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Effect of the velocity radial non-uniformity in the column apparatuses

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Abstract - A theoretical analysis of the effect of the velocity radial non-uniformity in the column apparatuses is presented. A numerical analysis shows, that average concentration model, where the radial velocity component is equal to zero (in the cases of a constant velocity radial non-uniformity along the column height), is possible to be used in the cases of an axial modification of the radial non-uniformity of the axial velocity component. The use of experimental data, for the average concentration at different points along the column height, for a concrete process, 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 model for modeling of different processes in the cases of different values of the column height, average velocity, reagent diffusivity and chemical reaction rate constant.

Keywords: Column apparatus, chemical reaction, convection-diffusion model, average concentration model, velocity radial non-uniformity.

I. INTRODUCTION

The complex processes in the column apparatuses have a combination of hydrodynamic processes, convective and diffusive mass (heat) transfer processes and chemical reactions between the reagents (components of the phases).

The fundamental problem in the column apparatuses modeling is result of the complicated hydrodynamic behavior of the flows in the columns and as a result the velocity distributions in the columns are unknown.

In the general case a multicomponent ($i = 1, 2, ..., i_0$) 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 [m^3.s^{-1}], the input velocities of the phases in the column u_j^0 [m.s^{-1}], $j = 1, 2, 3$ are possible to be defined as:

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

From (1) follows:

$$\varepsilon_j = \frac{F_j}{F_0}, \quad j = 1, 2, 3, \quad \sum_{j}^{3} \varepsilon_j = 1, \tag{2}$$

where ε_j, $j = 1, 2, 3$ are the parts of the column volume, occupied by the gas, liquid and solid phase, respectively, i.e., the phase volumes (m^3) in 1 m^3 of the column volume (hold-up coefficients of the phases).

II. CONVECTION-DIFFUSION MODEL

The column apparatuses is possible to be modeled, using a new approach (Boyadjiev, 2006; Boyadjiev, 2010; Doichinova et al, 2012; Boyadjiev, 2013) on the base of the physical approximations of the mechanics of continua, where the mathematical point is equivalent to a small

(elementary) physical volume, which is sufficiently small with respect to the apparatus volume, but at the same time sufficiently large with respect to the intermolecular volumes in the medium.
The physical elementary volumes will be presented as mathematical points in a cylindrical coordinate system (r, z), where r and z [m] are radial and axial coordinates. The concentrations [kg-mol.m^{-3}] of the reagents (components of the phases) are $c_{ij}, i=1,2,...,i_0, j=1,2,3$, i.e., the quantities of the reagents (kg-mol) in 1 m^3 of the column volume (no in the phase volumes in the column).
In the cases of a stationary fluids motion in cylindrical column apparatus $u_j(r,z), v_j(r,z), j=1,2,3$ [m.s^{-1}] are axial and radial velocity components of the phases in the elementary volumes.
The volume reactions [kg-mol.m^{-3}.s^{-1}] in the phases (homogeneous chemical reactions and interphase mass transfer, as a volume source or sink in the phase volumes in the column) are $Q_{ij}(c_{ij}),\ j=1,2,3,\ i=1,2,...,i_0$. They lead to different values of the reagent (substance) concentrations in the elementary volumes $c_{ij}(r,z)\ \left[\text{kg-mol.m}^{-3}\right]$ 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 mathematical model of the processes in the column apparatuses, in the physical approximations of the mechanics of continua, is mass balances in the phase volumes (phase parts in the elementary 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). In the stationary case, the convection-diffusion equations (as a mathematical structures of the mass transfer process models in the column apparatuses) (Boyadjiev, 2006; Boyadjiev, 2010; Doichinova et al, 2012; Boyadjiev, 2013) are:

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

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

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

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

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

The average values of the velocity at the column cross-sectional area can be presented as

$$\bar{u}(z)=\frac{2}{r_0^2}\int_0^{r_0} r u(r,z)\,dr,\quad \bar{v}(z)=\frac{2}{r_0^2}\int_0^{r_0} r v(r,z)\,dr.\qquad (6)$$

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The velocity distributions in (3), (4) assume to be presented by the average functions (6):

$$u(r,z)=\bar{u}(z)\tilde{u}(r,z), \quad v(r,z)=\bar{v}(z)\tilde{v}(r,z), \qquad (7)$$

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

$$\frac{2}{r_0^2}\int_0^{r_0} r\tilde{u}(r,z)\,dr=1, \quad \frac{2}{r_0^2}\int_0^{r_0} r\tilde{v}(r,z)\,dr=1. \qquad (8)$$

A differentiation of $u(r,z)$ in (7), with respect to z, leads to:

$$\frac{\partial u}{\partial z}=\frac{\partial \bar{u}}{\partial z}\tilde{u}+\bar{u}\frac{\partial \tilde{u}}{\partial z}. \qquad (9)$$

Practically, the cross-sectional area surface in the columns is a constant and the average velocity is a constant too $\left(\frac{\partial \bar{u}}{\partial z}=0, \quad \bar{u}=u^0\right)$, i.e. $\frac{\partial u}{\partial z}\equiv 0$ if $\frac{\partial \tilde{u}}{\partial z}\equiv 0$ $\left(u=u(r), \quad \tilde{u}=\tilde{u}(r)\right)$. In this case from (4) follows:

$$\frac{dv}{dr}+\frac{v}{r}=0; \quad r=r_0, \quad v=0 \qquad (10)$$

and the solution is $v(r,z)\equiv 0$. This leads to a new form of the convection - diffusion type model (Boyadjiev, 2006; Boyadjiev, 2010; Doichinova et al, 2012; Boyadjiev, 2013) and for a two components chemical reaction ($i=1,2$) has the form:

$$u\frac{\partial c_i}{\partial z}=D_i\left(\frac{\partial^2 c_i}{\partial z^2}+\frac{1}{r}\frac{\partial c_i}{\partial r}+\frac{\partial^2 c_i}{\partial r^2}\right)+Q_i\left(c_1,c_2\right);$$

$$r=0, \quad \frac{\partial c_i}{\partial r}\equiv 0; \quad r=r_0, \quad \frac{\partial c_i}{\partial r}\equiv 0; \qquad (11)$$

$$z=0, \quad c_i\equiv c_i^0, \quad u^0c_i^0\equiv uc_i^0-D_i\frac{\partial c_i}{\partial z}; \quad i=1,2.$$

From (6), (7), (8), (9) and (10) is seen, that if the radial non-uniformity of the axial velocity component is independent of the axial coordinate, the radial velocity component is equal to zero:

$$\frac{\partial \tilde{u}}{\partial z}\equiv 0, \quad v\equiv 0. \qquad (12)$$

From (11), (12) follows, that in the case of pseudo-first order chemical reaction, the convection-diffusion model has the form:

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

$$r=0, \quad \frac{\partial c}{\partial r}\equiv 0; \quad r=r_0, \quad \frac{\partial c}{\partial r}\equiv 0; \qquad (13)$$

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

The convection-diffusion model (13) permits to be made (Boyadjiev, 2006; Boyadjiev, 2010; Doichinova et al, 2012; Boyadjiev, 2013) a qualitative analysis of the process (model) for to be obtained the main, small and slight physical effects (mathematical operators), and to be rejected the slight effect (operators). As a result the process mechanism identification is possible to be made. The convection-diffusion model is a base of the average concentration models, which allow a quantitative analysis of the processes in column apparatuses.

III. AVERAGE CONCENTRATION MODEL

The average values of the velocity and concentration in (13), at the column cross-sectional area (Boyadjiev, 2006; Boyadjiev, 2010; Doichinova et al, 2012; Boyadjiev, 2013) are:

$$\bar{u}=\frac{2}{r_0^2}\int_0^{r_0} ru(r)\,dr,\quad \bar{c}(z)=\frac{2}{r_0^2}\int_0^{r_0} rc(r,z)\,dr. \qquad (14)$$

The functions $u(r), c(r,z)$ in (13) can be presented by the help of the average functions (14):

$$u(r)=\bar{u}\,\tilde{u}(r),\quad c(r,z)=\bar{c}(z)\,\tilde{c}(r,z), \qquad (15)$$

where $\tilde{u}(r)$ and $\tilde{c}(r,z)$ present the radial non-uniformity of the velocity and concentration and satisfy the next conditions:

$$\frac{2}{r_0^2}\int_0^{r_0} r\,\tilde{u}(r)\,dr=1,\quad \frac{2}{r_0^2}\int_0^{r_0} r\,\tilde{c}(r,z)\,dr=1. \qquad (16)$$

The average concentration model may be obtained if put (15) into (13), multiply by r and integrate over r in the interval $[0,r_0]$. As a result, the average concentration model has the form:

$$\begin{gathered}\alpha\bar{u}\frac{d\bar{c}}{dz}+\frac{d\alpha}{dz}\bar{u}\,\bar{c}=D\frac{d^2\bar{c}}{dz^2}-k\bar{c};\\ z=0,\quad \bar{c}(0)=c^0,\quad \frac{d\bar{c}}{dz}=0,\end{gathered} \qquad (17)$$

where

$$\alpha(z)=\frac{2}{r_0^2}\int_0^{r_0} r\,\tilde{u}(r)\tilde{c}(r,z)\,dr \qquad (18)$$

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

IV. GENERALIZED VARIABLES

In (13), (17), (18) is possible to be introduced the generalized variables:

$$\begin{gathered}r=r_0R,\quad z=lZ,\quad u(r)=\bar{u}U(R),\quad \tilde{u}(r)=\frac{u(r)}{\bar{u}}=U(R),\\ c(r,z)=c^0C(R,Z),\quad \bar{c}(z)=c^0\bar{C}(Z),\quad \bar{C}(Z)=2\int_0^1 RC(R,Z)dR,\\ \tilde{c}(r,z)=\frac{c(r,z)}{\bar{c}(z)}=\frac{C(R,Z)}{\bar{C}(Z)},\quad \alpha(z)=\alpha(lZ)=A(Z)=2\int_0^1 RU(R)\frac{C(R,Z)}{\bar{C}(Z)}dR\end{gathered} \qquad (19)$$

and as a result is obtained:

$$\begin{gathered}U\frac{\partial C}{\partial Z}=\mathrm{Fo}\left(\varepsilon\frac{\partial^2C}{\partial Z^2}+\frac{1}{R}\frac{\partial C}{\partial R}+\frac{\partial^2C}{\partial R^2}\right)-\mathrm{Da}\,C;\\ R=0,\quad \frac{\partial C}{\partial R}\equiv 0;\quad R=1,\quad \frac{\partial C}{\partial R}\equiv 0;\\ Z=0,\quad \mathrm{C}\equiv 1,\quad 1\equiv U-\mathrm{Pe}^{-1}\frac{\partial C}{\partial Z}.\end{gathered} \qquad (20)$$

$$\begin{gathered}A(Z)\frac{d\bar{C}}{dZ}+\frac{dA}{dZ}\bar{C}=\mathrm{Pe}^{-1}\frac{d^2\bar{C}}{dZ^2}-\mathrm{Da}\,\bar{C};\\ Z=0,\quad \bar{C}=1,\quad \frac{d\bar{C}}{dZ}=0,\end{gathered} \qquad (21)$$

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

$$\text{Fo} = \frac{Dl}{\bar{u}r_0^2}, \quad \text{Pe} = \frac{\bar{u}l}{D}, \quad \text{Da} = \frac{kl}{\bar{u}} \quad \varepsilon = \frac{r_0^2}{l^2} = \text{Fo}^{-1}\,\text{Pe}^{-1}. \qquad (22)$$

The theoretical analysis of the models (20), (21) shows, that the function $A(Z)$ in (19) is possible to be presented as a linear approximation:

$$A = a_0 + a_1 Z. \qquad (23)$$

The presented theoretical analysis shows that the basic approximation of the convection-diffusion model (13) and average concentration model (17) is $\partial\tilde{u}/\partial z \equiv 0$.

V. EFFECT OF THE AXIAL MODIFICATION OF THE RADIAL NON-UNIFORMITY OF THE VELOCITY

The radial non-uniformity of the axial velocity component in a column apparatus is the result of the fluid hydrodynamics at the column inlet, where it is 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.

Let's considers the velocity distribution

$$u_n(r, z_n) = \bar{u}\, \tilde{u}_n(r, z_n) \qquad (24)$$

and an axial step change of the radial non-uniformity of the axial velocity component in a column (fig. 1):

$$\begin{aligned} &\tilde{u}_n(r, z_n) = \tilde{u}_n(r_0 R, l Z_n) = U_n(R, Z_n) = a_n - b_n R^2, \\ &a_n = 2 - 0.1n, \quad b_n = 2(1 - 0.1n), \quad 0.2n \le Z_n \le 0.2(n+1) \quad n = 0,1,\ldots,4, \end{aligned} \qquad (25)$$

where $\tilde{u}_n(r, z_n)$ satisfy the equation:

$$\frac{2}{r_0^{\,2}} \int_0^{r_0} r\, \tilde{u}_n(r, z_n)\, dr = 1, \qquad (26)$$

i.e. $\bar{u} = const$.

If put (24), (25) in (13), the convection-diffusion model has the form:

$$U_n \frac{\partial C_n}{\partial Z_n} = \text{Fo}\left(\varepsilon \frac{\partial^2 C_n}{\partial Z_n^2} + \frac{1}{R}\frac{\partial C_n}{\partial R} + \frac{\partial^2 C_n}{\partial R^2}\right) - \text{Da}\, C_n; \quad 0.2n \le Z_n \le 0.2(n+1);$$

$$R = 0, \quad \frac{\partial C_n}{\partial R} \equiv 0; \quad R = 1, \quad \frac{\partial C_n}{\partial R} \equiv 0; \quad Z_n = 0.1n, \quad \text{C}_n(R, Z_n) = C_{n-1}(R, Z_n), \qquad (27)$$

$$1 \equiv U_n - \text{Pe}^{-1}\frac{\partial C_n}{\partial Z_n}; \quad n = 0,1,\ldots,4; \quad Z_0 = 0, \quad \text{C}_0(R, Z_0) \equiv 1.$$

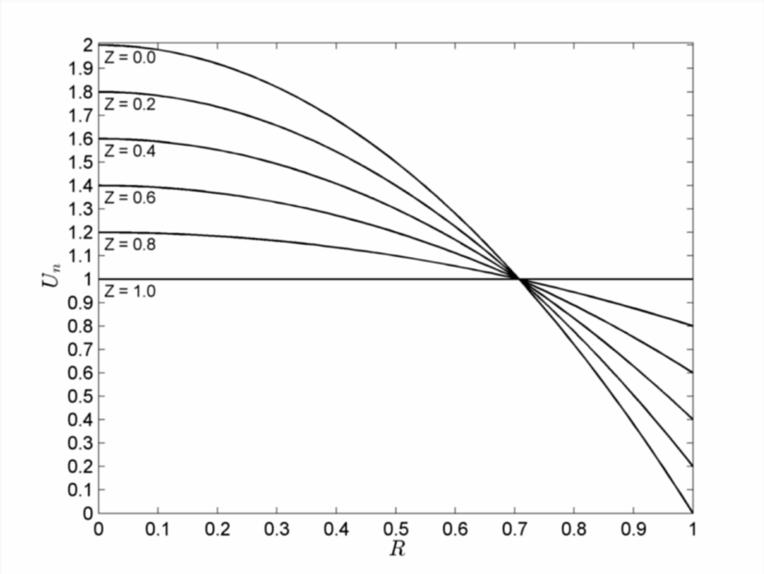

Fig. 1. Velocity distributions $U_n(R, Z_n), Z_n = 0.2n, n = 0,1,...,4.$

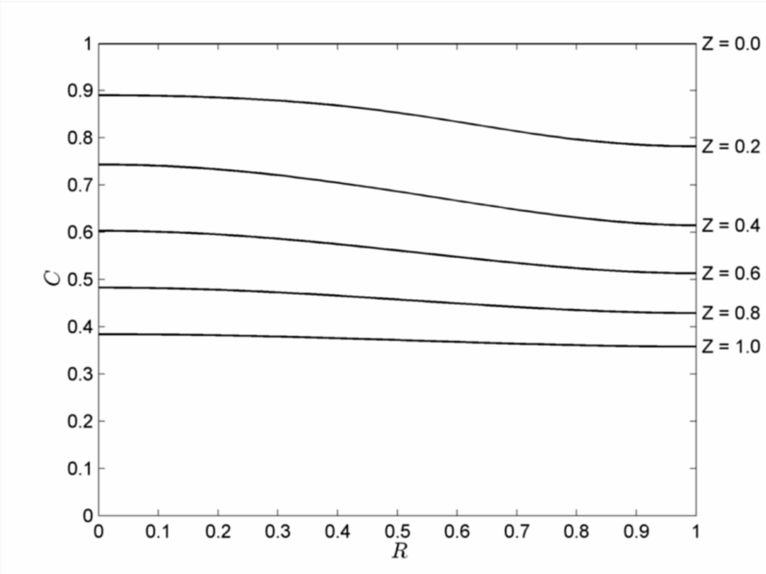

Fig. 2. Concentration distribution $C(Z) = C_n(Z_{n+1}), n = 0,1,...,4, \varepsilon = 0.05.$

In (27) ε is a small parameter and for the solution is possible to be used the perturbation method (Boyadjiev et al, 2015):

$$\mathrm{C}_n(R, Z_n) = C_n^0(R, Z_n) + \varepsilon C_n^1(R, Z_n), \tag{28}$$

where $C_n^0(R, Z_n)$ and $C_n^1(R, Z_n)$ are the solutions of the problems:

$$\begin{gathered} U_n \frac{\partial C_n^0}{\partial Z_n} = \mathrm{Fo}\left(\frac{1}{R}\frac{\partial C_n^0}{\partial R} + \frac{\partial^2 C_n^0}{\partial R^2}\right) - \mathrm{Da}\, C_n^0; \quad 0.2n \le Z_n \le 0.2(n+1); \\ R = 0, \quad \frac{\partial C_n^0}{\partial R} \equiv 0; \quad R = 1, \quad \frac{\partial C_n^0}{\partial R} \equiv 0; \\ Z_n = 0.1n, \quad \mathrm{C}_n^0(R, Z_n) = C_{n-1}^0(R, Z_n); \quad n = 0,1,...,4; \\ Z_0 = 0, \quad \mathrm{C}_0^0(R, Z_0) \equiv 1. \end{gathered} \tag{29}$$

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$$U_n \frac{\partial C_n^1}{\partial Z_n} = \mathrm{Fo}\left(\frac{\partial^2 C_n^0}{\partial Z_n^2} + \frac{1}{R}\frac{\partial C_n^1}{\partial R} + \frac{\partial^2 C_n^1}{\partial R^2}\right) - \mathrm{Da}\, C_n^1; \quad 0.2n \le Z_n \le 0.2(n+1);$$
$$R=0, \quad \frac{\partial C_n^1}{\partial R} \equiv 0; \quad R=1, \quad \frac{\partial C_n^1}{\partial R} \equiv 0; \tag{30}$$
$$Z_n = 0.1n, \quad \mathrm{C}_n^1(R,Z_n) = C_{n-1}^1(R,Z_n); \quad n=0,1,...,4;$$
$$Z_0 = 0, \quad \mathrm{C}_0^1(R,Z_0) \equiv 1.$$

The solution of (29) is possible to be presented as

$$\mathrm{C}_n^0(R,Z_n) = a_0(R) + a_1(R)Z_n + a_2(R)Z_n^2 + a_3(R)Z_n^3 + a_4(R)Z_n^4, \; n=0,1,...,4 \tag{31}$$

and in (30) must be replaced:

$$\frac{\partial^2 C_n^0}{\partial Z_n^2} = 2a_2(R) + 6a_3(R)Z_n + 12a_4(R)Z_n^2, \quad n=0,1,...,4. \tag{32}$$

A consistent solution of equations (27) in the cases:

$$\mathrm{Fo}=0.5, \quad \mathrm{Da}=1, \quad \varepsilon=0.05, \quad \mathrm{Pe}^{-1}=0.025, \tag{33}$$

permits to be obtained the concentration distributions $C(R,Z)$, average concentrations $\bar{C}(Z)$ in the column and function $A(Z)$ in (19) on every step:

$$C_n(R,Z_{n+1}), \quad \bar{C}_n(Z_{n+1}) = 2\int_0^1 RC_n(R,Z_{n+1})\,dR,$$
$$A_n(Z_{n+1}) = 2\int_0^1 RU_n(R)\frac{C_n(R,Z_{n+1})}{\bar{C}_n(Z_{n+1})}dR, \quad n=0,1,...,4, \tag{34}$$

which are presented on the figs. 2-4.

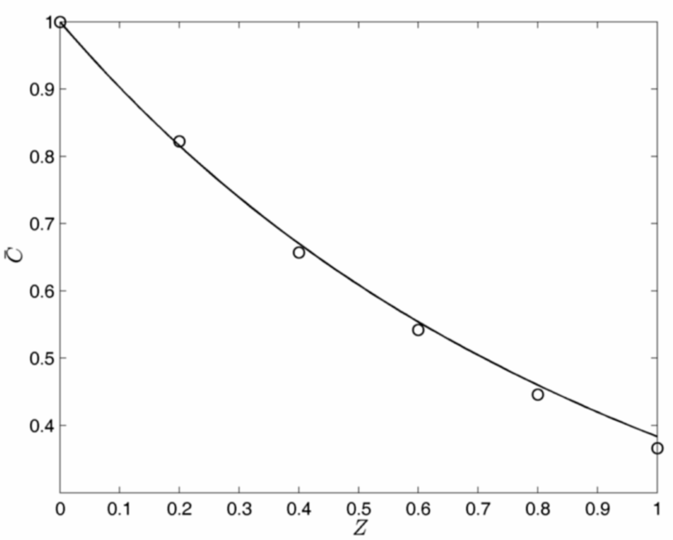

Fig. 3. Average concentration distribution $\bar{C}(Z) = \bar{C}_n(Z_{n+1}), n=0,1,...,4, \varepsilon=0.05$ ***(points);*** $\bar{C}(Z)$ ***as a solution of (36) for "theoretical" values of*** a_1, a_2 ***(line).***

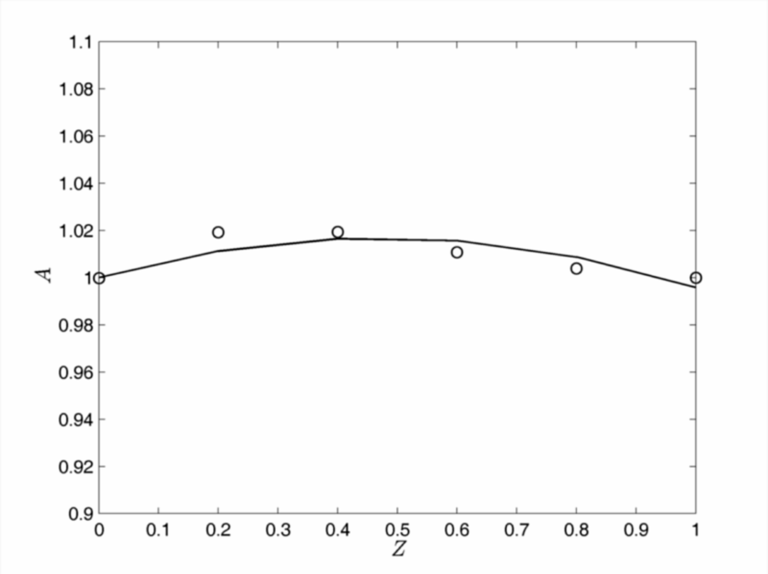

Fig. 4. Function $A_n\left(Z_{n+1}\right), n=0,1,\ldots,4, \varepsilon=0.05$ ***(points);***

$A(Z)$ ***as a quadratic approximation (35) (line).***

Table 1. Parameters a_1***,*** a_2***, Fo = 0.5, Da = 1, ε = 0.05,*** Pe^{-1} ***= 0.025.***

Parameters	"Theoretical" values	"Experimental" values
a_1	0,0716	0,0911
a_2	-0,0758	0,0328

From fig. 4 is seen, that the function $A_n\left(Z_{n+1}\right) n=0,1,\ldots 4$ is possible to be presented as a quadratic approximation:

$$A(Z)=1+a_1 Z+a_2 Z^2, \quad (35)$$

where the ("theoretical") values of a_1, a_2 are presented in the table 1.

As a result, in the case of axial modification of the radial non-uniformity of the velocity, the model (21) has the form:

$$\left(1+a_1 Z+a_2 Z^2\right)\frac{d\bar{C}}{dZ}+\left(a_1+2a_2 Z\right)\bar{C}=\mathrm{Pe}^{-1}\frac{d^2\bar{C}}{dZ^2}-Da\bar{C};$$
$$Z=0, \quad \bar{C}=1, \quad \frac{d\bar{C}}{dZ}=0, \quad (36)$$

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

In (36) Pe^{-1} is a small parameter and for the solution is possible to be used the perturbation method (Boyadjiev et al, 2015):

$$\bar{\mathrm{C}}(Z)=\bar{C}^0(Z)+\mathrm{Pe}^{-1}\varepsilon\bar{C}^1(Z), \quad (37)$$

where $C^0(Z)$ and $C^1(Z)$ are the solution of the equation set:

$$\frac{d\bar{C}^{(0)}}{dZ} = -\frac{\left(a_1 + 2a_2 Z + \mathrm{Da}\right)\bar{C}^{(0)}}{\left(1 + a_1 Z + a_2 Z^2\right)}, \quad \bar{C}^{(0)}\left(0\right) = 1,$$

$$\frac{d\bar{C}^{(1)}}{dZ} = \frac{\frac{d^2\bar{C}^{(0)}}{dZ^2} - \left(a_1 + 2a_2 Z + \mathrm{Da}\right)\bar{C}^{(1)}}{\left(1 + a_1 Z + a_2 Z^2\right)}, \quad \bar{C}^{(1)}\left(0\right) = 0, \qquad (38)$$

$$\frac{d^2\bar{C}^{(0)}}{dZ^2} = \frac{-2a_2\bar{C}^{(0)} - \left(a_1 + 2a_2 Z + \mathrm{Da}\right)\frac{d\bar{C}^{(0)}}{dZ} + \left(a_1 + 2a_2 Z + \mathrm{Da}\right)\left(a_1 + 2a_2 Z\right)\bar{C}^{(0)}}{\left(1 + a_1 Z + a_2 Z^2\right)^2}$$

The obtained the values of the function $\bar{C}_n\left(Z_{n+1}\right), n = 0,1,...,4$ (fig. 3) permits to be obtained the artificial experimental data for different values of Z_n :

$$\bar{C}^n_{\exp}\left(Z_{n+1}\right) = \left(0.95 + 0.1B_n\right)\bar{C}_n\left(Z_{n+1}\right), \quad Z_n = 0.2n, \quad n = 0,1,...,4, \quad \varepsilon = 0.05, (39)$$

where $0 \le B_n \le 1, n = 0,1,...,4$ are obtained by a generator of random numbers.

The obtained artificial experimental data (39) are used for the illustration of the parameters (a_1, a_2) identification in the average concentrations model (36) by the minimization of the least-squares function:

$$Q(a_1, a_2) = \sum_{n=0}^{4}\left[\bar{C}(Z_{n+1}, a_1, a_2) - \bar{C}^n_{\exp}(Z_{n+1})\right]^2, \qquad (40)$$
$$Z_n = 0.2n, \quad n = 0,1,...,4, \quad \varepsilon = 0.05,$$

where the values of $\bar{C}(Z_{n+1}, a_1, a_2), n = 0,1,...,4$ are obtained as solutions of (36). The obtained ("experimental") parameter values are compared with the "theoretical" values on the table 1.

The obtained ("experimental") parameter values are used for the solution of (36) and the result (the line) is compared with the artificial experimental data (39) on the fig. 5.

VI. INFLUENCE OF THE MODEL PARAMETERS

The model (36), with "experimental" parameters values of a_1, a_2 (for $\varepsilon = 0.05$, $\mathrm{Fo} = 0.5$, $\mathrm{Da} = 1$, $\mathrm{Pe}^{-1} = 0.025$), is used for the calculation the average concentrations in the cases:

1. $\varepsilon = 0$, $\mathrm{Fo} = 0.5$, $\mathrm{Da} = 1$, $\mathrm{Pe}^{-1} = 0.025$;
2. $\varepsilon = 0.05$, $\mathrm{Fo} = 0.1$, $\mathrm{Da} = 1$, $\mathrm{Pe}^{-1} = 0.005$;
3. $\varepsilon = 0.05$, $\mathrm{Fo} = 0.5$, $\mathrm{Da} = 2$, $\mathrm{Pe}^{-1} = 0.025$

and the results (lines) are compared (figs. 6-8) with the "experimental" data (39) (points) for these three cases.

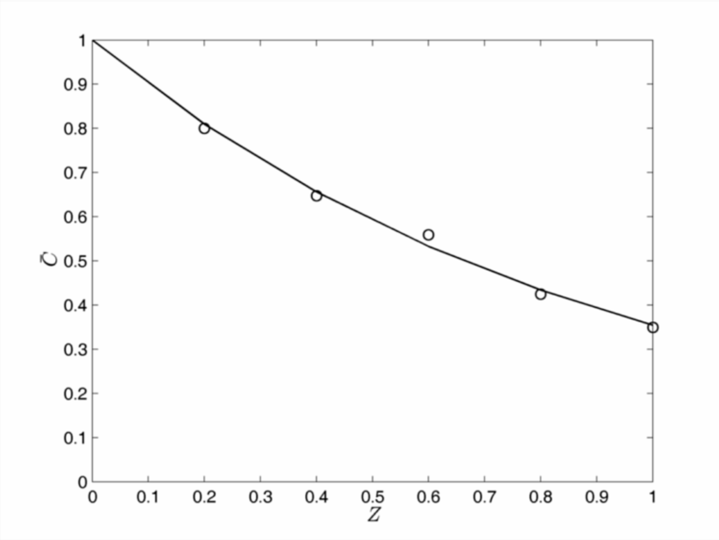

Fig. 5. Average concentration distribution $\bar{C}(Z), \varepsilon = 0.05$:
"Experimental" data (39) $\bar{C}(Z) = \bar{C}_n(Z_{n+1}), n = 0,1,\ldots,4$ ***(points);***
$\bar{C}(Z)$ ***as a solution of (36) for "experimental" values of*** a_1, a_2 ***(lines).***

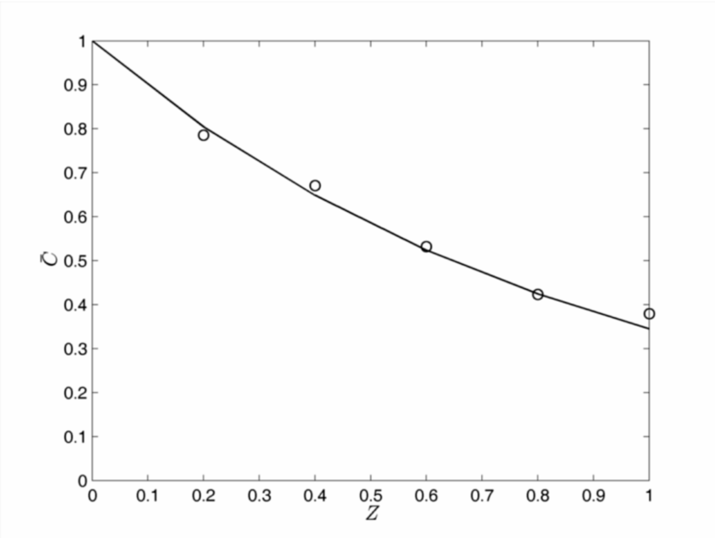

Fig. 6. Average concentration distribution $\bar{C}(Z)$ ***: effect of*** ε ***.***

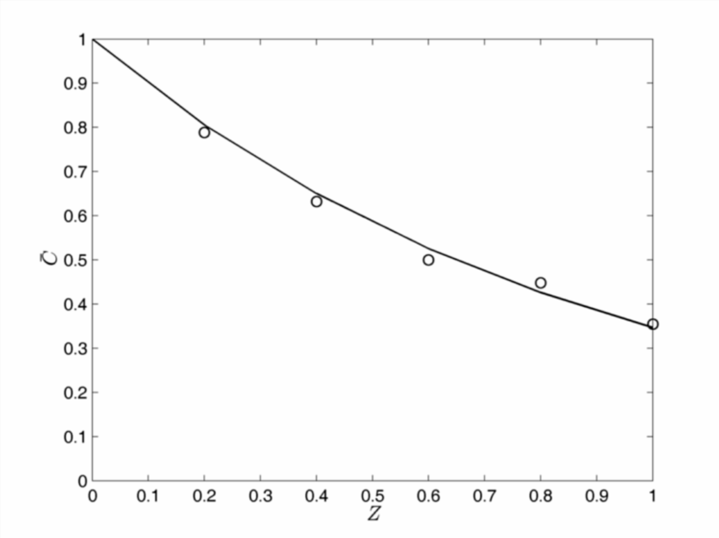

Fig. 7. Average concentration distribution $\bar{C}(Z)$ ***: effect of Fo.***

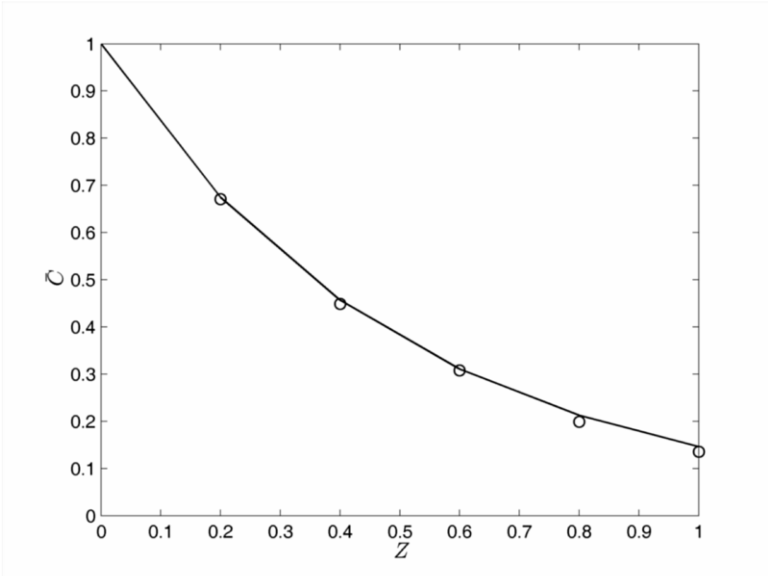

Fig. 8. Average concentration distribution $\bar{C}(Z)$: effect of Da.

VII. CONCLUSIONS

The presented numerical analysis shows, that average concentration model, where the radial velocity component is equal to zero (in the cases of a constant velocity radial non-uniformity along the column height), is possible to be used in the cases of an axial modification of the radial non-uniformity of the axial velocity component. The use of experimental data, for the average concentration at different points along the column height, for a concrete process, permits to be obtained the model parameters (a_1, a_2), related with the radial non-uniformity of the velocity. These parameter values permit to be used the average concentration model for modeling of different processes (different values of the parameters ε, Fo, Da, i.e. different values of the column height, average velocity, reagent diffusivity and chemical reaction rate constant).

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