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COMPUTER MODELING OF COLUMN APPARATUSES TWO COORDINATES SYSTEMS APPROACH

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Abstract: *The computer modelling of the mass transfer processes in column apparatuses on the base of a new approach is presented. A convection–diffusion type model and an average concentration type model are used for to be solved the calculation problems in the cases of counter-current gas-liquid or liquid-liquid processes. In these conditions the mass transfer process models are presented in two coordinates systems, because in one coordinate system one of the equations has not a solution by reason of the negative equation Laplacian value. A combination of iterative algorithms and MATLAB are used for the solutions of the equations set in different coordinate systems. As a result is shown, that the experimental data, obtained from the column with real radius and small height are useful for the parameters identifications in the average concentration type models.*

Key words: *Absorption, column apparatus, counter-current flow, two coordinates system approach*.

1. Introduction

The computer modelling of the mass transfer processes in column apparatuses is possible on the base of a new approach 1, using convection–diffusion type model 3, 5 in 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.

For the modelling of gas absorption processes must be used two equations model in a cylindrical coordinates system (r,z), i.e., mass balances in the gas $(j=1)$ and liquid $(j=2)$ phases, where according 4, 5, the radial velocity components are equal to zero:

$$\begin{aligned} & u_j \frac{\partial c_j}{\partial z_j} = D_j \left(\frac{\partial^2 c_j}{\partial z_j^2} + \frac{1}{r}\frac{\partial c_j}{\partial r} + \frac{\partial^2 c_j}{\partial r^2} \right) + Q_j\left(c_j\right); \\ & r=0, \quad \frac{\partial c_j}{\partial r} \equiv 0; \quad r=r_0, \quad \frac{\partial c_j}{\partial r} \equiv 0; \\ & z_j = 0, \quad c_j \equiv c_j^0, \quad u_j^0 c_j^0 \equiv u_j c_j^0 - D_j \left(\frac{\partial c_j}{\partial z_j} \right)_{Z_j=0}; \\ & j=1,2. \end{aligned} \tag{1}$$

In (1) $u_j = u_j(r)$ m.s^{-1} and $c_j = c_j\left(r,z_j\right)$ kg-mol.m^{-3} are the axial velocity components and absorbed substance concentrations in the phases, D_j m^2.s^{-1} and ε_j m^3.m^{-3} are the diffusivities and hold-up coefficients in the phases (parts of the gas and liquid phases in the elementary column volume), u_j^0 and c_j^0 are the inlet velocities and concentrations in the column, where $j=1,2$, $1=\varepsilon_1+\varepsilon_2$ (practically $c_2^0 \equiv 0$). The concentrations of the absorbed substance in the phases are presented as kg-mol of the absorbed substance in the phase in 1 m^3 of the column volume (no in 1 m^3 of the phase volume). The hold-up coefficients (m^3 of the phase volume in 1 m^3 of the column volume) and the inlet velocities in the column are obtained from the ratios $\varepsilon_j = F_j / F_0$ and $u_j^0 = F_j / \varepsilon_j \pi r_0^2$, where r_0 is the column radius m, F_j are the gas and liquid phase flow rates m^3.s^{-1} in the column, $j=1,2$. The volume reactions terms Q_j, $j=1,2$ kg-mol.m^{-3}s^{-1} are the rates of the interphase mass transfer and homogeneous chemical reaction, as a volume sources ($Q>0$) or sinks ($Q<0$) in the gas and liquid phase parts of the elementary column

volume and participate in the mass balance in the phase volumes (no in the column volume).

The model (1) is possible to be used for co-current two-phase flows ($z_1 = z_2 = z$) or for counter-current one ($z_1 + z_2 = l$, where l is the active zone height m of the column). In counter-current flows the mass transfer process models must be presented in two coordinates systems (r, z_j), $j = 1,2$ 1, because in one coordinate system one of the equations has not a solution by reason of the negative equation Laplacian value. The numerical solutions of an equations set in different coordinate systems is a problem, which will be solved in this paper.

2. Convection-diffusion type of model

As an example will be used a counter-current physical absorption process 1. The convection-diffusion type model is possible to be obtained from (1), where the rates of the interphase mass transfer terms Q_j, $j = 1,2$ have the forms:

$$Q_j = (-1)^j k(c_1 - \chi c_2), \quad j = 1,2, \qquad (2)$$

where k s^{-1} is interphase mass transfer coefficient, χ - the Henry's number, $c_1(c_2)$ kg-mol.m^{-3} - the concentration of the absorbed substance in the gas (liquid) phase, i.e., kg-mol of the absorbed substance in the gas (liquid) phase in 1 m^3 of the column volume. As a result from (1) and (2) follows:

$$u_j \frac{\partial c_j}{\partial z_j} = D_j \left(\frac{\partial^2 c_j}{\partial z_j^2} + \frac{1}{r}\frac{\partial c_j}{\partial r} + \frac{\partial^2 c_j}{\partial r^2} \right) + (-1)^j k(c_1 - \chi c_2); \quad j = 1,2. \qquad (3)$$

The boundary conditions of (3) have the form:

$$r = 0, \quad \frac{\partial c_1}{\partial r} = \frac{\partial c_2}{\partial r} \equiv 0; \quad r = r_0, \quad \frac{\partial c_1}{\partial r} = \frac{\partial c_2}{\partial r} \equiv 0;$$
$$z_1 = 0, \quad c_1(r,0) \equiv c_1^0,$$
$$u_1^0 c_1^0 \equiv u_1(r) c_1^0 - D_1 \left(\frac{\partial c_1}{\partial z_1} \right)_{z_1 = 0}; \qquad (4)$$
$$z_2 = 0, \quad c_2(r,0) \equiv 0, \quad \left(\frac{\partial c_2}{\partial z_2} \right)_{z_2 = 0} \equiv 0.$$

The presented convection-diffusion type model (3), (4) permits to be made a qualitative analysis of the physical absorption processes 4, 5, using dimensionless (generalized) variables:

$$R = \frac{r}{r_0}, \quad Z_j = \frac{z_j}{l}, \quad U_j = \frac{u_j}{u_j^0}, \quad j = 1,2,$$
$$C_1 = \frac{c_1}{c_1^0}, \quad C_2 = \frac{c_2 \chi}{c_1^0}. \qquad (5)$$

If put (5) into (3), (4), the model in generalized variables has the form:

$$U_j(R)\frac{\partial C_j}{\partial Z_j} = \mathrm{Fo}_j \left(\varepsilon \frac{\partial^2 C_j}{\partial Z_j^2} + \frac{1}{R}\frac{\partial C_j}{\partial R} + \frac{\partial^2 C_j}{\partial R^2} \right) + (-1)^j K_j (C_1 - C_2);$$
$$R = 0, \quad \frac{\partial C_i}{\partial R} \equiv 0; \quad R = 1, \quad \frac{\partial C_i}{\partial R} \equiv 0; \quad i = 1,2; \qquad (6)$$
$$Z_1 = 0, \quad C_1 \equiv 1, \quad 1 \equiv U_1(R) - \mathrm{Pe}_1^{-1} \left(\frac{\partial C_1}{\partial Z_1} \right)_{Z_1 = 0};$$
$$Z_2 = 0, \quad C_2 \equiv 0, \quad \left(\frac{\partial C_2}{\partial Z_2} \right)_{Z_2 = 0} \equiv 0.$$

where

$$K_1 = \frac{kl}{u_1^0}, \quad K_2 = \frac{kl\chi}{u_2^0}, \quad \mathrm{Pe}_j = \frac{u_j^0 l}{D_j},$$
$$\mathrm{Fo}_j = \frac{D_j l}{u_j^0 r_0^2}, \quad \varepsilon = \frac{r_0^2}{l^2} = \mathrm{Pe}_j^{-1}\mathrm{Fo}_j^{-1}, \quad j = 1,2. \qquad (7)$$

3. Qualitative analysis

For height columns the parameter ε is very small ($0 = \varepsilon \le 10^{-2}$) and the problem (6) is possible to be solved in zero approximation with respect to ε:

$$U_j(R)\frac{\partial C_j}{\partial Z_j} = \mathrm{Fo}_j \left(\frac{1}{R}\frac{\partial C_j}{\partial R} + \frac{\partial^2 C_j}{\partial R^2} \right) + (-1)^j K_j (C_1 - C_2);$$
$$R = 0, \quad \frac{\partial C_j}{\partial R} \equiv 0; \quad R = 1, \quad \frac{\partial C_j}{\partial R} \equiv 0; \quad j = 1,2; \qquad (8)$$
$$Z_1 = 0, \quad C_1 \equiv 1; \quad Z_2 = 0, \quad C_2 \equiv 0;$$

For big values of the average velocities $0 = \mathrm{Fo}_j \le 10^{-2}$, $j = 1,2$ and from (8) follows the convective type model:

$$U_j(R)\frac{\partial C_j}{\partial Z_j} = (-1)^j K_j (C_1 - C_2); \quad j = 1,2;$$
$$Z_1 = 0, \quad C_1 \equiv 1; \quad Z_2 = 0, \quad C_2 \equiv 0. \qquad (9)$$

4. Calculation problem

Let's consider the convection-diffusion type model of a counter-current absorption process (8), where the velocity distributions in the phases are

Poiseuille type 5 and difference between phases velocities is in the average velocities, only:

$$U_1 = U_2 = 2 - 2R^2. \qquad (10)$$

From (8) and (10) is possible to be obtained a particular form of the problem for computer modeling of the absorption processes in counter-current column apparatuses:

$$\left(2-2R^2\right)\frac{\partial C_1}{\partial Z_1} = \\ = \mathrm{Fo}_1\left(\frac{1}{R}\frac{\partial C_1}{\partial R} + \frac{\partial^2 C_1}{\partial R^2}\right) - K_1\left(C_1 - C_2\right); \\ R = 0, \quad \frac{\partial C_1}{\partial R} \equiv 0; \quad R = 1, \quad \frac{\partial C_1}{\partial R} \equiv 0; \\ Z_1 = 0, \quad C_1 \equiv 1. \qquad (11)$$

$$\left(2-2R^2\right)\frac{\partial C_2}{\partial Z_2} = \\ = \mathrm{Fo}_2\left(\frac{1}{R}\frac{\partial C_2}{\partial R} + \frac{\partial^2 C_2}{\partial R^2}\right) + K_2\left(C_1 - C_2\right); \\ R = 0, \quad \frac{\partial C_2}{\partial R} \equiv 0; \quad R = 1, \quad \frac{\partial C_2}{\partial R} \equiv 0; \\ Z_2 = 0, \quad C_2 \equiv 0. \qquad (12)$$

The numerical solution of the equations set (11), (12) is possible if MATLAB and an iterative procedure are used, where the concentration distributions in the column will be obtained in matrix forms on every iteration step s:

$$C_1^s\left(R, Z_1\right) = \left\| a_{\rho\zeta_1}^s \right\|, \\ \rho = 1,2,...,\rho^0, \quad \zeta_1 = 1,2,...,\zeta^0, \\ 0 \le R \le 1, \quad 0 \le Z_1 \le 1, \\ R = \frac{\rho - 1}{\rho^0 - 1}, \quad Z_1 = \frac{\zeta_1 - 1}{\zeta^0 - 1}, \quad \rho^0 = \zeta^0. \qquad (13)$$

$$C_2^s\left(R, Z_2\right) = \left\| b_{\rho\zeta_2}^s \right\|, \\ \rho = 1,2,...,\rho^0, \quad \zeta_2 = 1,2,...,\zeta^0, \\ 0 \le R \le 1, \quad 0 \le Z_2 \le 1, \\ R = \frac{\rho - 1}{\rho^0 - 1}, \quad Z_2 = \frac{\zeta_2 - 1}{\zeta^0 - 1}. \qquad (14)$$

The iterative procedure starts with the zero step $s = 0$:

$$C_2^0\left(R, Z_2\right) = \left\| b_{\rho\zeta_2}^0 \right\| \equiv 0, \\ \rho = 1,2,...,\rho^0, \quad \zeta_2 = 1,2,...,\zeta^0; \\ C_1^0\left(R, Z_1\right) = \left\| a_{\rho\zeta_1}^0 \right\|, \\ \rho = 1,2,...,\rho^0, \quad \zeta_1 = 1,2,...,\zeta^0; \qquad (15)$$

where $C_1^0\left(R, Z_1\right)$ is a solution of the problem:

$$\left(2-2R^2\right)\frac{\partial C_1^0}{\partial Z_1} = \mathrm{Fo}_1\left(\frac{1}{R}\frac{\partial C_1^0}{\partial R} + \frac{\partial^2 C_1^0}{\partial R^2}\right) - K_1 C_1^0; \\ R = 0, \quad \frac{\partial C_1^0}{\partial R} \equiv 0; \quad R = 1, \quad \frac{\partial C_1^0}{\partial R} \equiv 0; \\ Z_1 = 0, \quad C_1^0 \equiv 1. \qquad (16)$$

The solution of (16) permits to be obtained a new function:

$$C_1^0\left(R, Z_1\right) = C_1^0\left(R, 1 - Z_2\right) = \hat{C}_1^0\left(R, Z_2\right) = \left\| \hat{a}_{\rho\zeta_2}^0 \right\|, \\ \rho = 1,2,...,\rho^0, \quad \zeta_2 = 1,2,...,\zeta^0. \qquad (17)$$

The iterative step s is the solution of the problem:

$$\left(2-2R^2\right)\frac{\partial C_2^s}{\partial Z_2} = \\ = \mathrm{Fo}_2\left(\frac{1}{R}\frac{\partial C_2^s}{\partial R} + \frac{\partial^2 C_2^s}{\partial R^2}\right) + K_2\left(\hat{C}_1^{(s-1)} - C_2^s\right); \\ R = 0, \quad \frac{\partial C_2^s}{\partial R} \equiv 0; \quad R = 1, \quad \frac{\partial C_2^s}{\partial R} \equiv 0; \\ Z_2 = 0, \quad C_2^s \equiv 0, \qquad (18)$$

where

$$\hat{C}_1^{(s-1)}\left(R, Z_2\right) = \left\| \hat{a}_{\rho\zeta_2}^{(s-1)} \right\|, \\ \rho = 1,2,..,\rho^0, \quad \zeta_2 = 1,2,..,\zeta^0. \qquad (19)$$

The solution of (18) permits to be obtained a new function:

$$C_2^s\left(R, Z_2\right) = C_2^s\left(R, 1 - Z_1\right) = \hat{C}_2^s\left(R, Z_1\right) = \left\| \hat{b}_{\rho\zeta_1}^s \right\|, \\ \rho = 1,2,...,\rho^0, \quad \zeta_1 = 1,2,...,\zeta^0, \qquad (20)$$

which will be used for solution of (11) at the s iterative step:

$$\left(2-2R^2\right)\frac{\partial C_1^s}{\partial Z_1} = \\ = \mathrm{Fo}_1\left(\frac{1}{R}\frac{\partial C_1^s}{\partial R} + \frac{\partial^2 C_1^s}{\partial R^2}\right) - K_1\left(C_1^s - \hat{C}_2^s\right); \\ R = 0, \quad \frac{\partial C_1^s}{\partial R} \equiv 0; \quad R = 1, \quad \frac{\partial C_1^s}{\partial R} \equiv 0; \\ Z_1 = 0, \quad C_1^s \equiv 1. \qquad (21)$$

The solution of the problem (11), (12) was obtained using MATLAB program. It solves the equations (18), (21) through iterative procedure using the built-in MATLAB function *pdepe*, which solves initial-boundary value problems for parabolic partial differential equations. The obtained matrices C_1 (from (21)) and C_2 (from (18)) are introduced in (18) and (21) respectively, using the built-in MATLAB function *interp2*.

The stop criterion of the iterative procedure is the condition:

$$\left|\frac{a^{s}_{\rho\zeta_1}-a^{(s-1)}_{\rho\zeta_1}}{a^{s}_{\rho\zeta_1}}\right|\le 10^{-3}, \qquad (22)$$

$$\rho=1,2,...,\rho^{0}, \quad \zeta_1=1,2,...,\zeta^{0}.$$

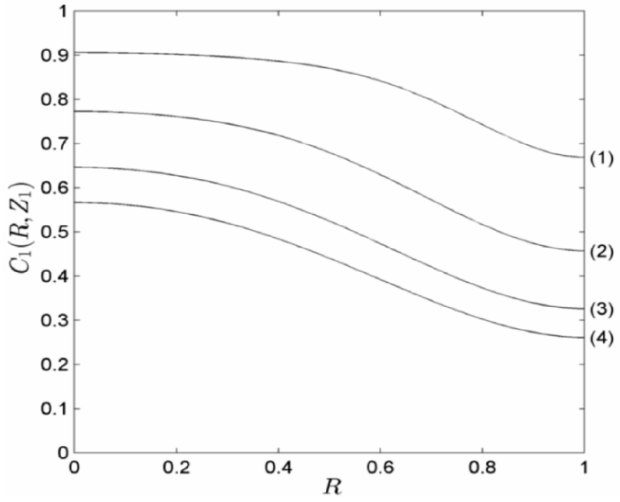

Fig. 1 *Concentration distributions* $C_1(R,Z_1)$ *at* Fo_1=0.*1,* K_1=1*:(1)-* $C_1(R,0.2)$*; (2)-* $C_1(R,0.5)$*; (3)-* $C_1(R,0.8)$*; (4)-* $C_1(R,1)$.

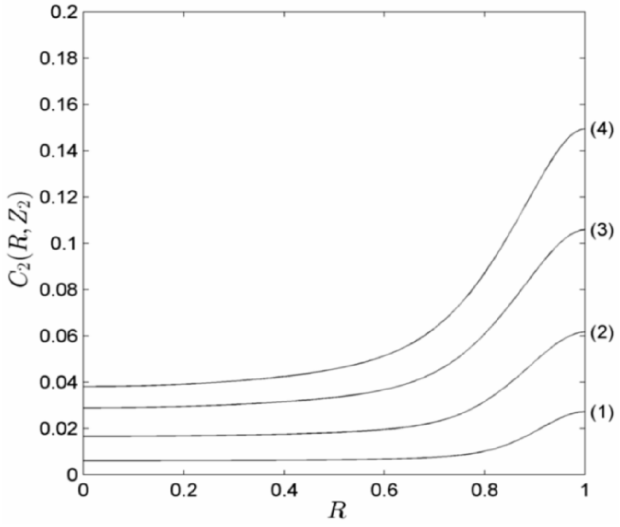

Fig. 2 *Concentration distributions* $C_2(R,Z_2)$ *at* Fo_2*=0.01,* K_2*=0.1:(1)-* $C_2(R,0.2)$*; (2)-* $C_2(R,0.5)$*; (3)-* $C_2(R,0.8)$*; (4)-* $C_2(R,1)$.

5. Concentration distributions

A solution of the problems (11), (12) is obtained for the case $\mathrm{Fo}_1=0.1$, $\mathrm{Fo}_2=0.01$, $K_1=1$, $K_2=0.1$ and the concentration distributions $C_j(R,Z_j)$ for $Z_j=0.2,0.5,0.8,1.0$, $j=1,2$ are presented in Fig.1 and Fig.2.

6. Absorption process efficiency

The absorption efficiency g and the gas absorption degree G in the column are possible to be obtained using the inlet and outlet average convective mass flux at the cross-sectional area surface in the column:

$$g=u_1^0c_1^0-\frac{2}{r_0^2}\int_0^{r_0} ru_1(r)c_1(r,l)\,dr, \quad G=\frac{g}{u_1^0c_1^0}. \qquad (23)$$

The absorption degree in generalized variables (5) has the form:

$$G=1-2\int_0^1 RU_1(R)C_1(R,1)\,dR. \qquad (24)$$

In the cases of absence of the velocity radial non-uniformity ($U_1=U_2\equiv 1$) the absorption degree has the form:

$$G_0=1-2\int_0^1 RC_1(R,1)\,dR \qquad (25)$$

and the reduction in the process efficiency due to the radial non-uniformity of the velocity is shown on Table 1.

Table 1 Process efficiency

Fo_1=0.1, K_1=1 Fo_2=0.01, K_2=0.1	$U_1=2-2R^2$ $U_2=2-2R^2$	$U_1=U_2\equiv 1$
G	0.5814	0.6336

7. Average concentration model

In the cases of unknown velocity distribution in the column, an average concentration model is possible to be used for absorption modeling in the column apparatuses.

The average values of the velocity and concentration for the cross-section's area of the column are:

$$\bar{u}_j=\frac{2}{r_0^2}\int_0^{r_0} ru_j(r)\,dr=u_j^0,$$
$$\bar{c}_j(z_j)=\frac{2}{r_0^2}\int_0^{r_0} rc_j(r,z_j)\,dr, \quad j=1,2. \qquad (26)$$

The functions in (3) may be presented by the help of the average function (26):

$$u_j(r)=\bar{u}_j\tilde{u}_j(r),$$
$$c_j(r,z_j)=\bar{c}_j(z_j)\,\tilde{c}(r,z_j), \quad j=1,2, \qquad (27)$$

where

$$\frac{2}{r_0^2}\int_0^{r_0} r\tilde{u}_j(r)\,dr=1,$$
$$\frac{2}{r_0^2}\int_0^{r_0} r\tilde{c}_j(r,z_j)\,dr=1, \quad j=1,2. \qquad (28)$$

The average concentration model may be obtained if put (27) in (3), (4), multiply with r and to integrate over r in the interval $0,r_0$. As a result is obtained:

$$\alpha_j \bar{u}_j \frac{d\bar{c}_j}{dz_j} + \frac{d\alpha_j}{dz_j} \bar{u}_j \bar{c}_j = $$

$$= D_j \frac{d^2 \bar{c}_j}{dz_j^2} + (-1)^j k\left(\bar{c}_1 - \chi \bar{c}_2\right), \quad j = 1,2, \tag{29}$$

where

$$\alpha_j = \alpha_j\left(z_j\right) = \frac{2}{r_0^2} \int_0^{r_0} r \tilde{u}_j(r) \tilde{c}_j\left(r, z_j\right) dr, \quad j = 1,2. \tag{30}$$

The boundary conditions of (29) have the form:

$$\begin{aligned} & z_1 = 0, \quad \bar{c}_1(0) \equiv c_1^0, \quad \left(\frac{d\bar{c}_1}{dz_1}\right)_{z_1=0} \equiv 0; \\ & z_2 = 0, \quad \bar{c}_2(0) \equiv 0, \quad \left(\frac{d\bar{c}_2}{dz_2}\right)_{z_2=0} \equiv 0. \end{aligned} \tag{31}$$

The presented average concentration model (29), (31) permits to be made a quantitative analysis of the physical absorption processes 4, using dimensionless (generalized) variables:

$$Z_j = \frac{z_j}{l}, \quad j = 1,2, \quad \bar{C}_1 = \frac{\bar{c}_1}{c_1^0}, \quad \bar{C}_2 = \frac{\bar{c}_2 \chi}{c_1^0}. \tag{32}$$

If put (32) into (29), (31), the model in generalized variables has the form:

$$\begin{aligned} & A_j \frac{d\bar{C}_j}{dZ_j} + \frac{dA_j}{dZ_j} \bar{C}_j = \mathrm{Pe}_j^{-1} \frac{d^2 \bar{C}_j}{dZ_j^2} + \\ & + (-1)^j K_j\left(\bar{C}_1 - \bar{C}_2\right); \quad j = 1,2; \\ & Z_1 = 0, \quad \bar{C}_1(0) \equiv 1, \quad \left(\frac{d\bar{C}_1}{dZ_1}\right)_{Z_1=0} \equiv 0; \\ & Z_2 = 0, \quad \bar{C}_2(0) \equiv 0, \quad \left(\frac{d\bar{C}_2}{dZ_2}\right)_{Z_2=0} \equiv 0, \end{aligned} \tag{33}$$

where

$$\begin{aligned} & A_j = A_j\left(Z_j\right) = \alpha_j\left(lZ_j\right) = \alpha_j\left(z_j\right), \\ & \mathrm{Pe}_j = \frac{\bar{u}_j l}{D_j}, \quad K_j = \frac{kl}{\bar{u}_j}, \quad j = 1,2. \end{aligned} \tag{34}$$

The functions $A_j = (Z_j),\ j = 1,2$ is possible to be obtained from (30), (32) after solution of (11), (12):

$$\begin{aligned} & A_j\left(Z_j\right) = 2\int_0^1 RU(R) \frac{C_j\left(R, Z_j\right)}{\bar{C}_j\left(Z_j\right)} dR, \\ & \bar{C}_j\left(Z_j\right) = 2\int_0^1 RC_j\left(R, Z_j\right) dR, \quad j = 1,2 \end{aligned} \tag{35}$$

and $\bar{C}_j\left(Z_j\right),\ A_j\left(Z_j\right),\ j = 1,2$, for $\mathrm{Fo}_1 = 0.1,\ \mathrm{Fo}_2 = 0.01,\ K_1 = 1,\ K_2 = 0.1$, are shown in Figs. 3-6.

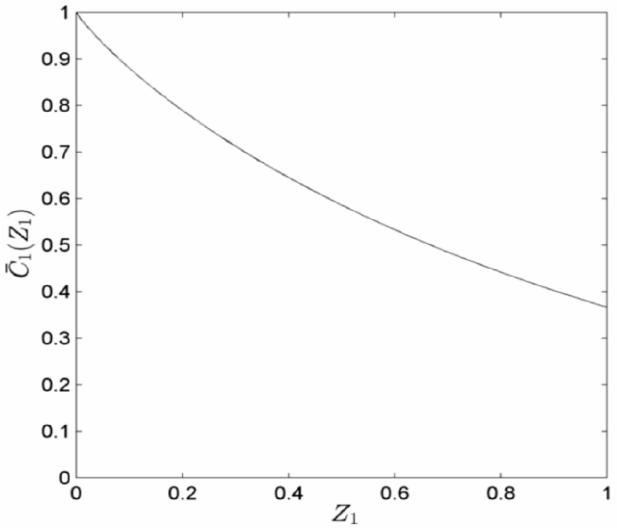

Fig. 3 *Average concentration* $\bar{C}_1\left(Z_1\right)$ *for* $\mathrm{Fo}_1 = 0.1,\ \mathrm{Fo}_2 = 0.01,\ K_1 = 1,\ K_2 = 0.1$.

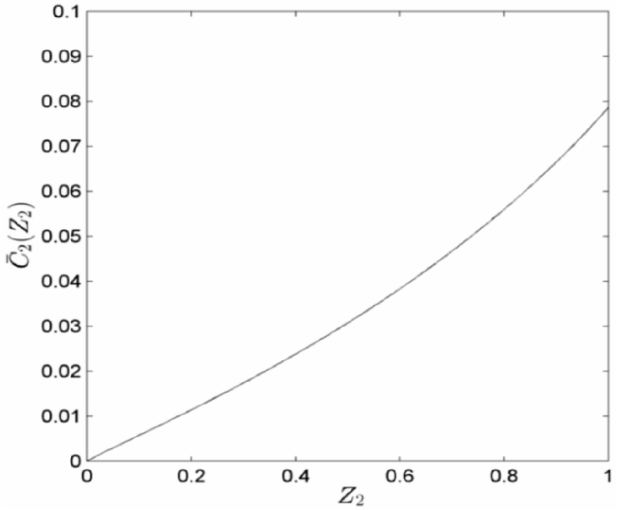

Fig. 4. *Average concentration* $\bar{C}_2\left(Z_2\right)$ *for* $\mathrm{Fo}_1 = 0.1,\ \mathrm{Fo}_2 = 0.01,\ K_1 = 1,\ K_2 = 0.1$

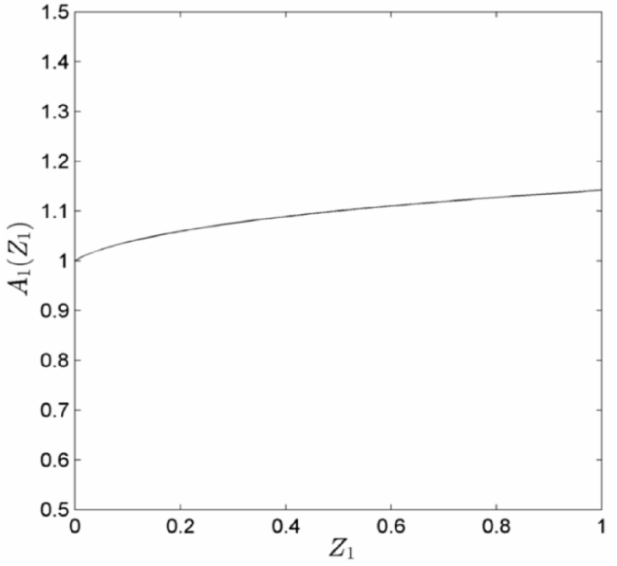

Fig. 5 *Function* $A_1\left(Z_1\right)$ *for* $\mathrm{Fo}_1 = 0.1,\ \mathrm{Fo}_2 = 0.01,\ K_1 = 1,\ K_2 = 0.1$

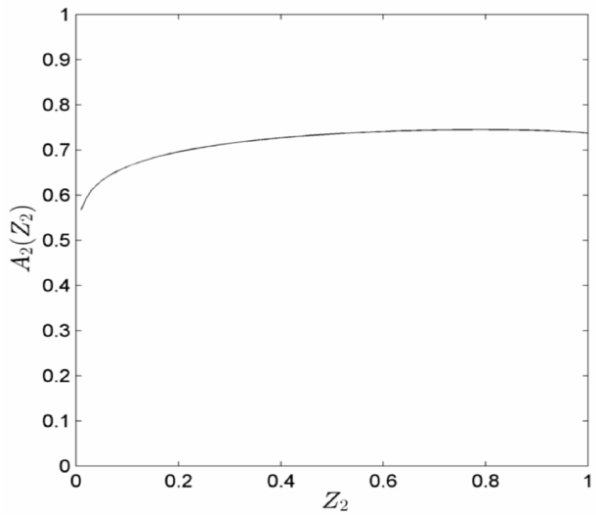

Fig. 6 *Function* $A_2(Z_2)$ *for* $\mathrm{Fo}_1 = 0.1,\ \mathrm{Fo}_2 = 0.01,\ K_1 = 1,\ K_2 = 0.1$.

For height columns the parameter ε is very small ($0 = \varepsilon \le 10^{-2},\ 0 = \mathrm{Pe}_j^{-1} = \varepsilon\,\mathrm{Fo}_j \le 10^{-2}$ for $\mathrm{Fo}_j \le 1,\ j = 1,2$) and the problem (33) is possible to be solved in zero approximation with respect to Pe_j^{-1}:

$$A_j \frac{d\bar{C}_j}{dZ_j} + \frac{dA_j}{dZ_j}\bar{C}_j = (-1)^j K_j\left(\bar{C}_1 - \bar{C}_2\right);\ j = 1,2; \quad (36)$$
$$Z_1 = 0,\quad \bar{\mathrm{C}}_1(0) \equiv 1;\quad Z_2 = 0,\quad \bar{C}_2(0) \equiv 0,$$

The presented functions $A_j = (Z_j),\ j = 1,2$ in Figs.3 and 4, show, that the linear approximations are possible to be used:

$$A_j = \omega_{0j} + \omega_{1j} Z_j,\quad j = 1,2 \quad (37)$$

and obtained (theoretical) parameters values ($\mathrm{Fo}_1 = 0.1,\ \mathrm{Fo}_2 = 0.01,\ K_1 = 1,\ K_2 = 0.1$) are presented on Table 2. As a result the average concentration model of a counter-current physical absorption process has the form:

$$\left(\omega_{01} + \omega_{11} Z_1\right)\frac{d\bar{C}_1}{dZ_1} + \omega_{11}\bar{C}_1 = -K_1\left(\bar{C}_1 - \bar{C}_2\right);$$
$$Z_1 = 0,\quad \bar{\mathrm{C}}_1(0) \equiv 1. \quad (38)$$

$$\left(\omega_{02} + \omega_{12} Z_2\right)\frac{d\bar{C}_2}{dZ_2} + \omega_{12}\bar{C}_2 = K_2\left(\bar{C}_1 - \bar{C}_2\right);$$
$$Z_2 = 0,\quad \bar{\mathrm{C}}_2(0) \equiv 0. \quad (39)$$

8. Model equations solution

The numerical solution of the equation set (38), (39) is possible if MATLAB and an iterative procedure are used, where the average concentration distributions in the column will be obtained in two vectors forms on every iteration step s:

$$\bar{C}_1^s(Z_1) = \left\| m_{\zeta_1}^s \right\|,\quad \zeta_1 = 1,2,...,\zeta^0,$$
$$0 \le Z_1 \le 1,\quad Z_1 = \frac{\zeta_1 - 1}{\zeta^0 - 1}. \quad (40)$$

$$\bar{C}_2^s(Z_2) = \left\| n_{\zeta_2}^s \right\|,\quad \zeta_2 = 1,2,...,\zeta^0,$$
$$0 \le Z_2 \le 1,\quad Z_2 = \frac{\zeta_2 - 1}{\zeta^0 - 1}. \quad (41)$$

The iterative procedure starts with the zero step $s = 0$:

$$\bar{C}_2^0(Z_2) = \left\| n_{\zeta_2}^0 \right\| \equiv 0,\quad \zeta_2 = 1,2,...,\zeta^0;$$
$$\bar{C}_1^0(Z_1) = \left\| m_{\zeta_1}^0 \right\|,\quad \zeta_1 = 1,2,...,\zeta^0; \quad (42)$$

where $\bar{C}_1^0(Z_1) = \left\| m_{\zeta_1}^0 \right\|$ is solution of the problem:

$$\left(\omega_{01} + \omega_{11} Z_1\right)\frac{d\bar{C}_1^0}{dZ_1} + \omega_{11}\bar{C}_1^0 = -K_1\bar{C}_1^0;$$
$$Z_1 = 0,\quad \bar{\mathrm{C}}_1^0(0) \equiv 1. \quad (43)$$

The iterative procedure s is the sequentially solving of the problems:

$$\left(\omega_{02} + \omega_{12} Z_2\right)\frac{d\bar{C}_2^s}{dZ_2} + \omega_{12}\bar{C}_2^s = K_2\left(\bar{C}_1^{(1-s)} - \bar{C}_2^s\right);$$
$$Z_2 = 0,\quad \bar{\mathrm{C}}_2^s(0) \equiv 0; \quad (44)$$

$$\left(\omega_{01} + \omega_{11} Z_1\right)\frac{d\bar{C}_1^s}{dZ_1} + \omega_{11}\bar{C}_1^s = -K_1\left(\bar{C}_1^s - \bar{C}_2^s\right);$$
$$Z_1 = 0,\quad \bar{\mathrm{C}}_1^s(0) \equiv 1. \quad (45)$$

The stop criterion of the iterative procedure is the condition:

$$\left|\frac{m_{\zeta_1}^s - m_{\zeta_1}^{(s-1)}}{m_{\zeta_1}^s}\right| \le 10^{-3},\quad \zeta_1 = 1,2,...,\zeta^0. \quad (46)$$

Table 2 Parameters values of ω for $\mathrm{Fo}_1 = 0.1,\ \mathrm{Fo}_2 = 0.01,\ K_1 = 1,\ K_2 = 0.1$

Theoretical values of ω	Experimental values of ω		
$\omega_{01} = 1.031$	$\omega_{01}^0 = 1.224$	$\omega_{01}^1 = 0.926$	$\omega_{01}^2 = 0.889$
$\omega_{11} = 0.123$	$\omega_{11}^0 = 0.476$	$\omega_{11}^1 = 0.156$	$\omega_{11}^2 = 0.080$
$\omega_{02} = 0.666$	$\omega_{02}^0 = 0.719$	$\omega_{02}^1 = 0.586$	$\omega_{02}^2 = 0.602$
$\omega_{12} = 0.104$	$\omega_{12}^0 = 0.022$	$\omega_{12}^1 = 0.110$	$\omega_{12}^2 = 0.129$

The solutions of the problems (38), (39) are obtained, where the theoretical parameters values of ω (Table 2) are used, for the case $\mathrm{Fo}_1 = 0.1,\ \mathrm{Fo}_2 = 0.01,\ K_1 = 1,\ K_2 = 0.1$, and the axial distributions of the average concentrations (the points) are presented in Figs. 5 and 6.

9. Parameter identification

The obtained concentrations $C_j(R, Z_j),\ j = 1,2$ in (11), (12), for the case of

$\mathrm{Fo}_1 = 0.1,\ \mathrm{Fo}_2 = 0.01,\ K_1 = 1,\ K_2 = 0.1,$ permit to be obtained the average concentrations $\bar{C}_j\left(Z_j\right), j = 1,2$ in (35) and artificial experimental data for different $Z_j, j = 1,2$:

$$\bar{C}^m_{\mathrm{jexp}}\left(Z_{j1n}\right) = \left(0.95 + 0.1S_m\right)\bar{C}_j\left(Z_{jn}\right),$$
$$m = 1,...10,\ Z_{jn} = 0.1n,\ n = 1,2,...,10,\ j = 1,2, \tag{47}$$

where $0 \le S_m \le 1, m = 1,...,10$ are obtained by a generator of random numbers. The obtained artificial experimental data (47) are used for the illustration of the parameter identification in the average concentrations models (38), (39) by the minimization of the least-squares functions $Q_n, n = 1,2$ and Q:

$$Q_n\left(Z_n, \omega^n_{01}, \omega^n_{11}, \omega^n_{02}, \omega^n_{12}\right) =$$
$$= \sum_{m=1}^{10}\left[\bar{C}_1(Z_{1n}, \omega_{01}, \omega_{11}) - \bar{C}^m_{1\mathrm{exp}}(Z_{1n})\right]^2 +$$
$$+\left[\bar{C}_2(Z_{2n}, \omega_{02}, \omega_{12}) - \bar{C}^m_{2\mathrm{exp}}(Z_{2n})\right]^2,$$
$$Z_n = Z_{1n} = Z_{2n} = 0.1n, \quad n = 1,2;$$
$$Q\left(\omega^0_{01}, \omega^0_{11}, \omega^0_{02}, \omega^0_{12}\right) = \sum_{n=1}^{10} Q_n(Z_n, \omega_{01}, \omega_{11}, \omega_{02}, \omega_{12}), \tag{48}$$

where the values of $\bar{C}_j\left(Z_{jn}, \omega^n_{01}, \omega^n_{11}, \omega^n_{02}, \omega^n_{12}\right)$ are obtained as solutions of (38), (39) for different $Z_{jn} = 0.1n,\ n = 1,2,...,10,\ j = 1,2$. The obtained (experimental) values $\left(\omega^0_{01}, \omega^0_{11}, \omega^0_{02}, \omega^0_{12}\right)$, $\left(\omega^1_{01}, \omega^1_{11}, \omega^1_{02}, \omega^1_{12}\right)$ and $\left(\omega^2_{01}, \omega^2_{11}, \omega^2_{02}, \omega^2_{12}\right)$ are presented on the Table 2. They are used for the calculation of the functions $\bar{C}^0_1\left(Z_1, \omega^0_{01}, \omega^0_{11}\right)$, $\bar{C}^1_1\left(Z_1, \omega^1_{01}, \omega^1_{11}\right)$, $\bar{C}^2_1\left(Z_1, \omega^2_{01}, \omega^2_{11}\right)$, (the lines in Fig. 7) and $\bar{C}^0_2\left(Z_2, \omega^0_{02}, \omega^0_{12}\right)$, $\bar{C}^1_2\left(Z_2, \omega^1_{02}, \omega^1_{12}\right)$, $\bar{C}^2_2\left(Z_2, \omega^2_{02}, \omega^2_{12}\right)$, (the lines in Fig. 8). The points in Figs. 7 and 8 are the artificial experimental data (47).

The comparison of the functions (lines) and experimental data (points) in Figs. 7 and 8 shows, that the experimental data, obtained from the column with real radius and small height ($Z_j = 0.1, j = 1,2$) are useful for the parameters identifications.

10. Conclusions

The computer modeling of the mass transfer processes in column apparatuses on the base of a new approach, using convection–diffusion type model and average concentration type model, leads to calculation problems in the cases of counter-current gas-liquid or liquid-liquid processes. In these conditions the mass transfer process models are presented in two coordinates systems, because in one coordinate system one of the equations has not a solution by reason of the negative equation Laplacian value. The numerical algorithms and solutions of equations set in different coordinate systems are presented. As a result is shown, that the experimental data, obtained from the column with real radius and small height are useful for the parameters identifications in the average concentration type models.

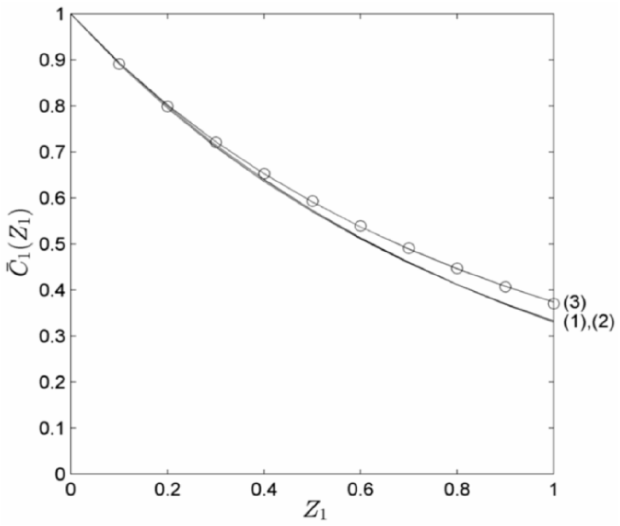

Fig. 7 *Comparison of concentration distributions (38): (1)-* $\bar{C}^1_1\left(Z_1, \omega^1_{01}, \omega^1_{11}\right)$; *(2)-* $\bar{C}^2_1\left(Z_1, \omega^2_{01}, \omega^2_{11}\right)$; *(3)-* $\bar{C}^0_1\left(Z_1, \omega^0_{01}, \omega^0_{11}\right)$; ○ *- experimental data (47).*

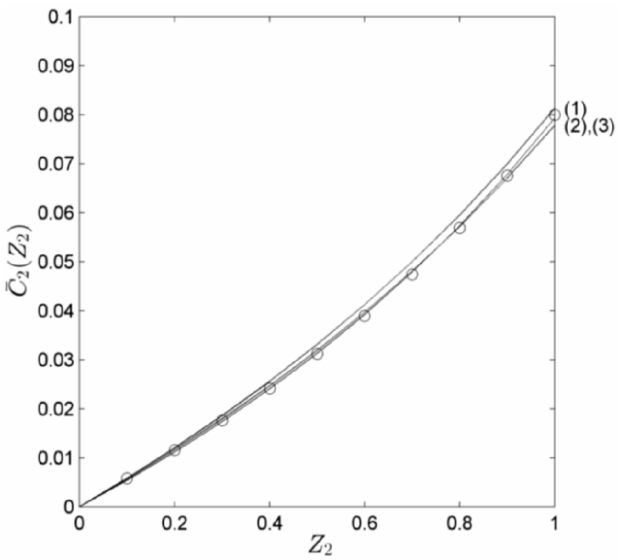

Fig. 8 *Comparison of concentration distributions (39) (1)-* $\bar{C}^1_2\left(Z_2, \omega^1_{02}, \omega^1_{12}\right)$; *(2)-* $\bar{C}^2_2\left(Z_2, \omega^2_{02}, \omega^2_{12}\right)$; *(3)-* $\bar{C}^0_2\left(Z_2, \omega^0_{02}, \omega^0_{12}\right)$; ○ *- experimental data (47).*

References

1. Boyadjiev Chr. Diffusion models and scale-up. Int. J. of Heat and Mass Transfer 2006;49: 796-799.

2.Boyadjiev Chr. Modeling of column apparatuses. Transactions of Academenergo 2009;№3:7-22.

3. Boyadjiev Chr. Theoretical Chemical Engineering. Modeling and simulation, Springer-Verlag, Berlin Heidelberg; 2010.

4. Doichinova M., Boyadjiev Chr. On the column apparatuses modeling. Int. J. Heat Mass Transfer 2012; 55: 6705-6715.

5. Boyadjiev Chr. A new approach for the column apparatuses modeling in chemical engineering. J. Appl. Math.:Advances and Aplications 2013; 10(2): 131-150.

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