

MASS TRANSFER IN COUNTER CURRENT FLOWS

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Abstract

A theoretical analysis of gas-liquid counter-current flow in laminar boundary layers with flat phase boundary based on similarity variables method has been done. The obtained numerical results for the energy dissipation, mass transfer rate and their ratio are compared with analogous results for co-current flows. A diffusion type of model is proposed for modeling of the mass transfer with chemical reaction in the column apparatuses in the cases of circulation zones. The presence of rising and descending flows (the change of the velocity direction) leads to using three coordinate systems. An iterative algorithm for the concentration distribution calculation is proposed. The influence of the zones breadths on the mass transfer efficiency in the column is investigated.

Key words: efficiency, mass transfer, velocity distribution, column apparatuses, circulation zones.

INTRODUCTION

Chemical technologies based on counter current flows in gas-liquid systems are widely encountered in practice. The analyses of such flows [1] reveal that there is a possibility to obtain asymptotic solutions for gas-liquid systems which are in agreement with the experimental data, obtained from thermoanemometrical measurements in the boundary layers. The correctness of the asymptotic method proposed in [1] was confirmed by numerical experiments concerning the exact solution of the problem [2]. The theoretical analysis of the counter current flow [3], for example, shows that it is a nonclassical problem of mathematical physics insufficiently discussed in the literature. The parabolic boundary value problem with changing direction of time [4, 5] is a typical problem of this type. It was shown in [3] that this nonclassical problem can be described as consisting of several classical subproblems.

The modelling problems in column apparatuses are result of the complicated hydrodynamic behaviour of the flows in the columns. The presence of different phases (gas, liquid and solid) lead to the necessity of a formulation of two or three phases hydrodynamic problem, where the equations at the face interphase (boundary conditions at the phase boundaries) are practically unknown. As a result the solution of the interphase mass transfer problem is not possible because the velocity function in the convection-diffusion equation is unknown.

For this purpose a convection-diffusion equation with volume reaction is used [6-9], where the convective transfer in the column apparatuses is a result of laminar or turbulent (large-scale pulsations) flows, while the diffusive transfer is molecular or turbulent (small-scale pulsations). The volume reaction is mass source (sink) as a result of chemical reactions or interphase mass transfer. This approach was used for modelling of airlift reactors [10, 11] and an airlift photobioreactor [12].

The theoretical analysis of the mass transfer with volume chemical reaction in the column apparatuses shows [13, 14] that process efficiency decrease as a result of the radial non-uniformity of the velocity distribution. This effect increase with the column radius increase and is named "scale effect".

In certain cases a change of the velocity direction exist [10-12, 15] and must be used different coordinate systems for convection-diffusion equation solution, because velocity must be positive only.

In some cases the change of the velocity direction is a result of the circulation flows in stagnation zone and the mass transfer efficiency decrease. The using of the diffusion type of models [6-9] permit to obtain the concentration distribution in these cases and the zones breadths influence on the mass transfer rate.

1 Velocity Distribution

The mathematical description of the counter current (see Fig. 1) flow in the boundary approximation is

$$\begin{aligned} u_j \frac{\partial u_j}{\partial x} + v_j \frac{\partial u_j}{\partial y} &= v_j \frac{\partial^2 u_j}{\partial y^2}, \quad \frac{\partial u_j}{\partial x} + \frac{\partial v_j}{\partial y} = 0, \quad j=1,2; \\ x=0, \quad y \geq 0, \quad u_1 &= u_1^\infty; \quad x=L, \quad y \leq 0, \quad u_2 = -u_2^\infty; \\ y \rightarrow \infty, \quad 0 \leq x \leq L, \quad u_1 &= u_1^\infty; \quad y \rightarrow -\infty, \quad 0 \leq x \leq l, \quad u_2 = -u_2^\infty; \\ y=0, \quad 0 < x < L, \quad u_1 &= u_2, \quad \mu_1 \frac{\partial u_1}{\partial y} = \mu_2 \frac{\partial u_2}{\partial y}, \quad v_1 = v_2 = 0. \end{aligned} \quad (1)$$

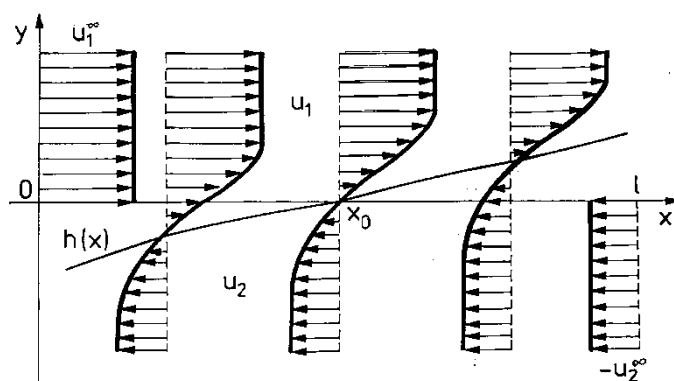


Fig. 1. Counter-current flow

Problem (1) can be represented in a dimensionless form using two different coordinate systems for the two phases. The flow in each phase is oriented along the longitudinal coordinate, which yields the following dimensionless variables and parameters:

$$\begin{aligned} x &= LX_1 = L - LX_2, \quad y = \delta_1 Y_1 = -\delta_2 Y_2, \\ u_1 &= u_1^\infty U_1, \quad v_1 = u_1^\infty \frac{\delta_1}{L} V_1, \quad u_2 = -u_2^\infty U_2, \quad v_2 = -u_2^\infty \frac{\delta_2}{L} V_2, \end{aligned}$$

$$\delta_j = \sqrt{\frac{v_j L}{u_j^\infty}}, \quad j=1,2, \quad \theta_1 = \frac{u_2^\infty}{u_1^\infty}, \quad \theta_2 = \left(\frac{\rho_1 \mu_1}{\rho_2 \mu_2} \right)^{\frac{1}{2}} \left(\frac{u_1^\infty}{u_2^\infty} \right)^{\frac{3}{2}}. \quad (2)$$

In the new coordinate systems, the model of counter current flows takes the form

$$\begin{aligned} U_j \frac{\partial U_j}{\partial X_j} + V_j \frac{\partial U_j}{\partial Y_j} &= \frac{\partial^2 U_j}{\partial Y_j^2}, \quad \frac{\partial U_j}{\partial X_j} + \frac{\partial V_j}{\partial Y_j} = 0; \\ X_j = 0, \quad U_j = 1; \quad Y_j \rightarrow \infty, \quad U_j = 1; \\ Y_1 = Y_2 = 0, \quad U_1 = -\theta_1 U_2, \quad \theta_2 \frac{\partial U_1}{\partial Y_1} &= \frac{\partial U_2}{\partial Y_2}, \quad V_j = 0; \quad j=1,2. \end{aligned} \quad (3)$$

Problem (3) cannot be solved directly, because the velocities $U_i (i=1,2)$ change their directions within the ranges $0 \leq X_i \leq 1$, $0 \leq Y_i < \infty$, $(i=1,2)$. This nonclassical problem of mathematical physics can be converted to a classical one by introduction of the following similarity variables:

$$U_j = f_j', \quad V_j = \frac{1}{2\sqrt{X_j}} (\eta_j f_j' - f_j), \quad f_j = f_j(\eta_j), \quad \eta_j = \frac{Y_j}{\sqrt{X_j}}. \quad (4)$$

The substitution of (4) into (3) yields

$$\begin{aligned} 2f_j''' + f_j f_j'' &= 0, \quad f_j(0) = 0, \quad f_j(\infty) = 1, \quad j=1,2, \\ f_1'(0) &= -\theta_1 f_2'(0), \quad \theta_2 \sqrt{\frac{X_2}{X_1}} f_1''(0) = f_2''(0), \quad X_1 + X_2 = 1. \end{aligned} \quad (5)$$

It is obvious from (5) that problem (3) has no solution in similarity variables.

However, problem (5) can be solved after the introduction of new parameter $\bar{\theta}_2$ for each $X_1 \in (0,1)$:

$$\bar{\theta}_2 = \theta_2 \sqrt{\frac{1-X_1}{X_1}}. \quad (6)$$

Hence, the problem has a local similarity solution. In this way problem (5) is substituted by several separate problems for each $X_1 \in (0,1)$.

The solutions of these separate problems can be obtained after the introduction of the function

$$F(a, b) = \int_6^7 (f_1' - 1)^2 d\eta_1 + \int_6^7 (f_2' - 1)^2 d\eta_2, \quad a = f_1'(0), \quad b = f_1''(0). \quad (7)$$

The solution of (5) for each $X_1 \in (0, 1)$ is obtained after searching for the minimum of the function $F(a, b)$. At each step of the minimization procedure, the boundary problem has to be solved:

$$2f_j''' + f_j f_j'' = 0, \quad f_j(0) = 0, \quad j = 1, 2, \quad f_1'(0) = a, \quad f_2'(0) = -\frac{a}{\theta_1}, \quad f_1''(0) = b, \quad f_2''(0) = \bar{\theta}_2 b. \quad (8)$$

Problem (8) was solved numerically for counter current gas and liquid flows for the following parameters values: $\theta_1 = 0.1$ and $\theta_2 = 0.152$. In accordance with the requirement for a minimum of $F(a, b)$ in (7), the boundary conditions a, b and $F(a, b)$ were determined [2].

The energy dissipated in the laminar boundary layer [16, 17] is described for both phases by the equations

$$e_j = \mu_j \int_0^l \int_0^{(-1)^{j+1}} \left(\frac{\partial u_j}{\partial y} \right)^2 dx dy, \quad E_j = - \int_0^1 \int_0^\infty \left(\frac{\partial U_j}{\partial Y_j} \right)^2 dY_j dX_j, \quad E_j = \frac{e_j \sqrt{u_j^\infty l / \nu_i}}{\nu_i \rho_i u_j^{\infty 2}}, \quad j = 1, 2. \quad (9)$$

For gas-liquid counter current flows, the introduction of similarity variables leads to

$$E_j = \int_0^1 \frac{1}{\sqrt{X_j}} \left[\int_0^\infty (f_j'')^2 d\eta_j \right] dX_j, \quad j = 1, 2. \quad (10)$$

In the case of co-current flows, the function f_j^{**} does not depend on X_j and for energy dissipation one can obtain

$$E_j^* = 2 \int_0^\infty (f_i^{**})^2 d\eta_i, \quad i = 1, 2. \quad (11)$$

Here $f_j^*(i = 1, 2)$ is the solution of equations (8) with boundary conditions for co-current flows:

$$\theta_1^* = -0.1, \quad \theta_2^* = \theta_2 = 0.152, \quad f_1'^*(0) = 0.0908, \quad f_1''^*(0) = 0.32765. \quad (12)$$

The comparison of the energy dissipated in the laminar boundary layer [16, 17] for the case of gas–liquid counter current and co-current flows is shown in Table 1. These results reveal that the energy dissipation for the gas phase in co-current flows is lower than that in counter current flows, whereas in the liquid phase there are no significant changes.

2 Concentration Distribution

The mathematical model of mass transfer in gas–liquid systems with counter current flow in a laminar boundary layer with a flat phase boundary takes the following form:

$$\begin{aligned} u_j \frac{\partial c_j}{\partial x} + v_j \frac{\partial c_j}{\partial y} &= D_j \frac{\partial^2 c_j}{\partial y^2}, \quad j=1,2; \\ x=0, \quad y \geq 0, \quad c_1 &= c_1^\infty; \quad x=L, \quad y \leq 0, \quad c_2 = c_2^\infty; \\ y \rightarrow \infty, \quad 0 \leq x \leq L, \quad c_1 &= c_1^\infty; \quad y \rightarrow -\infty, \quad 0 \leq x \leq L, \quad c_2 = c_2^\infty; \\ y=0, \quad 0 < x < L, \quad c_1 &= \chi c_2, \quad D_1 \frac{\partial c_1}{\partial y} = D_2 \frac{\partial c_2}{\partial y}. \end{aligned} \quad (13)$$

Here u_j and v_j ($j=1,2$) are the velocity components in the gas and in the liquid phase determined by the solution of (8).

The solution of (13) was performed [18] by introducing the following similarity variables:

$$\begin{aligned} \eta_j &= (-1)^{j+1} y \sqrt{\frac{u_j^\infty}{v_j L X_j}}, \quad X_1 = \frac{x}{L}, \quad X_2 = \frac{L-x}{L}, \quad X_1 + X_2 = 1, \\ u_j &= (-1)^{j+1} u_j^\infty f_j', \quad v_j = (-1)^{j+1} \frac{1}{2} \sqrt{\frac{v_j u_j^\infty}{L X_j}} (\eta_j f_j' - f_j), \quad f_j = f_j(\eta_j), \\ c_j &= c_j^\infty - \chi^{1-j} (c_1^\infty - \chi c_2^\infty) \psi_j, \quad \psi_j = \psi_j(\eta_j), \quad j=1,2. \end{aligned} \quad (14)$$

The substitution of equations (14) into equations (13) leads to

$$2f_j''' + f_j f_j'' = 0, \quad 2\psi_j'' + Sc_j f_j \psi_j' = 0, \quad j=1,2,$$

$$\begin{aligned} f_1(0) = 0, \quad f_1'(0) = a, \quad f_1''(0) = b, \quad f_2(0) = 0, \quad f_2'(0) = -\frac{a}{\theta_1}, \quad f_2''(0) = \bar{\theta}_2 b, \\ \psi_1(0) + \psi_2(0) = 1, \quad \bar{\theta}_3 \psi_1'(0) = \psi_2'(0), \quad \psi_j(\infty) = 0, \quad j = 1, 2, \end{aligned} \quad (15)$$

where

$$\begin{aligned} Sc_j = \frac{\nu_j}{D_j} \quad (j=1,2), \quad \theta_1 = \frac{u_2^\infty}{u_1^\infty}, \quad \theta_2 = \left(\frac{\rho_1 \mu_1}{\rho_2 \mu_2} \right)^{\frac{1}{2}} \left(\frac{u_1^\infty}{u_2^\infty} \right)^{\frac{3}{2}}, \\ \bar{\theta}_2 = \theta_2 \sqrt{\frac{X_2}{X_1}}, \quad \theta_3 = \chi \frac{D_1}{D_2} \sqrt{\frac{u_1^\infty \nu_2}{u_2^\infty \nu_1}}, \quad \bar{\theta}_3 = \theta_3 \sqrt{\frac{X_2}{X_1}}. \end{aligned} \quad (16)$$

The boundary conditions a and b are determined by (8).

Obviously, it is evident from (15) that it is possible to develop a similarity solution for different values of $X_1 = 1 - X_2$.

The solution of (15) was carried out [45] under new boundary conditions for ψ_j ($j = 1, 2$):

$$\psi_1(0) = \alpha, \quad \psi_1'(0) = \beta, \quad \psi_2(0) = 1 - \alpha, \quad \psi_2'(0) = \bar{\theta}_3 \beta. \quad (17)$$

Here α and β are determined for different values of $X_1 = 1 - X_2$, so the conditions $\psi_j(\infty) = 0$, ($j = 1, 2$) have to be satisfied.

The Sherwood number may be obtained as

$$Sh_j = -\sqrt{Re_j} \int_0^1 \frac{\psi_j'(0)}{\sqrt{X_j}} dX_j, \quad Re_j = \frac{u_j^\infty L}{\nu_j}, \quad j = 1, 2. \quad (18)$$

The dimensionless diffusive flux has the form

$$J_j = -\int_0^1 \frac{\psi_j'(0)}{\sqrt{X_j}} dX_j, \quad j = 1, 2. \quad (19)$$

3 Comparison between Co-current and Counter current Flows

The comparison between the mass transfer rates in the counter current and the co-current flow modes will be performed by solving equation (15) with parameters corresponding to the case of co-current flow, namely,

$$\begin{aligned} \theta_1 &= -0.1, \quad \theta_2 = 0.152, \quad f_1'(0) = 0.0908, \quad f_1''(0) = 0.37265, \\ \bar{\theta}_3 &= \theta_3, \quad J_j^* = -2\psi_j'(0), \quad j=1, 2. \end{aligned} \quad (20)$$

The results obtained for J_j^* ($j=1, 2$) are summarized in Table 1. These results definitely indicate that with the co-current flow the mass transfer rate is higher than that exhibited under the counter current flow conditions.

The numerical results allow us to determine the ratio (A) between the mass transfer rate (Sh) and the corresponding energy dissipation (E) with both flow modes, namely,

$$A_i = \frac{Sh_i}{E_i}, \quad A_i^* = \frac{Sh_i^*}{E_i^*}, \quad i=1, 2. \quad (21)$$

The data summarized in Table 1 indicate the better performance of the co-current flow mode with a higher mass transfer rate per unit energy dissipation required to perform the process. This theoretical analysis shows that the linear mass transfer theory permits us to predict the mass transfer resistance distribution in two-phase systems. In the diffusion boundary layer approximation, the mass transfer is governed by the parameter χ/ε_0 . The process is limited by the mass transfer in the first phase if $\chi/\varepsilon_0 \geq 10^2$; if $\chi/\varepsilon_0 \leq 10^{-2}$ the process is limited by the mass transfer in the second phase. The diffusion resistances are of the same order of magnitude if $\chi/\varepsilon_0 \sim 1$. In the film theory mass transfer approximation, the theory reveals that χ is the only governing parameter.

Table 1 Comparison between counter current and co-current flows

$\theta_3 = 0$		$\theta_3 \rightarrow \infty$		$\theta_3 = 1$			
J_1	J_1^*	J_2	J_2^*	J_1	J_1^*	J_2	J_2^*
0.554	0.720	4.380	4.822	0.432	0.626	0.432	0.626
A_1	A_1^*	A_2	A_2^*	A_1	A_1^*	A_2	A_2^*
1.06	1.57	739	750	0.82	1.37	72.8	97.3
E_1	E_1^*	E_2	E_2^*	E_1	E_1^*	E_2	E_2^*
0.525	0.458	0.00593	0.00643	0.525	0.458	0.01328	0.00643

The results obtained so far represent the linear mass transfer theory in the boundary layer approximation with a flat phase boundary. Such problems (the linear mass transfer theory) can be solved in similar manners (in the boundary layer approximation) with conditions imposed by different forms of the interphase surface (wavy, spherical, cylindrical, and other shapes) in processes involving film flows, droplets, bubbles, jets, etc.

4. On the scale effect and scale – up in the column apparatuses with circulation zones

Let's consider fluid motion in a column with radius R_0 , where the concentration of the fluid components decrease as a result of first order chemical reaction. The presence of solid barriers (see Fig.1) leads to circulation zone. As a mathematical model of the concentration distribution $c(r, z)$ in the column will be used convection–diffusion equation:

$$u \frac{\partial c}{\partial z} = D \left(\frac{\partial^2 c}{\partial z^2} + \frac{1}{r} \frac{\partial c}{\partial r} + \frac{\partial^2 c}{\partial r^2} \right) - kc \quad (22)$$

The solution of this equation is possible if the velocity distribution $u(r, z)$ is positive.

The change of the velocity direction (see Fig.2) lead to solution of Eq.(22) in different zone in the column: $0 \leq r \leq r_0$ ($u_1(r, z) \geq 0$) and $r_0 \leq r \leq R_0$ ($u_2(r, z) \leq 0$), where:

$$u = u_1(r) = \bar{u} \left(2 - 2 \frac{r^2}{r_0^2} \right), \quad u = u_2(r) = A \left[r_0^2 - r^2 + \frac{R_0^2 - r_0^2}{\ln(R_0/r_0)} \ln(r/r_0) \right] \quad (23)$$

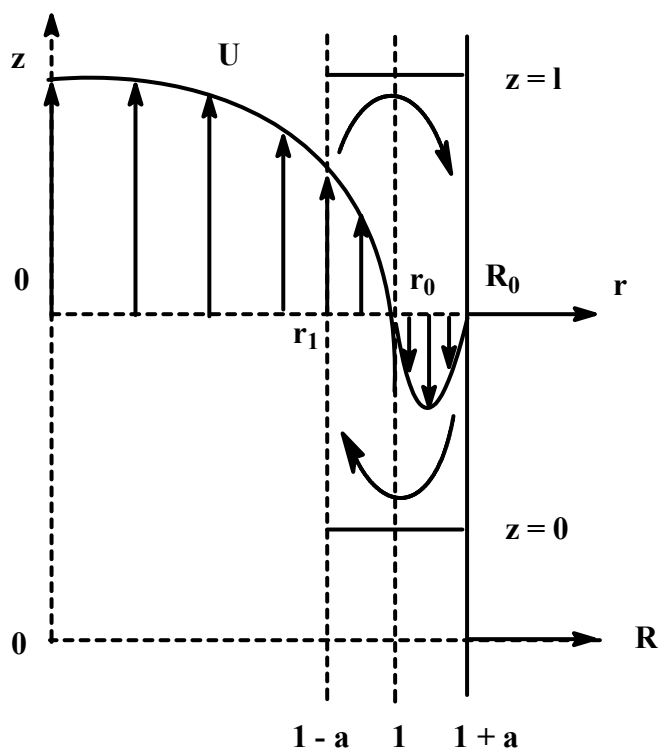


Fig.2 Circulation zones in column apparatuses

The parameter A must be obtained from the physical condition in the circulation zone, where the absolute values of the average velocities in the zones $r_1 \leq r \leq r_0$ and $r_0 \leq r \leq R_0$ are equals:

$$A = \frac{2\bar{u}(2a - a^2)}{\left[R_0^2 + r_0^2 - \frac{R_0^2 - r_0^2}{\ln(R_0/r_0)} \right]}, \quad (R_0 - r_0)/r_0 = a, \quad (24)$$

where $2ar_0$ is the breadth of the stagnation zone.

From Eqs.(23) is possible to be obtained the average velocities $\bar{u}_1$ and $\bar{u}_2$:

$$\bar{u}_1 = \bar{u}, \quad \bar{u}_2 = \frac{2}{R_0^2 - r_0^2} \int_{r_0}^{R_0} r u_2(r) dr = \frac{A}{2} \left[R_0^2 + r_0^2 - \frac{R_0^2 - r_0^2}{\ln(R_0/r_0)} \right] = \bar{u}(2a - a^2) \quad (25)$$

and dimensionless form of the velocities distributions:

$$U_1(R) = 2 - 2R^2, \quad U_2(R) = \frac{2(2a - a^2) \left[1 - R^2 + \frac{2a + a^2}{\ln(1+a)} \ln R \right]}{2 + 2a + a^2 - \frac{2a + a^2}{\ln(1+a)}}, \quad (26)$$

where

$$R = \frac{r}{r_0}, \quad \frac{R_0}{r_0} = 1 + a, \quad U_1(R) = \frac{u_1(r)}{\bar{u}}, \quad U_2(R) = \frac{u_2(r)}{\bar{u}} \quad (27)$$

The velocity distributions $U_1(R)$ and $U_2(R)$ are shown in the Fig.3.

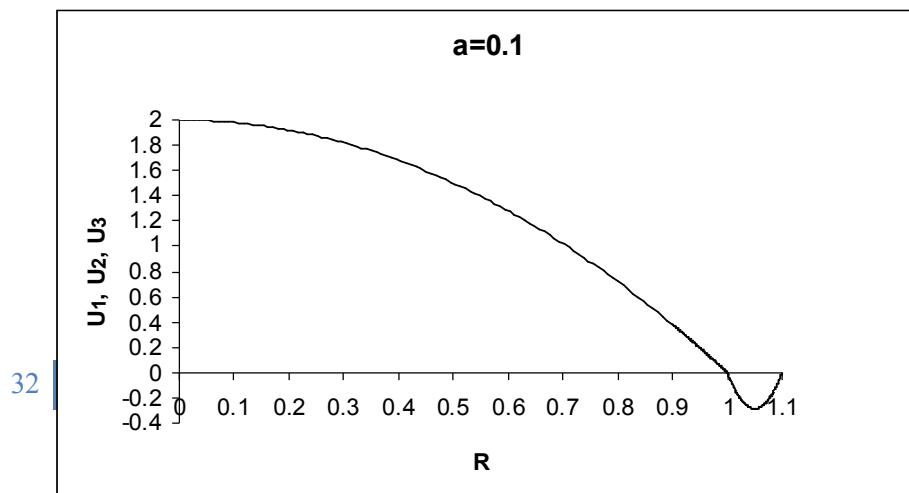


Fig. 3 Velocity distribution at $a=0.1$

The sign change of the velocity at $r = r_0$ lead to necessity the problem Eq.(22) to be presented in three problems in two coordinate systems (r, z_1) and (r, z_2) , where $z_1 + z_2 = l$ and l is the circulation zone height:

$$\begin{aligned}
 & \mathbf{1.} \quad u_1 \frac{\partial c_1}{\partial z_1} = D \left(\frac{1}{r} \frac{\partial c_1}{\partial r} + \frac{\partial^2 c_1}{\partial r^2} \right) - kc_1, \\
 & \quad (0 \leq r \leq r_1, 0 \leq z_1 \leq l, u_1 = u_1(r), c_1 = c_1(r, z_1)) \\
 & \quad z_1 = 0, c_1 = \bar{c}_0; \quad r = 0, \frac{\partial c_1}{\partial r} = 0; \quad r = r_1, c_1 = c_2, \frac{\partial c_1}{\partial r} = \frac{\partial c_2}{\partial r}. \\
 & \mathbf{2.} \quad u_1 \frac{\partial c_2}{\partial z_1} = D \left(\frac{1}{r} \frac{\partial c_2}{\partial r} + \frac{\partial^2 c_2}{\partial r^2} \right) - kc_2, \\
 & \quad (r_1 \leq r \leq r_0, 0 \leq z_1 \leq l, u_1 = u_1(r), c_2 = c_2(r, z_1)) \\
 & \quad z_1 = 0, c_2 = (\bar{c}_3)_{z_2=l}; \quad r = r_1, c_1 = c_2, \frac{\partial c_1}{\partial r} = \frac{\partial c_2}{\partial r}; \quad r = r_0, c_2 = c_3, \frac{\partial c_2}{\partial r} = \frac{\partial c_3}{\partial r}. \\
 & \mathbf{3.} \quad u_2 \frac{\partial c_3}{\partial z_2} = D \left(\frac{1}{r} \frac{\partial c_3}{\partial r} + \frac{\partial^2 c_3}{\partial r^2} \right) - kc_3, \\
 & \quad (r_0 \leq r \leq R_0, 0 \leq z_2 \leq l, u_2 = u_2(r), c_3 = c_3(r, z_2)) \\
 & \quad z_2 = 0, c_3 = (\bar{c}_2)_{z_1=l}; \quad r = r_0, c_2 = c_3, \frac{\partial c_2}{\partial r} = \frac{\partial c_3}{\partial r}, \quad r = R_0, \frac{\partial c_3}{\partial z} = 0. \tag{28}
 \end{aligned}$$

In Eqs. (28) $(\bar{c}_2)_{z_1=l}$ and $(\bar{c}_3)_{z_2=l}$ are the average concentrations:

$$(\bar{c}_2)_{z_1=l} = \frac{2}{r_0^2 - r_1^2} \int_{r_1}^{r_0} r c_2(r, l) dr, \quad (\bar{c}_3)_{z_2=l} = \frac{2}{R_0^2 - r_0^2} \int_{r_0}^{R_0} r c_3(r, l) dr \tag{29}$$

The solution of the problem Eqs.(28) permits to obtain the column mass transfer efficiency q in the case of circulation zone:

$$q = \bar{u}_1^{(0)} \bar{c}_0 - \frac{2}{r_1^2} \int_0^{\eta} r u_1 c_1(r, l) dr, \quad \bar{u}_1^{(0)} = \frac{2}{r_1^2} \int_0^{\eta} r u_1(r) dr = \bar{u} (1 + 2a - a^2), \quad (30)$$

where $\bar{u}_1^{(0)}$ is the average velocity of the convective mass flux in column with solid barriers.

Dimensionless problem solution

For the solution of Eqs.(28) must be used dimensionless variables:

$$r = r_0 R, \quad z = l Z_1 = l Z_2, \quad Z_1 + Z_2 = 1, \\ c_1 = \bar{c}_0 C_1(R, Z_1), \quad c_2 = \bar{c}_0 C_2(R, Z_1), \quad c_3 = \bar{c}_0 C_3(R, Z_2). \quad (31)$$

Introducing Eqs. (31) into Eqs. (28), lead to the next set of equations:

$$U_1 \frac{\partial C_1}{\partial Z_1} = Fo \left(\frac{1}{R} \frac{\partial C_1}{\partial R} + \frac{\partial^2 C_1}{\partial R^2} \right) - Da C_1 \quad (0 \leq R \leq 1-a) \\ Z_1 = 0, \quad C_1 = 1; \quad R = 0, \quad \frac{\partial C_1}{\partial R} = 0; \\ R = 1-a, \quad \frac{\partial C_1}{\partial R} = \delta_1(Z_1), \quad \delta_1(Z_1) = \frac{\partial C_2}{\partial R}. \quad (32) \\ U_1 \frac{\partial C_2}{\partial Z_1} = Fo \left(\frac{1}{R} \frac{\partial C_2}{\partial R} + \frac{\partial^2 C_2}{\partial R^2} \right) - Da C_2 \quad (1-a \leq R \leq 1) \\ Z_1 = 0, \quad C_2 = \alpha_2, \quad \alpha_2 = \frac{2}{2a+a^2} \int_1^{1+a} R C_3(R, 1) dR; \\ R = 1-a, \quad C_2(R, Z_1) = C_1(R, Z_1); \\ R = 1, \quad \frac{\partial C_2}{\partial Z_1} = \delta_2(Z_1), \quad \delta_2(Z_1) = \left(\frac{\partial C_3}{\partial Z_2} \right)_{Z_2=1-Z_1}. \quad (33) \\ U_2 \frac{\partial C_3}{\partial Z_2} = Fo \left(\frac{1}{R} \frac{\partial C_3}{\partial R} + \frac{\partial^2 C_3}{\partial R^2} \right) - Da C_3 \quad (1 \leq R \leq 1+a) \\ Z_2 = 0, \quad C_3 = \alpha_3, \quad \alpha_3 = \frac{2}{a} \int_{1-a}^1 R C_2(R, 1) dR;$$

$$R=1, C_3 = \delta_3, \delta_3(Z_2) = (C_2)_{Z_1=1-Z_2};$$

$$R=1+a, \frac{\partial C_3}{\partial R} = 0, \quad (34)$$

where Fo and Da are similar to the Fourier and Damkohler numbers:

$$Fo = \frac{Dl}{\bar{u}r_0^2}, \quad Da = \frac{kl}{\bar{u}}. \quad (35)$$

The column mass transfer efficiency Eq. (30) in dimensionless variables is:

$$Q = \frac{q}{u_1^{(0)} \bar{c}_0} = 1 - \frac{4}{(1-a)^2(1+2a-a^2)} \int_0^{1-a} R(1-R^2) C_1(R,1) dR. \quad (36)$$

The solution of the problem Eqs. (32-34) is possible to be obtained consecutively using the next algorithm:

1. The problem (32) is possible to be solved independently if put $\delta_1(Z_1) \equiv 0$. As a result the concentration $C_1(R, Z_1)$ is obtained.
2. The problem (33) is possible to be solved independently if put $\alpha_2 = 0$ and $\delta_2(Z_1) \equiv 0$. As a result are obtained the concentration $C_2(R, Z_1)$, $\delta_1(Z_1) = \left(\frac{\partial C_2}{\partial R} \right)_{R=1-a}$, $\delta_3(Z_2) = C_2(1, Z_1)$ (where $Z_1 = 1 - Z_2$) and $\alpha_3 = \frac{2}{2a-a^2} \int_{1-a}^1 RC_2(R,1) dR$.
3. The problem Eqs.(34) is possible to be solved independently if put $\alpha_2 = 0$ and $\delta_2(Z_1) \equiv 0$. As a result are obtained the concentration $C_3(R, Z_2)$, $\delta_2(Z_1) = \left(\frac{\partial C_3}{\partial Z_2} \right)_{R=1, Z_2=1-Z_1}$ and $\alpha_2 = \frac{2}{2a+a^2} \int_1^{1+a} RC_3(R,1) dR$.

The obtained initial approximations permit to make the next step of the algorithm:

4. Solution of Eqs. (32) and determination of $C_1(R, Z_1)$.
5. Solution of Eqs. (33) and determination of $C_2(R, Z_1)$ and α_3 .
6. Solution of Eqs. (34) and determination of $C_3(R, Z_2)$ and α_2, δ_2 and continue from 4.

The criterion of the iterative procedure stopping is the minimization of the difference (P_0) between concentration distributions of two consecutive iterations:

$$P_0 = \int_0^{1-a} (C_1^i - C_1^{i-1})^2 dR + \int_{1-a}^1 (C_2^i - C_2^{i-1})^2 dR + \int_1^{1+a} (C_3^i - C_3^{i-1})^2 dR.$$

The comparison of the results in the Fig.3 shows that the concentration distributions after the fourth iteration satisfy the differential equations and boundary conditions Eqs. (32-34) and the criterion of the iterative procedure stopping is $P_0 \leq 10^{-5}$. The same results are obtained in the cases: $a=0.05$, $a=0.13$, $a=0.15$ and in the Figs. 5a,b,c,d are shown the concentration distributions in the cases of a : a) $a=0.05$, b) $a=0.1$, c) $a=0.13$, d) $a=0.15$, at different cross section's areas $-Z=0.1$ ($Z_I=0.9$), $Z=0.3$ ($Z_I=0.7$), $Z=0.5$ ($Z_I=0.5$), $Z=0.7$ ($Z_I=0.3$), $Z=0.9$ ($Z_I=0.1$).

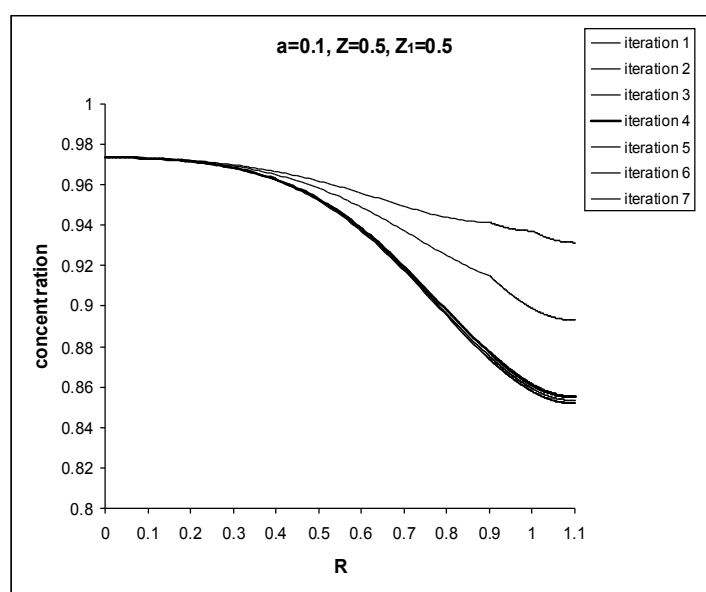
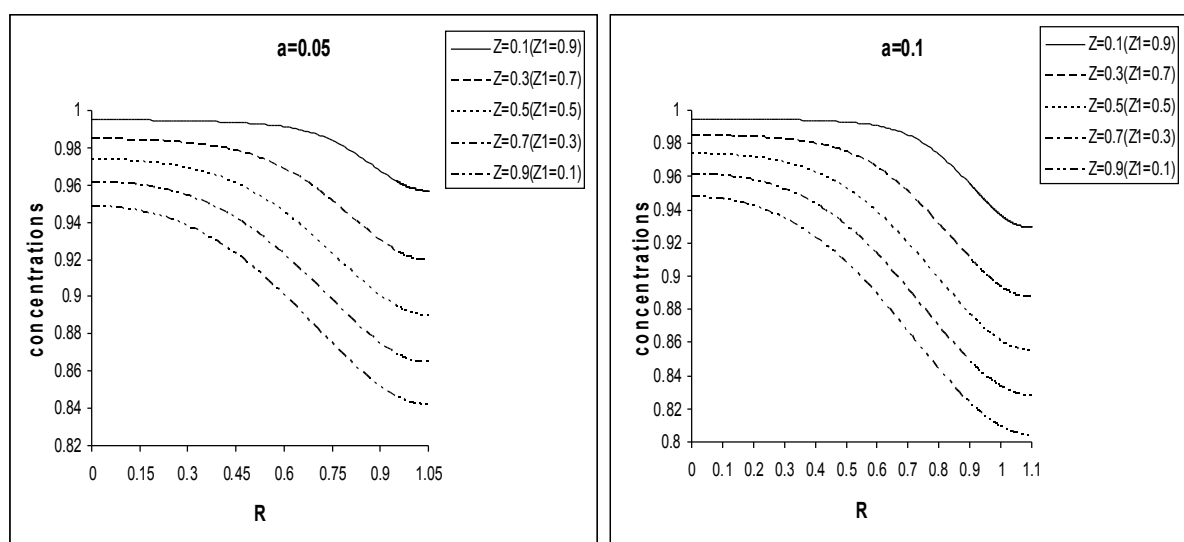


Fig. 4. Concentration distributions at different iterations, obtained from Eqs. (32-34)



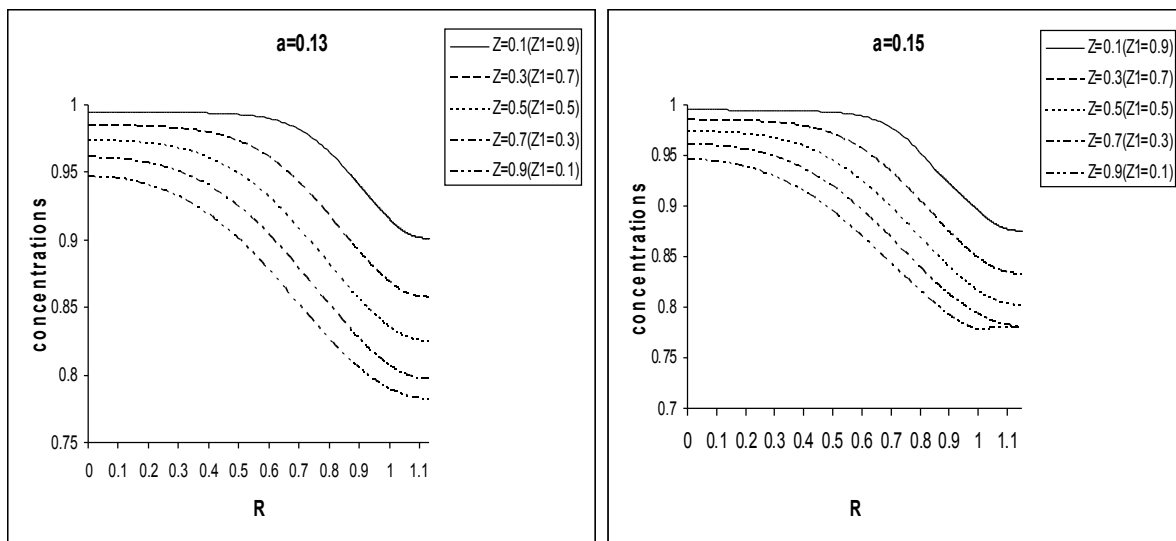


Fig.5c. Concentration distributions at different height of the column, when $a=0.13$

Fig.5d. Concentration distributions at different height of the column, when $a=0.15$

The influence of the stagnation zone breadths on the concentration distributions is shown in the Fig.6.

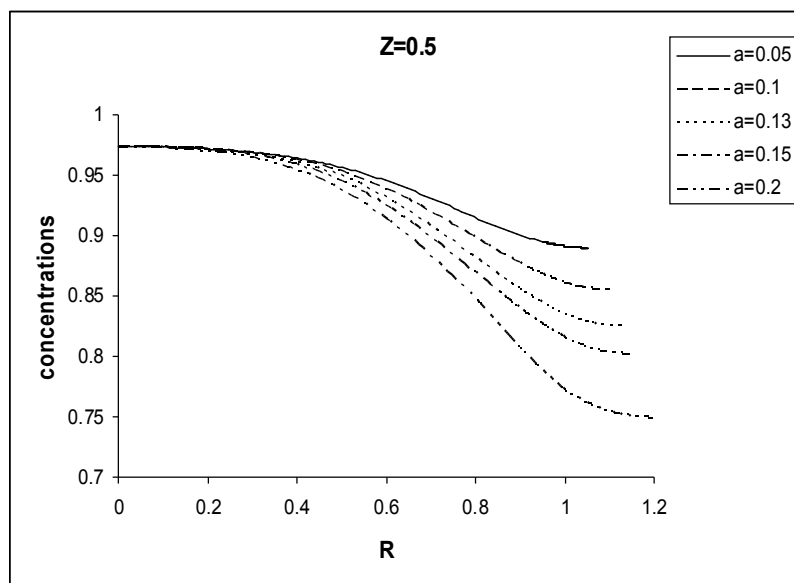


Fig. 6 Comparison of the concentration distributions for different stagnation zone breadths.

The fluid flow rate in the column with barriers is:

$$W = \bar{u}_1^{(0)} \pi r_1^2 = \bar{u}_0 \pi R_0^2,$$

where $\bar{u}_0$ is the average velocity in the column in the absence of the barriers and the flow is Poiseuille type:

$$\bar{u}_0 = \bar{u} (1 + 2a - a^2) \frac{(1-a)^2}{(1+a)^2}.$$

The velocity distribution in column without barriers is:

$$u_0 = 2\bar{u}_0 \left(1 - \frac{r^2}{R_0^2} \right) = 2\bar{u} (1 + 2a - a^2) \frac{(1-a)^2}{(1+a)^2} \left(1 - \frac{r^2}{R_0^2} \right).$$

The convection-diffusion equation in the case of absence of the barriers is possible to be obtained from (22) if replace $u = u_0$ and $c = c_0$:

$$u_0 \frac{\partial c_0}{\partial z} = D \left(\frac{\partial^2 c_0}{\partial z^2} + \frac{1}{r} \frac{\partial c_0}{\partial r} + \frac{\partial^2 c_0}{\partial r^2} \right) - k c_0 \quad (37)$$

with boundary conditions:

$$z = 0, c_1 = \bar{c}_0; \quad r = 0, \frac{\partial c_0}{\partial r} = 0; \quad r = R_0, \frac{\partial c_0}{\partial r} = 0. \quad (38)$$

The introducing of the dimensionless variable

$$r = r_0 R, \quad z = l Z, \quad c_0 = \bar{c}_0 C_0(R, Z), \quad u_0(r) = \bar{u} U_0(R), \quad (39)$$

leads to:

$$\begin{aligned}
 U_0 \frac{\partial C_0}{\partial Z_1} &= Fo \left(\frac{1}{R} \frac{\partial C_0}{\partial R} + \frac{\partial^2 C_0}{\partial R^2} \right) - Da C_0 \\
 Z = 0, C_0 &= 1; R = 0, \frac{\partial C_0}{\partial R} = 0; \\
 R = 1 + a, \frac{\partial C_0}{\partial R} &= 0.
 \end{aligned} \tag{40}$$

where

$$U_0(R) = (1 + 2a - a^2) \left(\frac{1-a}{1+a} \right)^2 \left[2 - \frac{2}{(1+a)^2} R^2 \right]. \tag{41}$$

The mass transfer efficiency in this case is possible to be presented as

$$q_0 = \bar{u}_0 \bar{c}_0 - \frac{2}{R_0^2} \int_0^{R_0} r u_0 c_0 dr \tag{42}$$

and in dimensionless form:

$$Q_0 = \frac{q_0}{\bar{u}_0 \bar{c}_0} = 1 - \frac{4}{(1+a)^2} \int_0^{1+a} R \left(1 - \frac{1}{(1+a)^2} R^2 \right) C_0(R,1) dR. \tag{43}$$

Let's consider the effect of the parameter a (who is related with the breadth of the stagnation zone) on the process efficiency in column and comparing it with process efficiency in column without stagnation zones and Poiseuille flow.

In the Table 2 are shown comparison results of the process efficiency (degree of the conversion) in column with (Q) and without (Q_0) stagnation zones (circulation flows as a result of the barriers) and relative column efficiency decrease (ΔQ) as a result of the stagnation zones:

$$\Delta Q = \frac{Q_0 - Q}{Q_0}. \tag{44}$$

The relative stagnation zone volume, with respect to the column volume

$$\Delta W = \frac{(R_0 - r_1)^2}{R_0^2} = \frac{4a^2}{(1+a)^2} \quad (45)$$

and the relative influence of the stagnation zone volume on the column efficiency $\frac{\Delta Q}{\Delta W}$ are demonstrated in Table 2:

Table 2 Process efficiency in column with (Q) and without (Q_0) stagnation zones, relative column efficiency (ΔQ) and relative stagnation zone volume (ΔW).

a	Q_0	Q	ΔQ	ΔW	$\Delta Q/\Delta W$
0.05	0.1042	0.0865	0.1699	0.009	18.67
0.10	0.1165	0.0803	0.3107	0.033	9.39
0.13	0.1253	0.0770	0.3855	0.053	7.29
0.15	0.1317	0.0751	0.4298	0.068	6.31
0.20	0.1502	0.0707	0.5293	0.111	4.76

The proposed method for modeling of the mass transfer in column apparatuses with change of the velocity sign permit to analyze the influence of the stagnation zones on the mass transfer processes efficiency in column apparatuses.

The results obtained show, that the increase of the stagnation zone breadth lead to the column efficiency Q decrease, while Q_0 increase as a result of the average velocity $\bar{u}_0$ decrease. The relative stagnation zone volume ΔW increase lead to the relative column efficiency ΔQ increase, while the relative influence of the stagnation zone volume on the column efficiency $\frac{\Delta Q}{\Delta W}$ decreases.

The elimination of the negative effect of the stagnation zone is possible on the base of very well distribution of the solid particles (filling or catalyzer particles) in the column volume or absence of solid barriers in the empty columns.

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