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ON THE SCALE EFFECT AND SCALE – UP IN THE COLUMN APPARATUSES. 3. CIRCULATION ZONES

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Abstract

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.

Keywords: *column apparatuses, mass transfer, velocity distribution, circulation zones*.

1. INTRODUCTION

The modeling 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 [1-4], 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 modeling of airlift reactors [5,6] and an airlift photobioreactor [7].

The theoretical analysis of the mass transfer with volume chemical reaction in the column apparatuses shows [8, 9] 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 [5-7,10] 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 [1-4] permit to obtain the concentration distribution in these cases and the zones breadths influence on the mass transfer rate.

2. MATHEMATICAL MODEL

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:

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

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

The change of the velocity direction (see Fig.1) lead to solution of Eq.(1) in different zone in the column: $0 \le r \le r_0$ ($u_1(r,z) \ge 0$) and $r_0 \le r \le R_0$ ($u_2(r,z) \le 0$), where:

$$u = u_1(r) = \bar{u}\left(2 - 2\frac{r^2}{r_0^2}\right),$$

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

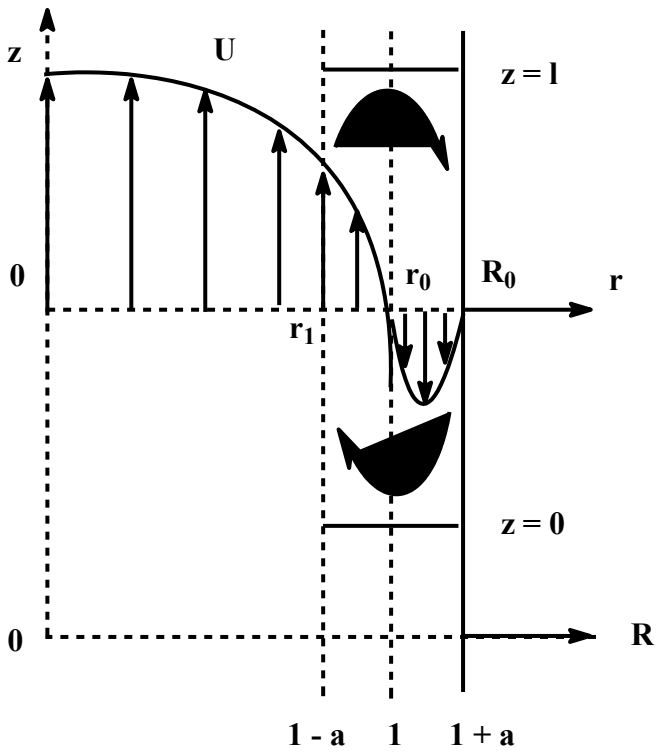

Fig.1 Circulation zones in column apparatuses

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 $r_1 \le r \le r_0$ and $r_0 \le r \le R_0$ are equals:

$$A = \frac{2\bar{u}\left(2a - a^2\right)}{\left[R_0^2 + r_0^2 - \dfrac{R_0^2 - r_0^2}{\ln\left(R_0 / r_0\right)}\right]}, \qquad (R_0 - r_0)/r_0 = a, \tag{3}$$

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

From Eqs.(2) is possible to be obtained the average velocities $\bar{u}_1$ and $\bar{u}_2$:

$$\bar{u}_1 = \bar{u}, \qquad \bar{u}_2 = \frac{2}{R_0^2 - r_0^2}\int_{r_0}^{R_0} r\,u_2(r) = \frac{A}{2}\left[R_0^2 + r_0^2 - \frac{R_0^2 - r_0^2}{\ln\left(R_0 / r_0\right)}\right] = \bar{u}\left(2a - a^2\right) \tag{4}$$

and dimensionless form of the velocities distributions:

$$U_1(R) = 2 - 2R^2, \qquad U_2(R) = \frac{2\left(2a - a^2\right)\left[1 - R^2 + \dfrac{2a + a^2}{\ln(1+a)}\ln R\right]}{2 + 2a + a^2 - \dfrac{2a + a^2}{\ln(1+a)}}, \tag{5}$$

where

$$R = \frac{r}{r_0}, \quad \frac{R_0}{r_0} = 1 + a, \quad U_1(R) = \frac{u_1(r)}{\bar{u}}, \quad U_2(R) = \frac{u_2(r)}{\bar{u}} \tag{6}$$

The velocity distributions $U_1(R)$ and $U_2(R)$ are shown in the Fig.2.

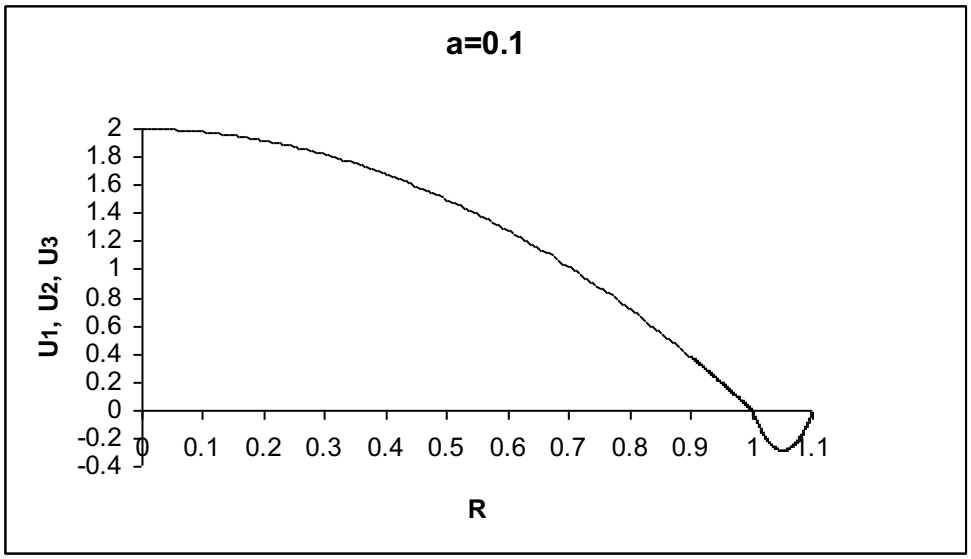

Fig. 2 Velocity distribution at a=0.1

The sign change of the velocity at $r = r_0$ lead to necessity the problem Eq.(1) 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:

$$1.\quad u_1\frac{\partial c_1}{\partial z_1} = D\left(\frac{1}{r}\frac{\partial c_1}{\partial r} + \frac{\partial^2 c_1}{\partial r^2}\right) - kc_1,$$

$$(0 \le r \le r_1,\ 0 \le z_1 \le l,\ u_1 = u_1(r),\ c_1 = c_1(r,z_1))$$

$$z_1 = 0,\ c_1 = \bar{c}_0;\ r = 0,\ \frac{\partial c_1}{\partial r} = 0;\ r = r_1,\ c_1 = c_2,\ \frac{\partial c_1}{\partial r} = \frac{\partial c_2}{\partial r}.$$

$$2.\quad u_1\frac{\partial c_2}{\partial z_1} = D\left(\frac{1}{r}\frac{\partial c_2}{\partial r} + \frac{\partial^2 c_2}{\partial r^2}\right) - kc_2,$$

$$(r_1 \le r \le r_0,\ 0 \le z_1 \le l,\ u_1 = u_1(r),\ c_2 = c_2(r,z_1))$$

$$z_1 = 0,\ c_2 = (\bar{c}_3)_{z_2=l};\ r = r_1,\ c_1 = c_2,\ \frac{\partial c_1}{\partial r} = \frac{\partial c_2}{\partial r};\qquad r = r_0,\ c_2 = c_3,\ \frac{\partial c_2}{\partial r} = \frac{\partial c_3}{\partial r}.$$

$$3.\quad u_2\frac{\partial c_3}{\partial z_2} = D\left(\frac{1}{r}\frac{\partial c_3}{\partial r} + \frac{\partial^2 c_3}{\partial r^2}\right) - kc_3,$$

$$(r_0 \le r \le R_0,\ 0 \le z_2 \le l,\ u_2 = u_2(r),\ c_3 = c_3(r,z_2))$$

$$z_2 = 0,\ c_3 = (\bar{c}_2)_{z_1=l};\ r = r_0,\ c_2 = c_3,\ \frac{\partial c_2}{\partial r} = \frac{\partial c_3}{\partial r},\qquad r = R_0,\ \frac{\partial c_3}{\partial z} = 0. \qquad (7)$$

In Eqs. (7) $(\bar{c}_2)_{z_1=l}$ and $(\bar{c}_3)_{z_2=l}$ are the average concentrations:

$$(\bar{c}_2)_{z_1=l}=\frac{2}{r_0^2-r_1^2}\int_{r_1}^{r_0} rc_2(r,l)dr,\quad (\bar{c}_3)_{z_2=l}=\frac{2}{R_0^2-r_0^2}\int_{r_0}^{R_0} rc_3(r,l)dr \tag{8}$$

The solution of the problem Eqs.(7) permits to obtain the column mass transfer efficiency q in the case of circulation zone:

$$q=\bar{u}_1^{(0)}\bar{c}_0-\frac{2}{r_1^2}\int_0^{r_1} ru_1c_1(r,l)dr,\quad \bar{u}_1^{(0)}=\frac{2}{r_1^2}\int_0^{r_1} ru_1(r)dr=\bar{u}\left(1+2a-a^2\right), \tag{9}$$

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

3. DIMENSIONLESS PROBLEM SOLUTION

For the solution of Eqs.(7) must be used dimensionless variables:

$$r=r_0R,\ z=lZ_1=lZ_2,\ Z_1+Z_2=1,$$
$$c_1=\bar{c}_0C_1(R,Z_1),\ c_2=\bar{c}_0C_2(R,Z_1),\ c_3=\bar{c}_0C_3(R,Z_2). \tag{10}$$

Introducing Eqs. (10) into Eqs. (7), lead to the next set of equations:

$$U_1\frac{\partial C_1}{\partial Z_1}=Fo\left(\frac{1}{R}\frac{\partial C_1}{\partial R}+\frac{\partial^2 C_1}{\partial R^2}\right)-DaC_1 \qquad (0\le R\le 1-a)$$

$$Z_1=0,\ C_1=1;\ R=0,\ \frac{\partial C_1}{\partial R}=0;$$

$$R=1-a,\ \frac{\partial C_1}{\partial R}=\delta_1(Z_1),\ \delta_1(Z_1)=\frac{\partial C_2}{\partial R}. \tag{11}$$

$$U_1\frac{\partial C_2}{\partial Z_1}=Fo\left(\frac{1}{R}\frac{\partial C_2}{\partial R}+\frac{\partial^2 C_2}{\partial R^2}\right)-DaC_2 \qquad (1-a\le R\le 1)$$

$$Z_1=0,\ C_2=\alpha_2,\ \alpha_2=\frac{2}{2a+a^2}\int_1^{1+a} RC_3(R,1)dR;$$

$$R=1-a,\ C_2(R,Z_1)=C_1(R,Z_1);$$

$$R=1,\ \frac{\partial C_2}{\partial Z_1}=\delta_2(Z_1),\ \delta_2(Z_1)=\left(\frac{\partial C_3}{\partial Z_2}\right)_{Z_2=1-Z_1}. \tag{12}$$

$$U_2\frac{\partial C_3}{\partial Z_2}=Fo\left(\frac{1}{R}\frac{\partial C_3}{\partial R}+\frac{\partial^2 C_3}{\partial R^2}\right)-DaC_3 \qquad (1\le R\le 1+a)$$

$$Z_2=0,\ C_3=\alpha_3,\ \alpha_3=\frac{2}{a}\int_{1-a}^{1}RC_2(R,1)dR;$$

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

$$R=1+a,\ \frac{\partial C_3}{\partial R}=0, \tag{13}$$

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

$$Fo=\frac{Dl}{\bar{u}r_0^2},\quad Da=\frac{kl}{\bar{u}}. \tag{14}$$

The column mass transfer efficiency Eq. (9) in dimensionless variables is:

$$Q=\frac{q}{u_1^{(0)}\bar{c}_0}=1-\frac{4}{(1-a)^2(1+2a-a^2)}\int_0^{1-a}R(1-R^2)C_1(R,1)dR. \tag{15}$$

The solution of the problem Eqs. (11-13) is possible to be obtained consecutively using the next algorithm:

1. The problem (11) 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 (12) 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.(13) 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. (11) and determination of $C_1(R,Z_1)$.
5. Solution of Eqs. (12) and determination of $C_2(R,Z_1)$ and α_3.
6. Solution of Eqs. (13) 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. (11-13) 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 on the Figs. 4a,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 –$Z=0.1$ ($Z_1=0.9$), $Z=0.3$ ($Z_1=0.7$), $Z=0.5$ ($Z_1=0.5$), $Z=0.7$ ($Z_1=0.3$), $Z=0.9$ ($Z_1=0.1$).

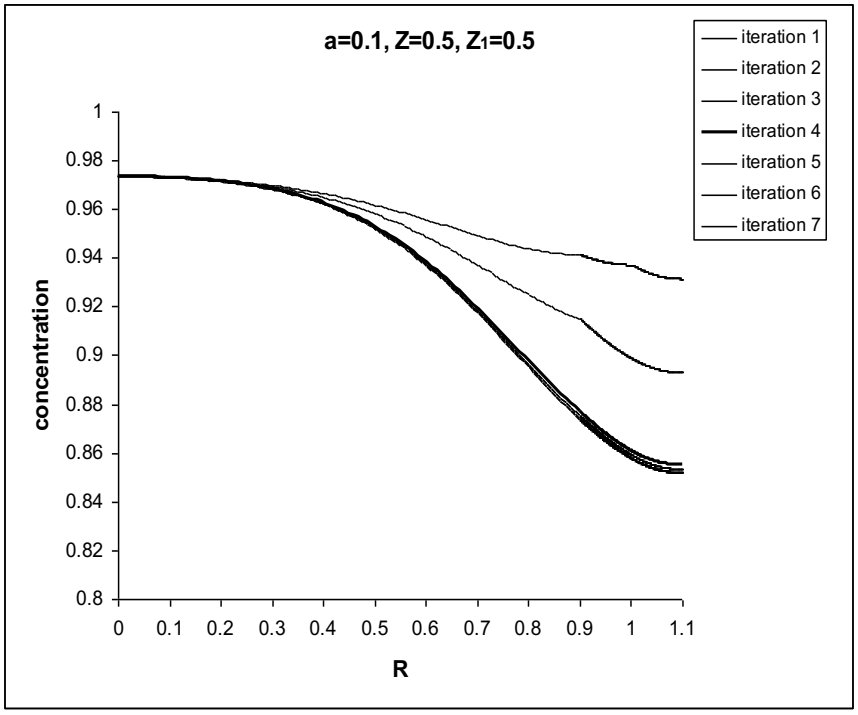

Fig. 3. Concentration distributions at different iterations, obtained from Eqs. (11-13)

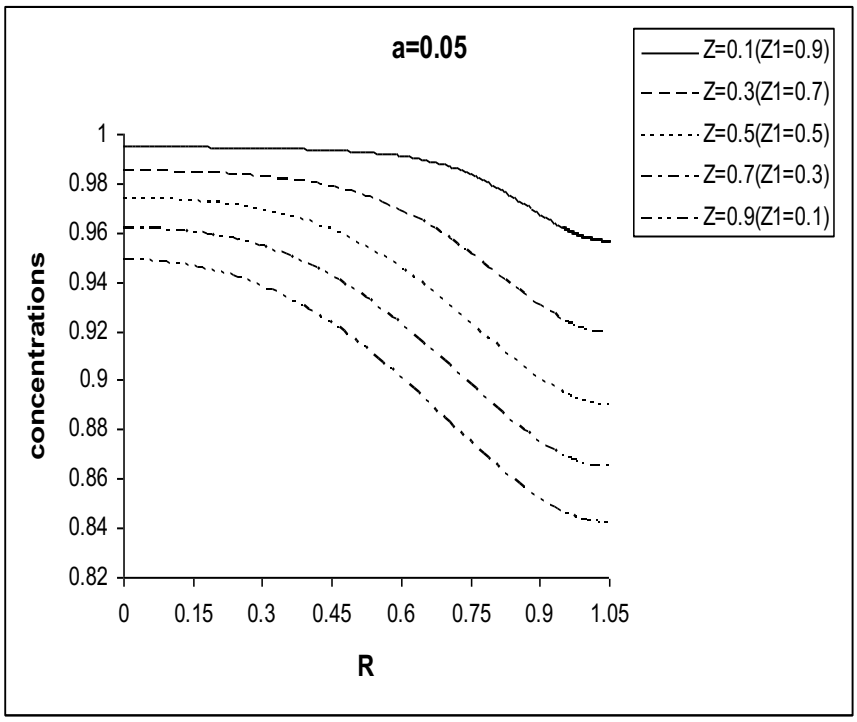

Fig.4a. Concentration distributions at different height of the column, when *a*=0.05

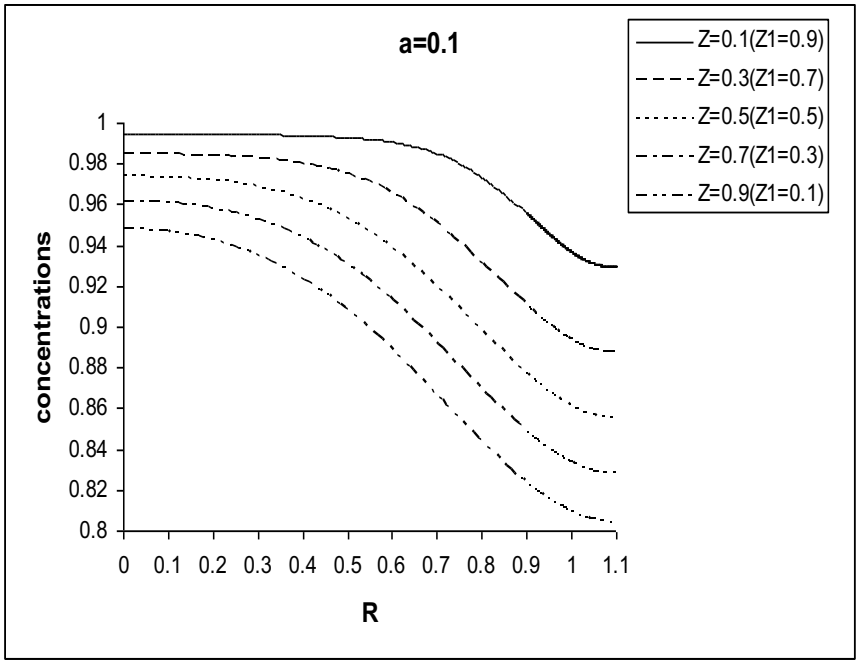

Fig.4b. Concentration distributions at different height of the column, when *a*=0.1

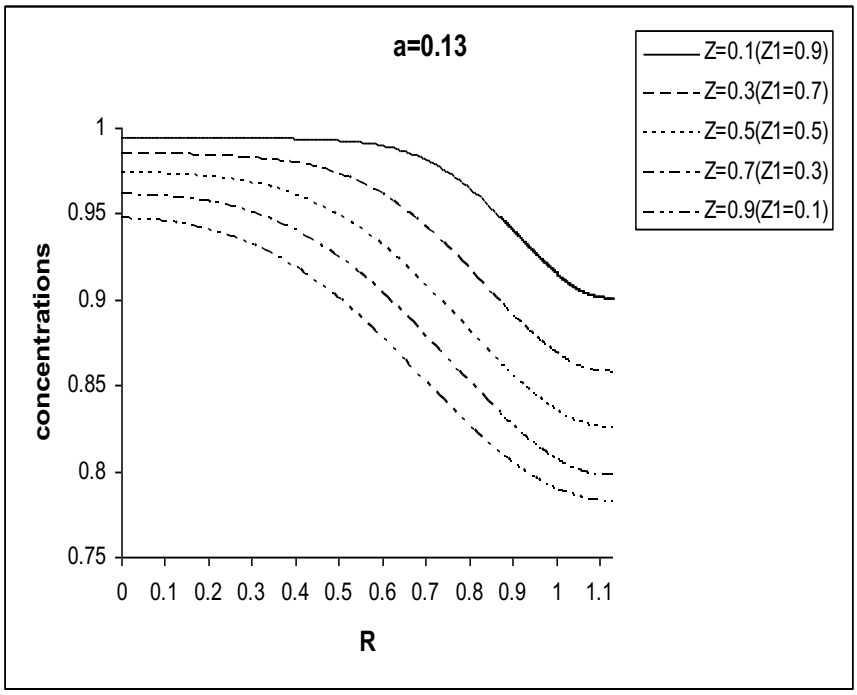

Fig.4c. Concentration distributions at different height of the column, when *a*=0.13

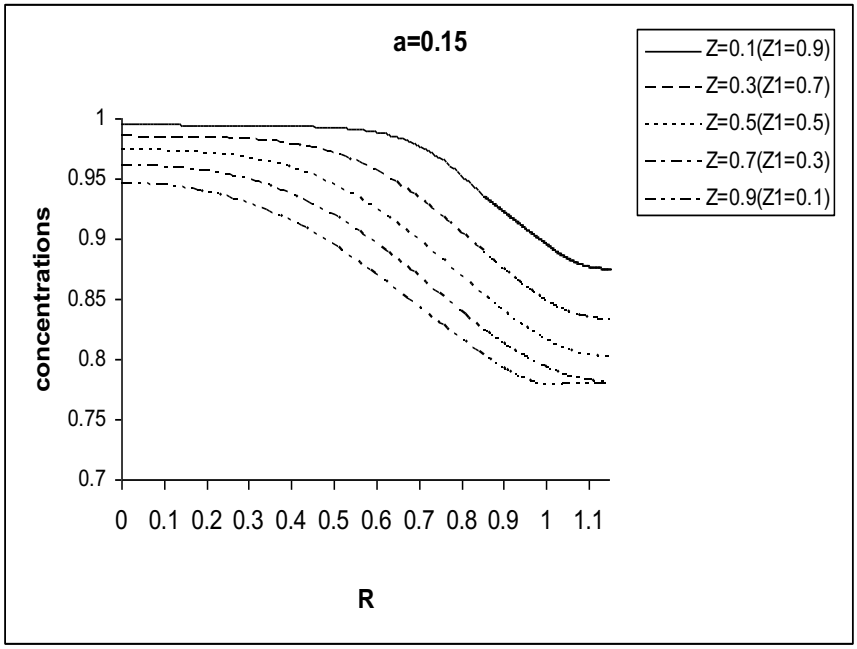

Fig.4d. Concentration distributions at different height of the column, when *a*=0.15

The influence of the stagnation zone breadths on the concentration distributions is shown in the Fig.5.

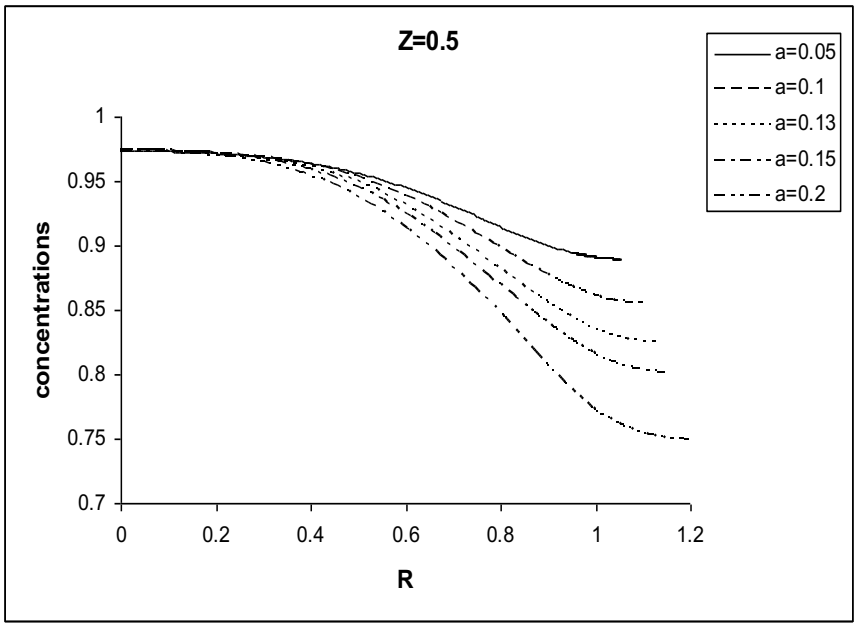

Fig. 5 Comparison of the concentration distributions for different stagnation zone breadths.

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:

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

The velocity distribution in column without barriers is:

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

The convection-diffusion equation in the case of absence of the barriers is possible to be obtained from (1) if replace $u = u_0$ and $c = c_0$:

$$u_0 \frac{\partial c_0}{\partial z} = D\left(\frac{\partial^2 c_0}{\partial z^2} + \frac{1}{r}\frac{\partial c_0}{\partial r} + \frac{\partial^2 c_0}{\partial r^2}\right) - kc_0 \tag{16}$$

with boundary conditions:

$$z = 0,\ c_1 = \bar{c}_0;\ r = 0,\ \frac{\partial c_0}{\partial r} = 0;\ r = R_0,\ ,\ \frac{\partial c_0}{\partial r} = 0. \tag{17}$$

The introducing of the dimensionless variable

$$r = r_0 R,\ z = lZ,\ c_0 = \bar{c}_0 C_0(R, Z),\ u_0(r) = \bar{u} U_0(R), \tag{18}$$

lead to:

$$U_0 \frac{\partial C_0}{\partial Z_1} = Fo\left(\frac{1}{R}\frac{\partial C_0}{\partial R} + \frac{\partial^2 C_0}{\partial R^2}\right) - DaC_0$$

$$Z = 0,\ C_0 = 1;\ R = 0,\ \frac{\partial C_0}{\partial R} = 0;$$

$$R = 1 + a,\ \frac{\partial C_0}{\partial R} = 0. \tag{19}$$

where

$$U_0(R) = (1 + 2a - a^2)\left(\frac{1-a}{1+a}\right)^2\left[2 - \frac{2}{(1+a)^2}R^2\right]. \tag{20}$$

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

$$q_0 = \bar{u}_0 \bar{c}_0 - \frac{2}{R_0^2} \int_0^{R_0} r u_0 c_0 dr \tag{21}$$

and in dimensionless form:

$$Q_0 = \frac{q_0}{\bar{u}_0 \bar{c}_0} = 1 - \frac{4}{(1+a)^2} \int_0^{1+a} R\,(1 - \frac{1}{(1+a)^2} R^2) C_0(R,1)\, dR\,. \tag{22}$$

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 1 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:

$$\Delta Q = \frac{Q_0 - Q}{Q_0}. \tag{23}$$

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

$$\Delta W = \frac{(R_0 - r_1)^2}{R_0^2} = \frac{4a^2}{(1+a)^2} \tag{24}$$

and the relative influence of the stagnation zone volume on the column efficiency $\frac{\Delta Q}{\Delta W}$ are demonstrated in Table 1:

Table 1 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

4. CONCLUSION

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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