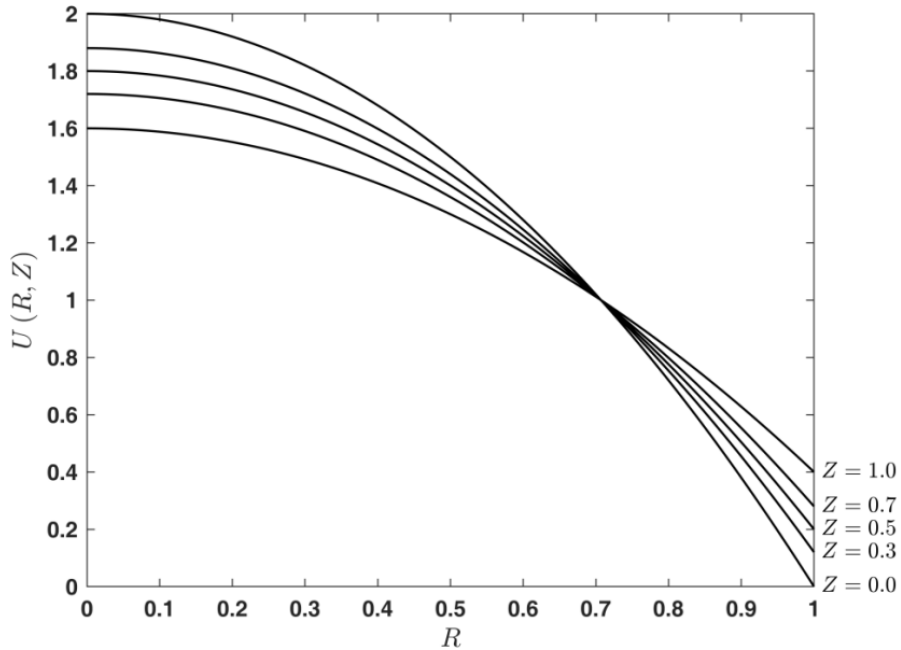


Fig. 8. Axial velocity component  $U(R, Z)$  for different  $Z = 0, 0.3, 0.5, 0.7, 1.0$

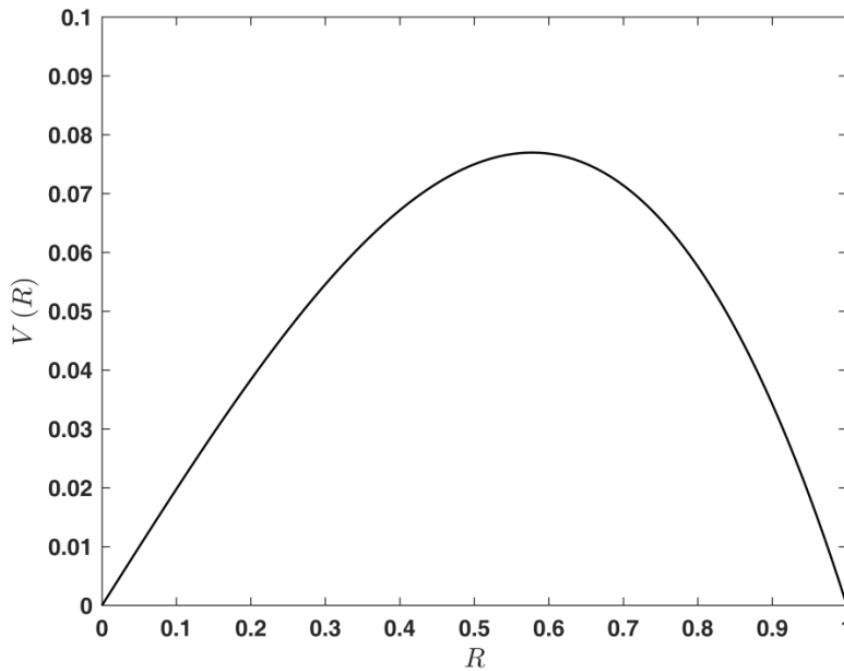


Fig. 9. Radial velocity component  $V(R)$

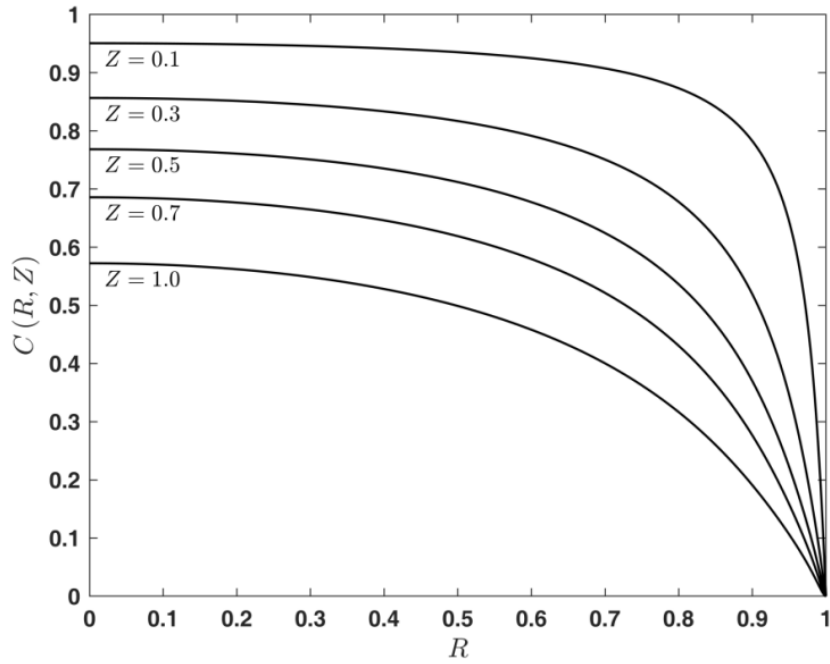


Fig. 10. Concentration distributions  $C(R, Z)$  for different  $Z = 0.1, 0.3, 0.5, 0.7, 1.0$

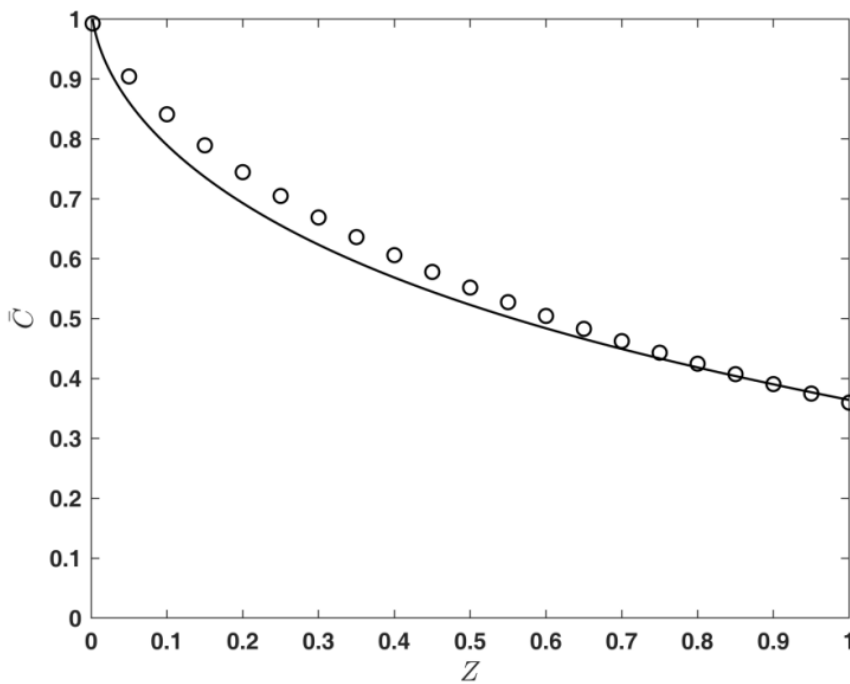


Fig. 11. Average concentrations  $\bar{C}(Z)$ : “theoretical” values  $\bar{C}(Z_n), Z_n = 0.1(n+1), n = 0, 1, \dots, 9$  (points); solution of (49) (lines)

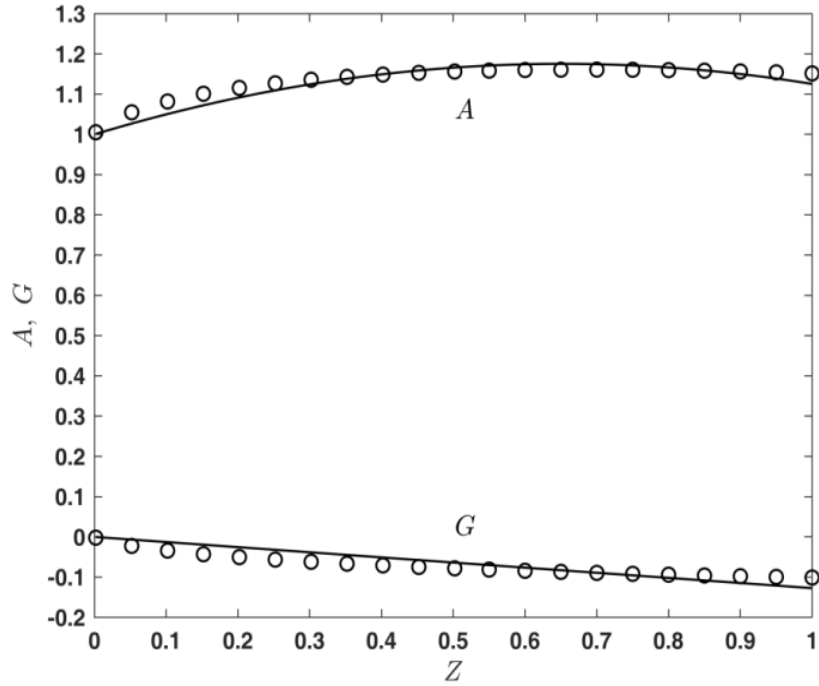


Fig. 12. Functions  $A(Z_n), G(Z_n), Z_n = 0.1(n+1), n = 0, 1, \dots, 9$  (points) and their quadratic and linear approximations (53) (lines)

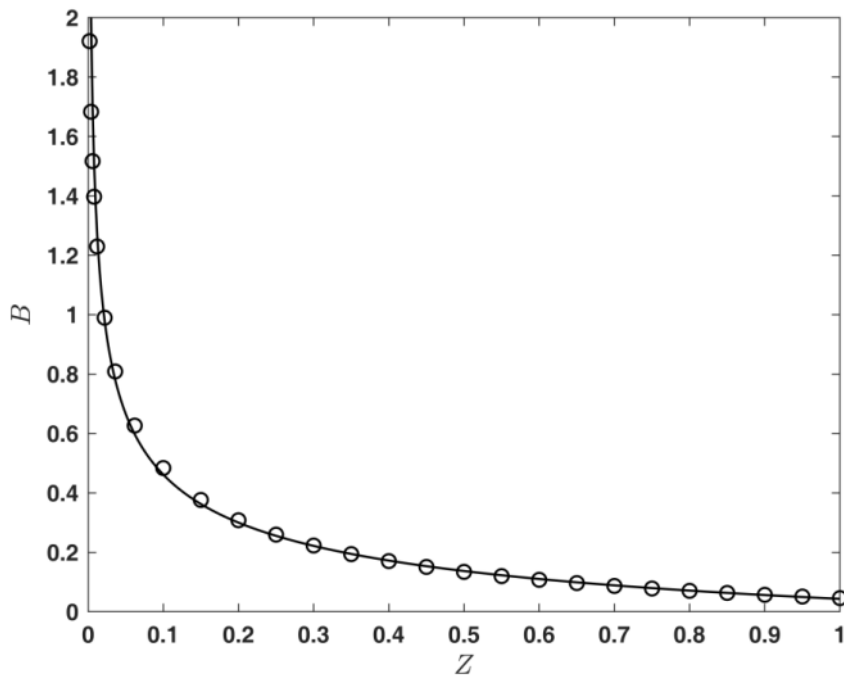


Fig. 13. Functions  $B(Z_n), Z_n = 0.1(n+1), n = 0, 1, \dots, 9$  (points) and its parabolic approximation (53) (line).

component is initiated. In generalized variables (7) is possible to be used the model:

$$\begin{aligned} U &= (2 - 0.4Z) - 2(1 - 0.4Z)R^2, \\ V &= 0.2(R - R^3), \end{aligned} \quad (50)$$

where the velocity components satisfy the equation (42). The velocity components (50) are presented on the Figs. 8, 9. From Fig. 9 is seen, that  $V < 0.1$  and must be presented with the help of a small parameter  $0.1 = \alpha \ll 1$ , i.e.

$$V = \alpha V_0, \quad V_0 = 0.2(R - R^3)\alpha^{-1} \quad (51)$$

As a result, the problem (43) has the form:

$$\begin{aligned} U \frac{\partial C}{\partial Z} + \alpha V_0 \frac{\partial C}{\partial R} &= -Da C; \quad R=1, \quad \frac{\partial C}{\partial R} \equiv 0; \\ Z=0, \quad C &\equiv 1, \end{aligned} \quad (52)$$

where  $0.1 = \alpha \ll 1$  is a small parameter and (52) must be solved by the perturbation method [1, 9].

The solutions of (52) in the case  $Da = 1$ , and  $0.1 = \alpha \ll 1$ , lead to  $C(R, Z)$  which is presented on Fig. 10.

The solution of (51, 52) and (47) permits to be obtained the average concentrations ("theoretical" values)  $\bar{C}(Z_n)$  and functions  $A(Z_n)$ ,  $B(Z_n)$ ,  $G(Z_n)$ ,  $Z_n = 0.1(n+1)$ ,  $n = 0, 1, \dots, 9$ , which are presented (points) on Figs. 11-13.

From Figs. 12, 13 is seen, that the functions  $A(Z)$ ,  $B(Z)$ ,  $G(Z)$  are possible to be presented as the next approximations:

$$\begin{aligned} A(Z) &= 1 + a_1 Z + a_2 Z^2, \quad B(Z) = b_0 + b_1 Z^{b_2}, \\ G(Z) &= gZ \end{aligned} \quad (53)$$

As a result, the model (49) has the form:

$$\begin{aligned} (1 + a_1 Z + a_2 Z^2) \frac{d\bar{C}}{dZ} + (b_0 + b_1 Z^{b_2} + gZ) \bar{C} &= -Da \bar{C}; \\ Z=0, \quad \bar{C} &= 1, \end{aligned} \quad (54)$$

where the parameters  $P(a_1, a_2, b_0, b_1, b_2, g)$  must be obtained using experimental data.

The value of the function  $\bar{C}(1)$  obtained from (51, 52) and (47) permits to be obtained the artificial experimental data  $\bar{C}_{\text{exp}}^m(1)$  for the column end ( $Z = 1$ ):

$$\bar{C}_{\text{exp}}^m(1) = (0.95 + 0.1B_m) \bar{C}(1), \quad m = 1, \dots, 10, \quad (55)$$

where  $0 \leq B_m \leq 1$ ,  $m = 0, 1, \dots, 10$  are obtained by a generator of random numbers.

The obtained artificial experimental data (55) is possible to be used for the illustration of the parameters  $P$  identification in the average concentrations model (54) by the minimization of the least-squares function:

$$Q(P) = \sum_{m=1}^{10} [\bar{C}(1, P) - \bar{C}_{\text{exp}}^m(1)]^2, \quad (56)$$

where the values of  $\bar{C}(1, P)$  are obtained after the solution of (54) for  $Z = 1$ .

The obtained ("experimental") parameter values are used for the solution of (54) and the results (the lines) are compared with the average ("theoretical") concentration values

$\bar{C}(Z_n)$ ,  $Z_n = 0.1(n+1)$ ,  $n = 0, 1, \dots, 9$  (points) on Fig. 11.

## GAS ABSORPTION IN COLUMN APPARATUS

### Convection-diffusion model

The new approach of the processes modeling in the column apparatuses [1-3] permits to be created the convection-diffusion model of the co-current physical absorption process in the case, when the radial velocity component is not equal to zero:

$$\begin{aligned} u_j \frac{\partial c_j}{\partial z} + v_j \frac{\partial c_j}{\partial r} &= D_j \left( \frac{\partial^2 c_j}{\partial z^2} + \frac{1}{r} \frac{\partial c_j}{\partial r} + \frac{\partial^2 c_j}{\partial r^2} \right) + \\ &+ (-1)^{(2-j)} k(c_1 - \chi c_2); \\ r=0, \quad \frac{\partial c_j}{\partial r} &\equiv 0; \quad r=r_0, \quad \frac{\partial c_j}{\partial r} \equiv 0; \quad j=1, 2; \\ z=0, \quad c_1 &\equiv c_1^0, \quad c_2 \equiv 0, \\ u_1^0 c_1^0 &\equiv u_1 c_1^0 - D_1 \left( \frac{\partial c_1}{\partial z} \right)_{z=0}, \quad \left( \frac{\partial c_2}{\partial z} \right)_{z=0} = 0. \end{aligned} \quad (57)$$

$$\begin{aligned} \frac{\partial u_j}{\partial z} + \frac{\partial v_j}{\partial r} + \frac{v_j}{r} &= 0; \\ r=r_0, \quad v_j(r_0, z) &\equiv 0; \\ z=0, \quad u_j &= u_j(r, 0); \quad j=1, 2. \end{aligned} \quad (58)$$

In (57, 58) the generalized variables can be introduced:

$$\begin{aligned} r &= r_0 R, \quad z = lZ, \\ u_j(r, z) &= u_j(r_0 R, lZ) = u_j^0 U_j(R, Z), \\ v_j(r, z) &= v_j(r_0 R, lZ) = u_j^0 \varepsilon V_j(R, Z), \quad j=1, 2, \\ c_1(r, z) &= c_1(r_0 R, lZ) = c_1^0 C_1(R, Z), \\ c_2(r, z) &= c_2(r_0 R, lZ) = \frac{c_2^0}{\chi} C_2(R, Z) \end{aligned} \quad (59)$$

and as a result is obtained:

$$\begin{aligned}
 U_j \frac{\partial C_j}{\partial Z} + V_j \frac{\partial C_j}{\partial R} &= \text{Fo}_j \left( \varepsilon^2 \frac{\partial^2 C_j}{\partial Z^2} + \frac{1}{R} \frac{\partial C_j}{\partial R} + \right. \\
 &\left. + \frac{\partial^2 C_j}{\partial R^2} \right) + (-1)^{(2-j)} K_j (C_1 - C_2); \\
 R=0, \quad \frac{\partial C_j}{\partial R} &\equiv 0, \quad j=1,2; \\
 R=1, \quad \frac{\partial C_j}{\partial R} &\equiv 0, \quad j=1,2; \\
 Z=0, \quad C_1 &\equiv 1, \quad C_2 \equiv 0, \\
 1 &\equiv U_1 - \text{Pe}_1^{-1} \frac{\partial C_1}{\partial Z}, \quad \frac{\partial C_2}{\partial Z} \equiv 0. \\
 \frac{\partial U_j}{\partial Z} + \frac{\partial V_j}{\partial R} + \frac{V_j}{R} &= 0; \\
 R=1, \quad V_j(1,Z) &\equiv 0; \quad Z=0, \quad U_j = U_j(R,0).
 \end{aligned} \tag{60}$$

In industrial conditions the model (60) has a convective form:

$$\begin{aligned}
 U_j \frac{\partial C_j}{\partial Z} + V_j \frac{\partial C_j}{\partial R} &= (-1)^{(2-j)} K_j (C_1 - C_2); \\
 R=1, \quad \frac{\partial C_j}{\partial R} &\equiv 0; \quad j=1,2; \\
 Z=0, \quad C_1 &\equiv 1, \quad C_2=0.
 \end{aligned} \tag{61}$$

#### Average-concentration model

The functions

$$\begin{aligned}
 u_j(r,z), v_j(r,z), c_j(r,z), \quad j=1,2 \text{ in (57) can be} \\
 \text{presented with the help of the average functions:} \\
 u_j(r,z) = \bar{u}_j U_j(R,Z), \quad v_j(r,z) = \varepsilon \bar{u}_j V_j(R,Z), \\
 c_j(r,z) = \bar{c}_j(z) \tilde{c}_j(r,z), \quad j=1,2.
 \end{aligned} \tag{62}$$

As a result, the following is obtained:

$$\begin{aligned}
 \alpha_j(z) \bar{u}_j \frac{d\bar{c}_j}{dz} + [\beta_j(z) + \gamma_j(z)] \bar{u}_j \bar{c}_j &= \\
 = D_j \frac{d^2 \bar{c}_j}{dz^2} + (-1)^{(2-j)} k (\bar{c}_1 - \chi \bar{c}_2); \\
 z=0, \quad \bar{c}_j(0) &\equiv (2-j)c_j^0, \quad \frac{d\bar{c}_j}{dz} \equiv 0; \quad j=1,2.
 \end{aligned} \tag{63}$$

where

$$\begin{aligned}
 \alpha_j(z) &= \frac{2}{r_0^2} \int_0^{r_0} r U_j \tilde{c}_j dr, \\
 \beta_j(z) &= \frac{2}{r_0^2} \int_0^{r_0} r U_j \frac{\partial \tilde{c}_j}{\partial z} dr, \\
 \gamma_j(z) &= \frac{2}{r_0^2} \int_0^{r_0} r V_j \frac{\partial \tilde{c}_j}{\partial r} dr, \\
 U_j &= U_j(R,Z), \quad V_j = V_j(R), \\
 \tilde{c}_j(r,z) &= \tilde{C}_j(R,Z), \quad j=1,2.
 \end{aligned} \tag{64}$$

The theoretical analysis of the model (63) will be made, using the next generalized variables and functions:

$$\begin{aligned}
 r = r_0 R, \quad z = lZ, \quad \bar{c}_j(z) &= c_j^0 \bar{C}_j(Z), \quad c_2^0 = \frac{c_1^0}{\chi}, \\
 \bar{C}_j(Z) &= 2 \int_0^1 R C_j(R,Z) dR, \\
 \tilde{c}_j(r,z) &= \frac{c_j(r,z)}{\bar{c}_j(z)} = \frac{C_j(R,Z)}{\bar{C}_j(Z)} = \tilde{C}_j(R,Z), \\
 \alpha_j(z) &= A_j(Z) = 2 \int_0^1 R U_j(R,Z) \tilde{C}_j(R,Z) dR, \\
 \beta_j(z) &= B_j(Z) = 2 \int_0^1 R U_j(R,Z) \frac{\partial \tilde{C}_j}{\partial Z} dR, \\
 \gamma_j(z) &= G_j(Z) = 2 \int_0^1 R V_j(R) \frac{\partial \tilde{C}_j}{\partial R} dR, \quad j=1,2,
 \end{aligned} \tag{65}$$

and as a result the model (63) has the form:

$$\begin{aligned}
 A_j(Z) \frac{d\bar{C}_j}{dZ} + [B_j(Z) + G_j(Z)] \bar{C}_j &= \\
 = \text{Pe}_j^{-1} \frac{d^2 \bar{C}_j}{dZ^2} + (-1)^{(2-j)} K_j (\bar{C}_1 - \bar{C}_2); \\
 Z=0, \quad \bar{C}_1 &= 1, \quad \bar{C}_2 = 0, \\
 \frac{d\bar{C}_1}{dZ} &= 0, \quad \frac{d\bar{C}_2}{dZ} = 0; \quad j=1,2.
 \end{aligned} \tag{66}$$

In industrial conditions the model (66) has the convective form:

$$\begin{aligned}
 A_j(Z) \frac{d\bar{C}_j}{dZ} + [B_j(Z) + G_j(Z)] \bar{C}_j &= \\
 = (-1)^{(2-j)} K_j \omega^{(j-1)} (\bar{C}_1 - \bar{C}_2); \\
 Z=0, \quad \bar{C}_1 &= 1, \quad \bar{C}_2=0; \quad j=1,2.
 \end{aligned} \tag{67}$$

#### Axial and radial velocity components

The theoretical analysis of the effect of the radial velocity components in a column can be made by an appropriate hydrodynamic model. In generalized

variables, as an example, is possible to be used the next velocity distributions, where the difference between the gas and liquid flows is in the average (inlet) velocities, only:

$$\begin{aligned} U_j &= (2 - 0.4Z) - 2(1 - 0.4Z)R^2, \\ V_j &= 0.2(R - R^3), \quad j=1,2, \end{aligned} \quad (68)$$

where  $V_j < 0.1$ ,  $j=1,2$  and must be presented with the help of a small parameter  $0.1 = \alpha \ll 1$ , i.e.

$$V_j = \alpha V_{j0}, \quad V_{j0} = 0.2(R - R^3)\alpha^{-1}, \quad j=1,2. \quad (69)$$

In the cases of physical absorption) of an average soluble gas ( $\omega \ll 1$ ) in an industrial absorption column, the convection-diffusion and average-concentration models (61, 67) have the forms:

$$\begin{aligned} U_1 \frac{dC_1}{dZ} + \alpha V_{10} \frac{dC_1}{dR} &= -K_1(C_1 - C_2); \\ U_2 \frac{dC_2}{dZ} + \alpha V_{20} \frac{dC_2}{dR} &= \omega K_1(C_1 - C_2); \end{aligned} \quad (70)$$

$$R = 1, \quad \frac{\partial C_j}{\partial R} \equiv 0, \quad j = 1, 2;$$

$$Z = 0, \quad C_1 \equiv 1, \quad C_2 = 0.$$

$$\begin{aligned} (1 + a_{11}Z + a_{12}Z^2) \frac{d\bar{C}_1}{dZ} + \\ + (b_{10} + b_{11}Z^{b_{12}} + g_1Z) \bar{C}_1 &= -K_1(\bar{C}_1 - \bar{C}_2); \end{aligned}$$

$$Z = 0, \quad \bar{C}_1 \equiv 1;$$

$$\begin{aligned} (a_{20} + a_{21}Z + a_{22}Z^2) \frac{d\bar{C}_2}{dZ} + (b_{20} + b_{21}Z^{b_{22}} + \\ + g_{20} + g_{21}Z) \bar{C}_2 &= \omega K_1(\bar{C}_1 - \bar{C}_2); \end{aligned}$$

$$Z = 0, \quad \bar{C}_2 \equiv 0; \quad (71)$$

where the parameters  $a_{j0}, a_{j1}, a_{j2}, b_{j0}, b_{j1}, b_{j2}, g_{j0}, g_{j1}, j=1,2, K_1$  must be obtained using experimental data.

The solution of (70), in the case  $K_1 = 1, \omega = 1$ , is obtained with the help of the perturbation method [10]. The solution of (70) and (65) permits to be obtained the average concentrations in the phases  $\bar{C}_j(Z), i=1,2$  ("theoretical" values, the points in Fig. 14).

The values of the functions  $\bar{C}_j(Z), j=1,2$  permit to be obtained the values of  $\bar{C}_j(1), j=1,2$  and the artificial experimental data (36), which are used for the parameters  $P(a_{j0}, a_{j1}, a_{j2}, b_{j0}, b_{j1}, b_{j2}, g_{j0}, g_{j1}, K_1), j=1,2$  identification in the average concentrations model (71), by the minimization of the least-squares function (37) with respect to  $P$ , where the values of  $\bar{C}_j(1, P), j=1,2$  are obtained as solution of (71).

The ("experimental") values of the parameters  $a_{j0}, a_{j1}, a_{j2}, b_{j0}, b_{j1}, b_{j2}, g_{j0}, g_{j1}, K_1, j=1,2$  are obtained for the solution of (71) and the results (lines) are compared (Fig 14) with the solution (points) of (70) and (65).

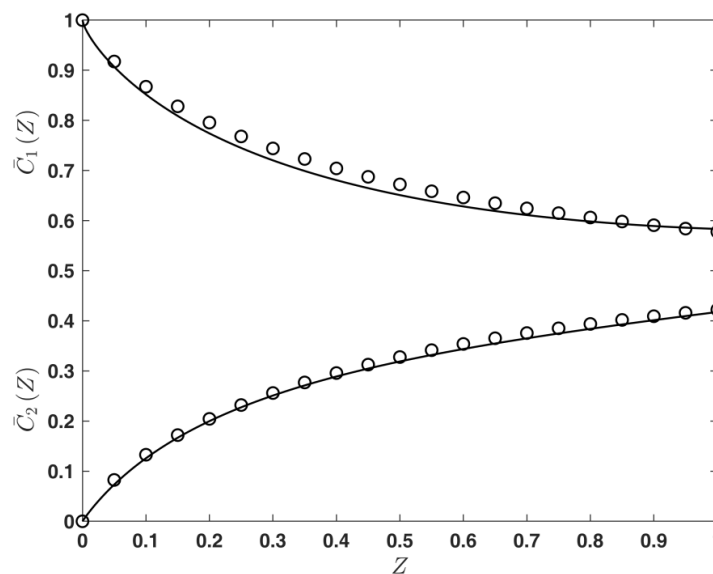


Fig. 14. Concentration distributions  $\bar{C}_j(Z), j=1,2$ : solution of (71) (lines); solution (points) of (70) and (65).



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## НОВ ПОДХОД ЗА МОДЕЛИРАНЕ И СИМУЛАЦИЯ НА ХИМИЧНИ И МАСОПРЕНОСНИ ПРОЦЕСИ В КОЛОННИ АПАРАТИ

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(Резюме)

Класическата теория на масопреенасяне не е приложима за моделиране на масопреенасянето при химически, абсорбционни, адсорбционни и каталитични процеси в колонни апарати, където разпределението на скоростите и междуфазовите граници са неизвестни. Моделирането на тези процеси е свързано със създаването на нов тип конвективно-дифузионни модели (за качествен анализ) и модели на средната концентрация (за количествен анализ), където повърхностните реакции са заменени с еквивалентна обемна реакция, а скоростта и разпределението на концентрациите са заменени със средна скорост и концентрации. Влиянието на радиалната неравномерност на скоростта в моделите на средната концентрация се въвежда чрез моделни параметри, които трябва да се определят експериментално. Новите конвекционно-дифузионни модели и тези на средната концентрация са получени в случаи на различни процеси в колонните апарати: прости и сложни химични реакции, физична и химична абсорбция, физична и химична адсорбция, хетерогенни каталитични процеси (физичен и химичен адсорбционен механизъм). Тези модели са представени в монографията на Хр. Бояджиев, М. Дойчинова, Б. Бояджиев, П. Попова-Крумова „Моделиране на процеси в колонни апарати”, второ издание, изд. Springer, Берлин-Хайделберг, 2018 г. Разгледани са две хидродинамични ситуации, когато радиалният скоростен компонент е равен на нула в случаите на аксиално модифициране на радиалната неравномерност на аксиалния скоростен компонент и когато радиалният скоростен компонент е различен от нула. Използването на експериментални данни за средните концентрации в края на колоната, за конкретен процес и колона, позволява да се получат параметрите на модела, свързани с радиалната неравномерност на скоростта. Стойностите на тези параметри позволяват да се използват модели на средната концентрация за моделиране на различни процеси.