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New Models of Industrial Column Absorbers. 2. Counter-current absorption process

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A theoretical analysis of the effect of the velocity radial non-uniformity on the counter-current absorption processes in the column apparatuses is presented. The 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 used in the cases of an axial modification of the radial non-uniformity of the axial velocity components in the gas and liquid phases. The modeling problem in the counter-current flows is complicated, because the model equations has to be presented in two-coordinate systems (in a one-coordinate system one of the equations has no solution due to the negative Laplacian value).

The use of experimental data, for the average concentrations in the gas and liquid phases at the column end in the cases of highly and lightly soluble gases, permits to be obtained the gas and liquid phases model parameters, related with the radial non-uniformity of the velocities. These parameter values permit to be used the average concentration models for different absorption processes modeling in counter-current columns.

Keywords: Column apparatus, gas absorption, counter-current flows, convection-diffusion model, average concentration model, velocity radial non-uniformity.

INTRODUCTION

In two papers [1, 2] was shown, 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 the column end, for a concrete process and column, permits to be obtained the model parameters, related with the radial non-uniformity of the velocity. These parameter values permit to be used the average concentration 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. This possibility will be used for modeling of the gas absorption processes in the counter-current columns, where the problem is complicated [3], because the mass transfer process models has to be presented in two-coordinate systems (in a one-coordinate system one of the equations has no s

Counter-current absorption processes

The modeling of the counter-current absorption processes uses two cylindrical coordinate systems $\left(r, z_j\right), j=1,2$ in the gas $\left(j=1\right)$ and liquid $\left(j=2\right)$ phases, i.e. the axial coordinates in the co-current models [2] must be replaced by $z=z_1, z=z_2$ in the gas and liquid phases, respectively. As a result, the convection-diffusion and average concentration models of the counter-current chemical absorption processes have the forms:

$$\begin{aligned}
& u_1 \frac{\partial c_1}{\partial z_1} = D_1\left(\frac{\partial^2 c_1}{\partial z_1^2} + \frac{1}{r}\frac{\partial c_1}{\partial r} + \frac{\partial^2 c_1}{\partial r^2}\right) - \\
& -k\left(c_1 - \chi c_2\right); \\
& u_2 \frac{\partial c_2}{\partial z_2} = D_2\left(\frac{\partial^2 c_2}{\partial z_2^2} + \frac{1}{r}\frac{\partial c_2}{\partial r} + \frac{\partial^2 c_2}{\partial r^2}\right) + \\
& +k\left(c_1 - \chi c_2\right) - k_0 c_2; \\
& r = 0, \quad \frac{\partial c_j}{\partial r} \equiv 0; \\
& r = r_0, \quad \frac{\partial c_j}{\partial r} \equiv 0; \quad j = 1,2; \\
& z_1 = 0, \quad c_1 \equiv c_1^0, \\
& u_1^0 c_1^0 \equiv u_1 c_1^0 - D_1\left(\frac{\partial c_1}{\partial z}\right)_{z=0}; \\
& z_2 = 0, \quad c_2 \equiv 0, \quad \left(\frac{\partial c_2}{\partial z}\right)_{z=0} = 0.
\end{aligned} \qquad (1)$$

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$$\alpha_1(z)\bar{u}_1\frac{d\bar{c}_1}{dz_1}+\frac{d\alpha_1}{dz_1}\bar{u}_1\bar{c}_1=D_1\frac{d^2\bar{c}_1}{dz_1^2}-k\left(\bar{c}_1-\chi\bar{c}_2\right);$$
$$\alpha_2(z)\bar{u}_2\frac{d\bar{c}_2}{dz_2}+\frac{d\alpha_2}{dz_2}\bar{u}_2\bar{c}_2=D_2\frac{d^2\bar{c}_2}{dz_2^2}+$$
$$+k\left(\bar{c}_1-\chi\bar{c}_2\right)-k_0\bar{c}_2;$$
$$z_1=0,\quad \bar{c}_1(0)\equiv c_1^0,\quad \frac{d\bar{c}_1}{dz}\equiv 0; \tag{2}$$
$$z_2=0,\quad \bar{c}_2(0)\equiv 0,\quad \frac{d\bar{c}_2}{dz}\equiv 0;$$
$$\alpha_j(z_j)=\frac{2}{r_0^2}\int_0^{r_0} r\tilde{u}_j\tilde{c}_j\,dr,\quad \tilde{u}_j(r)=\frac{u_j(r)}{\bar{u}_j},$$
$$\tilde{c}_j(r,z_j)=\frac{c_j(r,z_j)}{\bar{c}_j(z)},\quad j=1,2.$$

In (1, 2) $u_j(r), c_j(r,z_j), D_j, j=1,2$ are the velocities, concentrations and diffusivities in the gas and liquid phases, $\bar{u}_j, \bar{c}_j(z_j), j=1,2$ - the average velocities and concentrations at the column cross-sectional area, $\tilde{u}_j(r), \tilde{c}_j(r,z_j), j=1,2$ - the radial non-uniformities of the velocities and concentrations.

Generalized variables

In (1, 2) is possible to be introduced the generalized variables [4-7]:

$$r=r_0R,\quad z_1=lZ_1,\quad z_2=lZ_2,\quad u_j(r)=\bar{u}_jU_j(R),$$
$$\tilde{u}_j(r)=\frac{u_j(r)}{\bar{u}_j}=U_j(R),\quad j=1,2;$$
$$c_1(r,z_1)=c_1^0C_1(R,Z_1),\quad \bar{c}_1(z_1)=c_1^0\bar{C}_1(Z_1), \tag{3}$$
$$c_2(r,z_2)=\frac{c_1^0}{\chi}C_2(R,Z_2),\quad \bar{c}_2(z_2)=\frac{c_1^0}{\chi}\bar{C}_2(Z_2)$$

and as a result is obtained:

$$U_1\frac{\partial C_1}{\partial Z_1}=\mathrm{Fo}_1\left(\varepsilon\frac{\partial^2C_1}{\partial Z_1^2}+\frac{1}{R}\frac{\partial C_1}{\partial R}+\frac{\partial^2C_1}{\partial R^2}\right)-$$
$$-K_1\left(C_1-C_2\right);$$
$$U_2\frac{\partial C_2}{\partial Z_2}=\mathrm{Fo}_2\left(\varepsilon\frac{\partial^2C_2}{\partial Z_2^2}+\frac{1}{R}\frac{\partial C_2}{\partial R}+\frac{\partial^2C_2}{\partial R^2}\right)+$$
$$+\omega K_1\left(C_1-C_2\right)-\mathrm{Da}\,C_2; \tag{4}$$
$$R=0,\quad \frac{\partial C_j}{\partial R}\equiv 0;\quad R=1,\quad \frac{\partial C_j}{\partial R}\equiv 0;\quad j=1,2;$$
$$Z_1=0,\quad C_1\equiv 1,\quad 1\equiv U_1-\mathrm{Pe}_1^{-1}\frac{\partial C_1}{\partial Z_1};$$
$$Z_2=0,\quad C_2=0,\quad \frac{\partial C_2}{\partial Z_2}\equiv 0.$$
$$A_1(Z_1)\frac{d\bar{C}_1}{dZ_1}+\frac{dA_1}{dZ_1}\bar{C}_1=\mathrm{Pe}_1^{-1}\frac{d^2\bar{C}_1}{dZ_1^2}-K_1\left(\bar{C}_1-\bar{C}_2\right);$$
$$A_2(Z_2)\frac{d\bar{C}_2}{dZ_2}+\frac{dA_2}{dZ_2}\bar{C}_2=\mathrm{Pe}_2^{-1}\frac{d^2\bar{C}_2}{dZ_2^2}+$$
$$+\omega K_1\left(\bar{C}_1-\bar{C}_2\right)-\mathrm{Da}\,\bar{C}_2; \tag{5}$$
$$Z_1=0,\quad \bar{C}_1=1,\quad \frac{d\bar{C}_1}{dZ}=0;$$
$$Z_2=0,\quad \bar{C}_2=0,\quad \frac{d\bar{C}_2}{dZ}=0.$$

In (4, 5) Fo, Da and Pe are the Fourier, Damkohler and Peclet numbers, respectively:

$$\mathrm{Fo}_j=\frac{D_jl}{\bar{u}_jr_0^2},\quad \mathrm{Pe}_j=\frac{\bar{u}_jl}{D_j},\quad \mathrm{Da}=\frac{k_0l}{\bar{u}_2}, \tag{6}$$
$$\varepsilon=\mathrm{Fo}_j^{-1}\mathrm{Pe}_j^{-1},\quad K_1=\frac{kl}{\bar{u}_1},\quad \omega=\frac{\bar{u}_1\chi}{\bar{u}_2},\quad j=1,2.$$

In the cases of a physical absorption $\mathrm{Da}=0$.

In (5) are used the functions:

$$\bar{C}_j(Z_j)=2\int_0^1 RC_j(R,Z_j)\,dR,$$
$$\tilde{c}_j(r,z_j)=\frac{c_j(r,z_j)}{\bar{c}_j(z_j)}=\frac{C_j(R,Z_j)}{\bar{C}_j(Z_j)}, \tag{7}$$
$$\alpha_j(z_j)=\alpha_j(lZ_j)=A_j(Z_j)=$$
$$=2\int_0^1 RU_j(R)\frac{C_j(R,Z_j)}{\bar{C}_j(Z_j)}\,dR,\quad j=1,2.$$

The convection-diffusion model (4) permits to be made [1-4] 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. On this base are possible to be obtained different approximations for high column ($0=\varepsilon\le 10^{-2}$), big average velocities ($0=\mathrm{Fo}_j\le 10^{-2}$, $j=1,2$), small ($0=\mathrm{Da}\le 10^{-2}$) or big ($0=\mathrm{Da}^{-1}\le 10^{-2}$) chemical reaction rate, highly soluble ($0=\omega\le 10^{-2}$) or lightly soluble ($0=\omega^{-1}\le 10^{-2}$) gas. In the industrial absorption column [2], the model parameters have very small values:

$$\begin{aligned}&\mathrm{Fo}_1\sim 10^{-6},\quad \mathrm{Fo}_2\sim 10^{-10},\\ &\mathrm{Pe}_1^{-1}\sim 10^{-6},\quad \mathrm{Pe}_2^{-1}\sim 10^{-10}\end{aligned}\tag{8}$$

and the models (4, 5) have the convective forms:

$$\begin{aligned}&U_1\frac{dC_1}{dZ_1}=-K_1\left(C_1-C_2\right);\\ &U_2\frac{dC_2}{dZ_2}=\omega K_1\left(C_1-C_2\right)-\mathrm{Da}\,C_2;\\ &Z_1=0,\quad C_1\equiv 1;\quad Z_2=0,\quad C_2=0.\end{aligned}\tag{9}$$

$$\begin{aligned}&A_1\left(Z_1\right)\frac{d\bar{C}_1}{dZ_1}+\frac{dA_1}{dZ_1}\bar{C}_1=-K_1\left(\bar{C}_1-\bar{C}_2\right);\\ &A_2\left(Z_2\right)\frac{d\bar{C}_2}{dZ_2}+\frac{dA_2}{dZ_2}\bar{C}_2=\omega K_1\left(\bar{C}_1-\bar{C}_2\right)-\mathrm{Da}\,\bar{C}_2;\\ &Z_1=0,\quad \bar{C}_1=1;\quad Z_2=0,\quad \bar{C}_2=0.\end{aligned}\tag{10}$$

Physical absorption of the average soluble gases

In the case of physical absorption ($\mathrm{Da}=0$) of an average soluble gas ($\omega\sim 1$) from (9, 10) follows

$$\begin{aligned}&U_1\frac{dC_1}{dZ_1}=-K_1\left(C_1-C_2\right);\\ &U_2\frac{dC_2}{dZ_2}=\omega K_1\left(C_1-C_2\right);\\ &Z_1=0,\quad C_1\equiv 1;\quad Z_2=0,\quad C_2=0.\end{aligned}\tag{11}$$

$$\begin{aligned}&A_1\left(Z_1\right)\frac{d\bar{C}_1}{dZ_1}+\frac{dA_1}{dZ_1}\bar{C}_1=-K_1\left(\bar{C}_1-\bar{C}_2\right);\\ &A_2\left(Z_2\right)\frac{d\bar{C}_2}{dZ_2}+\frac{dA_2}{dZ_2}\bar{C}_2=\omega K_1\left(\bar{C}_1-\bar{C}_2\right);\\ &Z_1=0,\quad \bar{C}_1=1;\quad Z_2=0,\quad \bar{C}_2=0.\end{aligned}\tag{12}$$

The theoretical analysis of the model (12) shows [3-7], that the functions $A_j\left(Z_j\right)$, $j=1,2$ is possible to be presented as linear approximations:

$$A_j=\alpha_{j0}+\alpha_{j1}Z_j,\quad j=1,2,\tag{13}$$

where the model parameters α_{j0},α_{j1}, $j=1,2$ is possible to be obtained, using experimental data for a short column ($Z_j=0.1$, $j=1,2$).

The presented theoretical analysis shows, that the basic approximations of the convection-diffusion models (4, 9) and average concentration model (5, 10) are $\dfrac{\partial\tilde{u}_j}{\partial z_j}\equiv 0$, $j=1,2$.

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

Let's considers the velocity distributions [2]:

$$u_{jn}\left(r,z_{jn}\right)=\bar{u}_j\tilde{u}_{jn}\left(r,z_{jn}\right),\quad j=1,2\tag{14}$$

and axial step changes of the radial non-uniformity of the axial velocity components in the column:

$$\begin{aligned}&\tilde{u}_{jn}\left(r,z_{jn}\right)=\tilde{u}_{jn}\left(r_0R,lZ_{jn}\right)=\\ &\qquad=U_{jn}\left(R,Z_{jn}\right)=a_{jn}-b_{jn}R^2,\\ &a_{jn}=2-0.1n,\quad b_{jn}=2\left(1-0.1n\right),\\ &0.1n\le Z_{jn}\le 0.1\left(n+1\right),\quad n=0,1,...,9,\quad j=1,2,\end{aligned}\tag{15}$$

where the average velocities at the cross section of the column are constants, while the maximal velocities (and as a result the radial non-uniformity of the axial velocity components too) decrease along the column height.

If put (15) in (11), the model has the form:

$$\begin{aligned}&U_{1n}\frac{dC_{1n}}{dZ_{1n}}=-K_1\left(C_{1n}-C_{2n}\right),\\ &0.1n\le Z_{1n}\le 0.1\left(n+1\right);\\ &U_{2n}\frac{dC_{2n}}{dZ_{2n}}=\omega K_1\left(C_{1n}-C_{2n}\right),\\ &0.1n\le Z_{2n}\le 0.1\left(n+1\right);\\ &Z_{jn}=0.1n,\quad C_{jn}\left(R,Z_{jn}\right)=C_{j(n-1)}\left(R,Z_{jn}\right);\\ &n=0,1,...,9;\quad j=1,2;\\ &Z_{10}=0,\quad C_{10}\left(R,Z_{10}\right)\equiv 1;\\ &Z_{20}=0,\quad C_{20}\left(R,Z_{20}\right)\equiv 0.\end{aligned}\tag{16}$$

The solution of (16), using the method in [2, 8], for concrete process ($\omega=1$) and "theoretical" value of $K_1=1$, permits to be obtained the concentration distributions $C_{jn}\left(R,Z_{jn}\right)$, $j=1,2$ for different $Z_{jn}=0.1\left(n+1\right)$, $j=1,2$, $n=0,1,...,9$. These results and (7) permit to be obtained the "theoretical" average concentration values $\bar{C}_{jn}\left(Z_{jn}\right)$, $Z_{jn}=0.1\left(n+1\right)$, $j=1,2$, $n=0,1,...,9$ (the points on Fig. 1) and the function values $A_{jn}\left(Z_{jn}\right)$, $j=1,2$ (the points on Fig. 2) for different $Z_{jn}=0.1\left(n+1\right)$, $j=1,2$, $n=0,1,...,9$.

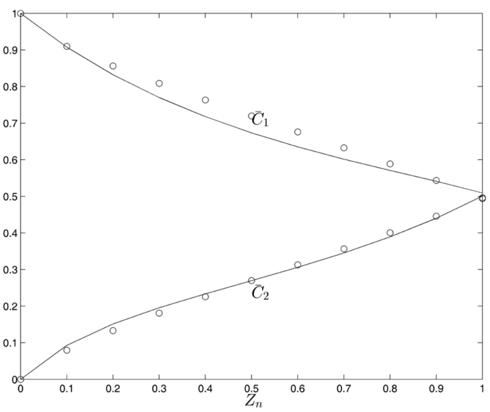

Fig. 1. Average concentration $\bar{C}_j\left(Z_j\right), j=1,2$ in the case $\omega=K_1=1$: "theoretical" values $\bar{C}_j\left(Z_j\right)=\bar{C}_{jn}\left(Z_{jn}\right), j=1,2$ as solutions of (16) and (7) for different $Z_{jn}=0.1(n+1), j=1,2, n=0,1,...,9$ (points); $\bar{C}_j\left(Z_j\right), j=1,2$ as a solution of (18), using the "experimental" parameter values $a_{j0}, a_{j1}, a_{j2}, j=1,2, K_1=K_2=\dfrac{K_1+K_2}{2}=1.05$ in the Table 1 (lines).

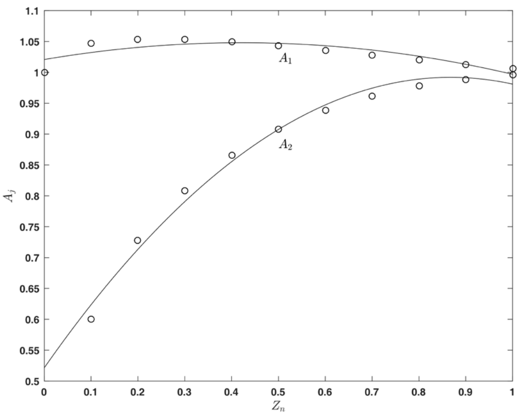

Fig. 2. Function $A_{jn}\left(Z_{jn}\right)$ for different $Z_{jn}=0.1(n+1), j=1,2, n=0,1,...,9$ (points); $A_j\left(Z_j\right), j=1,2$ as a quadratic approximation (17) (line).

From Fig. 2 is seen, that the functions $A_{jn}\left(Z_{jn}\right), n=0,1,...,4, j=1,2$ are possible to be presented as quadratic approximations:

$$A_j\left(Z_j\right)=a_{j0}+a_{j1}Z_j+a_{j2}Z_j^2, \quad j=1,2, \tag{17}$$

where the ("theoretical") values of $a_{j0}, a_{j1}, a_{j2}, j=1,2$ 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 (10) has the form:

$$\begin{gathered}\left(a_{10}+a_{11}Z_1+a_{12}Z_1^2\right)\frac{d\bar{C}_1}{dZ_1}+\\+\left(a_{11}+2a_{12}Z_1\right)\bar{C}_1=-K_1\left(\bar{C}_1-\bar{C}_2\right);\\ \left(a_{20}+a_{21}Z_2+a_{22}Z_2^2\right)\frac{d\bar{C}_2}{dZ_2}+\\+\left(a_{21}+2a_{22}Z_2\right)\bar{C}_2=\omega K_1\left(\bar{C}_1-\bar{C}_2\right);\\ Z_1=0, \quad \bar{C}_1=1; \quad Z_2=0, \quad \bar{C}_2=0.\end{gathered} \tag{18}$$

Physical absorption of highly soluble gas ($\omega=\mathrm{Da}=0$)

In the cases of physical absorption of highly soluble gas ($\omega=\mathrm{Da}=0$), from (16, 18) follows $C_{2n}=\bar{C}_{2n}\equiv 0$, and as a result the models (16, 18) have the forms:

$$\begin{gathered}U_{1n}\frac{dC_{1n}}{dZ_{1n}}=-K_1C_{1n}; \quad 0.1n\le Z_{1n}\le 0.1(n+1);\\ Z_{1n}=0.1n, \quad \mathrm{C}_{1n}\left(R,Z_{1n}\right)=C_{1(n-1)}\left(R,Z_{1n}\right);\\ n=0,1,...,9; \quad Z_{10}=0, \quad \mathrm{C}_{10}\left(R,Z_{10}\right)\equiv 1.\end{gathered} \tag{19}$$

$$\begin{gathered}\left(a_{10}+a_{11}Z_1+a_{12}Z_1^2\right)\frac{d\bar{C}_1}{dZ_1}+\left(a_{11}+2a_{12}Z_1\right)\bar{C}_1=\\ =-K_1\bar{C}_1;\\ Z_1=0, \quad \bar{C}_1=1.\end{gathered} \tag{20}$$

The solution of (19) for "theoretical" value of $K_1=1$ permits to be obtained the "theoretical" concentration distributions $C_{1n}\left(R,Z_{1n}\right)$ for different $Z_{1n}=0.1(n+1), n=0,1,...,9$. This solution of (19) and (7) permit to be obtained the "theoretical" average concentrations $\bar{C}_{1n}\left(Z_{1n}\right)$ for different $Z_{1n}=0.1(n+1), n=0,1,...,9$ (the points on the Fig. 3).

Parameters identification in the gas phase

The obtained the values of the function $\bar{C}_{1n}\left(Z_{1n}\right), Z_{1n}=0.1(n+1), n=0,1,...,9$ (using the solution of (19) and (7)), for the concrete process ($\omega=\mathrm{Da}=0$) and "theoretical" value of $K_1=1$, permit to be obtained the concentration values $\bar{C}_1(1)$ and the artificial experimental data:

$$\bar{C}_{1\exp}^m(1)=\left(0.95+0.1B_m\right)\bar{C}_1(1), \quad m=1,...,10, \tag{21}$$

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

The obtained artificial experimental data (21) are used for the parameters ($a_{10}, a_{11}, a_{12}, K_1$)

identification in the average concentrations model (20) by the minimization of the least-squares function Q_1 with respect to $a_{10}, a_{11}, a_{12}, K_1$:

$$Q_1\left(a_{10},a_{11},a_{12},K_1\right)= \\ =\sum_{m=1}^{10}\left[\bar{C}_1\left(1,a_{10},a_{11},a_{12},K_1\right)-\bar{C}^m_{1\exp}(1)\right]^2, \qquad (22)$$

where the values of $\bar{C}_1(1,a_{10},a_{11},a_{12},K_1)$ are obtained as solutions of (20), using the method in [8]. The obtained after the minimization "experimental" parameter values $a_{10}, a_{11}, a_{12}, K_1$ are compared with the "theoretical" values on the Table 1.

The obtained ("experimental") parameter values $a_{10}, a_{11}, a_{12}, K_1$ are used for the solution of (20) with the help of the method in [8] and the result (the line) is compared on Fig. 3 with the "theoretical" average concentrations $\bar{C}_{1n}\left(Z_{1n}\right)$ for different $Z_{1n}=0.1(n+1), n=0,1,...,9$ (the points).

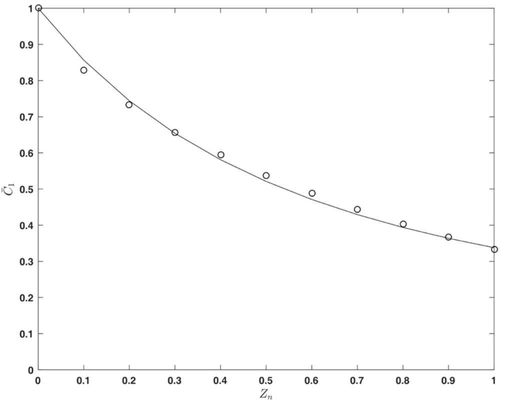

Fig. 3. Average concentration distribution $\bar{C}_1(Z)$ in the case $\omega=\mathrm{Da}=0$: "theoretical" values of $\bar{C}_{1n}\left(Z_1\right)$ for different $Z_{1n}=0.2(n+1)$, $n=0,1,...,9$ (points); $\bar{C}_1(Z)$ as solutions of (20) for "experimental" values of $a_{10}, a_{11}, a_{12}, K_1$ (line).

Physical absorption of lightly soluble gas ($\omega^{-1}=0, \mathrm{Da}=0$)

The models (16, 18) is possible to be presented as:

$$\begin{aligned}
&U_{1n}\frac{dC_{1n}}{dZ_{1n}}=-\omega^{-1}K_2\left(C_{1n}-C_{2n}\right),\\
&0.1n\le Z_{1n}\le 0.1(n+1);\\
&U_{2n}\frac{dC_{2n}}{dZ_{2n}}=K_2\left(C_{1n}-C_{2n}\right)-\mathrm{Da}\,C_{2n},\\
&0.1n\le Z_{2n}\le 0.1(n+1); \qquad (23)\\
&Z_{jn}=0.1n,\quad \mathrm{C}_{jn}\left(R,Z_n\right)=C_{j(n-1)}\left(R,Z_{jn}\right);\\
&n=0,1,...,9;\quad j=1,2;\\
&Z_{10}=0,\quad \mathrm{C}_{10}\left(R,Z_{10}\right)\equiv 1;\\
&Z_{20}=0,\quad C_{20}\left(R,Z_0\right)=0.
\end{aligned}$$

$$\begin{aligned}
&\left(a_{10}+a_{11}Z+a_{12}Z^2\right)\frac{d\bar{C}_1}{dZ_1}+\left(a_{11}+2a_{12}Z\right)\bar{C}_1=\\
&\qquad=-\omega^{-1}K_2\left(\bar{C}_1-\bar{C}_2\right);\\
&\left(a_{20}+a_{21}Z+a_{22}Z^2\right)\frac{d\bar{C}_2}{dZ_2}+\left(a_{21}+2a_{22}Z\right)\bar{C}_2= \qquad (24)\\
&\qquad=K_2\left(\bar{C}_1-\bar{C}_2\right)-\mathrm{Da}\,\bar{C}_2;\\
&Z_1=0,\quad \bar{C}_1=1;\quad Z_2=0,\quad \bar{C}_2=0.
\end{aligned}$$

In (23, 24) $K_2=\omega K_1$.

In the case of physical absorption of lightly soluble gas ($\omega^{-1}=0$, $\mathrm{Da}=0$), from (23, 24) follows $C_{1n}\equiv 1, n=0,1,...,9$ and as a result from (23, 24) is possible to be obtained:

$$\begin{aligned}
&U_{2n}\frac{dC_{2n}}{dZ_{2n}}=K_2\left(1-C_{2n}\right);\quad 0.1n\le Z_{2n}\le 0.1(n+1);\\
&Z_{2n}=0.1n,\quad \mathrm{C}_{2n}\left(R,Z_{2n}\right)=C_{2(n-1)}\left(R,Z_{2n}\right);\\
&n=0,1,...,9;\quad Z_{20}=0,\quad C_{20}\left(R,Z_{20}\right)=0.\\
&\qquad (25)
\end{aligned}$$

$$\begin{aligned}
&\left(a_{20}+a_{21}Z_2+a_{22}Z_2^2\right)\frac{d\bar{C}_2}{dZ_2}+\left(a_{21}+2a_{22}Z_2\right)\bar{C}_2=\\
&\qquad=K_2\left(1-\bar{C}_2\right);\quad (26)\\
&Z_2=0,\quad \bar{C}_2=0.
\end{aligned}$$

The solution of (25) for "theoretical" value of $K_2=1$ (dimensionless interphase mass transfer coefficient in the liquid phase) permits to be obtained the "theoretical" concentration distributions $C_{2n}\left(R,Z_{2n}\right)$ for different $Z_{2n}=0.1(n+1), n=0,1,...,9$. This solution of (25) and (7) permit to be obtained the "theoretical" average concentration values $\bar{C}_{2n}\left(Z_{2n}\right)$ for different $Z_{2n}=0.1(n+1)$, $n=0,1,...,9$ (the points on the Fig. 4).

Parameters identification in the liquid phase

The obtained the values of the function $\bar{C}_{2n}\left(Z_{2n}\right), Z_{2n}=0.1(n+1), n=0,1,\ldots,9$ (using the solution of (25) and (7)), for the concrete process ($\omega^{-1}=0, \mathrm{Da}=0$) and "theoretical" value of $K_2=1$, permit to be obtained the concentration values $\bar{C}_2(1)$ and the artificial experimental data:

$$\bar{C}_{2\exp}^{m}(1)=\left(0.95+0.1B_m\right)\bar{C}_2(1), \quad m=1,\ldots,10, \quad (27)$$

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

The obtained artificial experimental data (27) are used for the parameters ($a_{20}, a_{21}, a_{22}, K_2$) identification in the average concentrations model (26) by the minimization of the least-squares function Q_2 with respect to $a_{20}, a_{21}, a_{22}, K_2$:

$$Q_2\left(a_{20}, a_{21}, a_{22}, K_2\right)= =\sum_{m=1}^{10}\left[\bar{C}_2\left(1, a_{20}, a_{21}, a_{22}, K_2\right)-\bar{C}_{2\exp}^{m}(1)\right]^2, \quad (28)$$

where the values of $\bar{C}_2(1, a_{20}, a_{21}, a_{22}, K_2)$ are obtained as solutions of (26), using the method in [8]. The obtained after the minimization "experimental" parameter values $a_{20}, a_{21}, a_{22}, K_2$ are compared with the "theoretical" values on the Table 1.

The obtained ("experimental") parameter values $a_{20}, a_{21}, a_{22}, K_2$ are used for the solution of (26) with the help of the method in [8] and the result (the line) is compared on Fig. 4 with the "theoretical" average concentrations $\bar{C}_{2n}\left(Z_{2n}\right)$ for different $Z_{2n}=0.1(n+1), n=0,1,\ldots,9$ (the points).

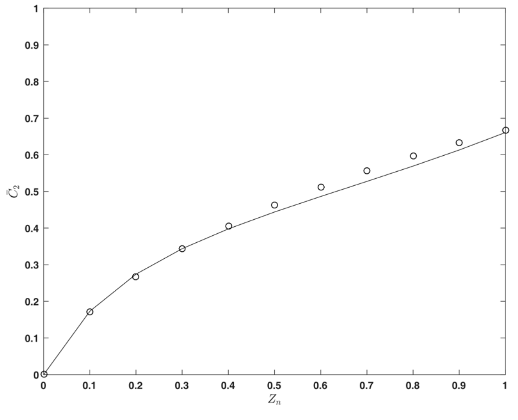

Fig. 4. Average concentration distribution $\bar{C}_2(Z)$ in the case $\omega^{-1}=0, \mathrm{Da}=0$: "theoretical" values of $\bar{C}_{2n}\left(Z_2\right)$ for different $Z_{2n}=0.2(n+1)$, $n=0,1,\ldots,9$ (points); $\bar{C}_2(Z)$ as solutions of (26) for "experimental" values of $a_{20}, a_{21}, a_{22}, K_2$ in the Table 1 (line).

Model parameters in the cases of average soluble gases

The parameters $a_{j0}, a_{j1}, a_{j2}, j=1,2,$ in the model (18) are related with the velocity nonuniformity in the column, only. Their "experimental" values are obtained in the cases of absorption of highly and lightly gases (Table 1). The parameter K_1 in (18) must be obtained from the experimental values of K_1 and K_2 in the Table 1 as $K_1=\dfrac{K_1+K_2}{2}=1.05$. The solution of (18), using the experimental parameter values in Table 1 and $K_1=1.05$, leads to the average concentrations in the Fig. 1 (lines).

Effect of the gas solubility

The procedure for determining the concentrations in (18) is repeated for different values of the Henry's number ($\chi=0.5, 1.5$) and the results are presented on the Figs. 5, 6.

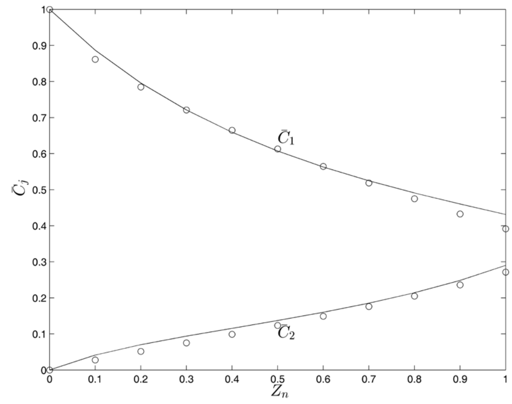

Fig. 5. Average concentration $\bar{C}_j\left(Z_j\right), j=1,2$ in the cases $\omega=0.5, K_1=1$: "theoretical" values $\bar{C}_j\left(Z_j\right)=\bar{C}_{jn}\left(Z_{jn}\right), j=1,2$ as solutions of (11) and (7) for different $Z_{jn}, n=0,1,\ldots,9$ (points); $\bar{C}_j\left(Z_j\right), j=1,2$ as solutions of (16) for "experimental" values of $a_{j0}, a_{j1}, a_{j2}, j=1,2, K_1=1.05$ in the Table 1 (lines).

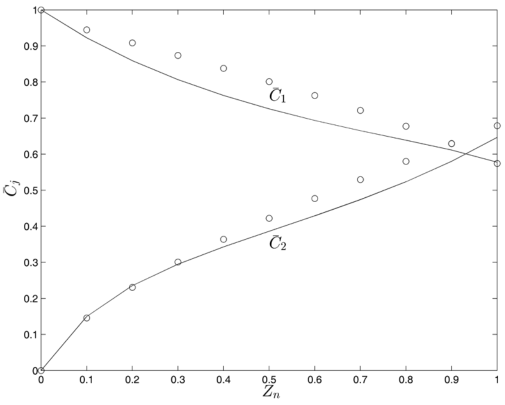

Fig. 6. Average concentration $\bar{C}_j\left(Z_j\right), j=1,2$ in the cases $\omega=1.5, K_1=1$: “theoretical” values $\bar{C}_j\left(Z_j\right)=\bar{C}_{jn}\left(Z_{jn}\right), j=1,2$ as solutions of (11) and (7) for different $Z_{jn}, n=0,1,...,9$ (points); $\bar{C}_j\left(Z_j\right), j=1,2$ as solutions of (16) for “experimental” values of $a_{j0}, a_{j1}, a_{j2}, j=1,2, K_1=1.05$ in the Table 1 (lines).

Table 1. Parameters $a_{j0}, a_{j1}, a_{j2}, K_j, j=1,2,$ (physical absorption).

Parameters	“Theoretical” values	“Experimental” values
a_{10}	0.919	0.567
a_{11}	0.420	0.443
a_{12}	–0.427	–0.420
a_{20}	0.433	0.414
a_{21}	1.105	0.910
a_{22}	–0.632	–0.766
K_1	1	1.077
K_2	1	1.029

Chemical absorption

In the case of chemical absorption, from (9, 10, 16, 18) follow the models:

$$\begin{aligned}
&U_{1n}\frac{dC_{1n}}{dZ_{1n}}=-K_1\left(C_{1n}-C_{2n}\right),\\
&0.1n\le Z_{1n}\le 0.1\left(n+1\right);\\
&U_{2n}\frac{dC_{2n}}{dZ_{2n}}=\omega K_1\left(C_{1n}-C_{2n}\right)-\mathrm{Da}\,C_{2n},\\
&0.1n\le Z_{2n}\le 0.1\left(n+1\right);\\
&Z_{jn}=0.1n,\quad \mathrm{C}_{jn}\left(R,Z_n\right)=C_{j(n-1)}\left(R,Z_{jn}\right);\\
&n=0,1,...,9;\quad j=1,2;\\
&Z_{10}=0,\quad \mathrm{C}_{10}\left(R,Z_{10}\right)\equiv 1;\\
&Z_{20}=0,\quad C_{20}\left(R,Z_0\right)=0.
\end{aligned} \qquad (28)$$

$$\begin{aligned}
&\left(a_{10}+a_{11}Z+a_{12}Z^2\right)\frac{d\bar{C}_1}{dZ_1}+\left(a_{11}+2a_{12}Z\right)\bar{C}_1=\\
&\qquad\qquad=-K_1\left(\bar{C}_1-\bar{C}_2\right);\\
&\left(a_{20}+a_{21}Z+a_{22}Z^2\right)\frac{d\bar{C}_2}{dZ_2}+\left(a_{21}+2a_{22}Z\right)\bar{C}_2=\\
&\qquad\qquad=\omega K_1\left(\bar{C}_1-\bar{C}_2\right)-\mathrm{Da}\,\bar{C}_2;\\
&Z_1=0,\quad \bar{C}_1=1;\quad Z_2=0,\quad \bar{C}_2=0.
\end{aligned} \qquad (29)$$

The solution of (28) for a concrete processes ($\omega=1, \mathrm{Da}=1,2$) and a “theoretical” value of $K_1=1$ permits to be obtained the concentration distributions $C_{jn}\left(R,Z_{jn}\right), j=1,2$ for different $Z_{jn}=0.1\left(n+1\right), j=1,2, n=0,1,...,9$. This solution of (28) and (7) permit to be obtained the “theoretical” average concentration $\bar{C}_{jn}\left(Z_{jn}\right), Z_{jn}=0.1\left(n+1\right), j=1,2, n=0,1,...,9$ (the points in the Figs. 7, 8).

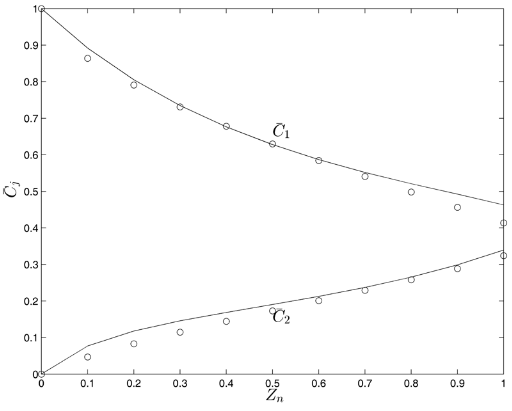

Fig. 7. Average concentration $\bar{C}_j\left(Z_j\right), j=1,2$ in the cases $\omega=1, \mathrm{Da}=1$: “theoretical” values $\bar{C}_j\left(Z_j\right)=\bar{C}_{jn}\left(Z_{jn}\right), j=1,2$ as solutions of (28) and (7) for different $Z_{jn}=0.1\left(n+1\right), j=1,2, n=0,1,...,9$

(points); $\bar{C}_j\left(Z_j\right), j=1,2$ as a solution of (29), using the "experimental" parameter values $a_{j0}, a_{j1}, a_{j2}, j=1,2$ in the Table 1 (lines) and the "experimental" value of $K_1=1.05$.

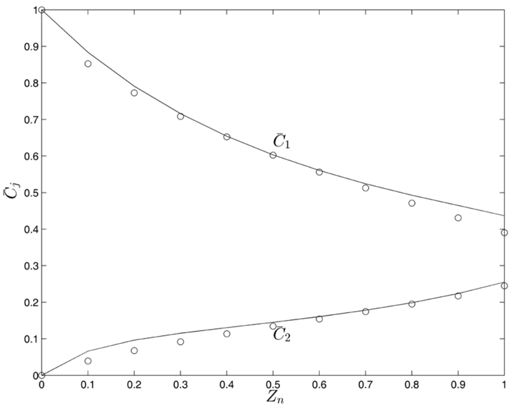

Fig. 8. Average concentration $\bar{C}_j\left(Z_j\right), j=1,2$ in the cases $\omega=1, \mathrm{Da}=2$: "theoretical" values $\bar{C}_j\left(Z_j\right)=\bar{C}_{jn}\left(Z_{jn}\right), j=1,2$ as solutions of (28) and (7) for different $Z_{jn}=0.1(n+1), j=1,2, n=0,1,...,9$ (points); $\bar{C}_j\left(Z_j\right), j=1,2$ as a solution of (29), using the "experimental" parameter values $a_{j0}, a_{j1}, a_{j2}, j=1,2$ in the Table 1 (lines) and the "experimental" value of $K_1=1.05$.

CONCLUSIONS

The modeling of the counter-current processes in column apparatuses is complicated because the hydrodynamic models has to be presented in two-coordinate system (in a one-coordinate system one of the equations has no solution due to the negative Laplacian value). The presented numerical analysis of a counter-current absorption process in column apparatus shows, that the average concentration model, where the radial velocity components in the phases are equal to zero (in the cases of constant velocity radial non-uniformities along the column height), is possible to be used in the cases of an axial modification of the radial non-uniformities of the axial velocity components.

The use of experimental data, for the average concentrations in the gas and liquid phases at the column end in the cases of highly and lightly soluble gases, permits to be obtained the gas and liquid phases model parameters, related with the radial non-uniformity of the velocities. These parameter values permit to be used the average concentration models for different absorption processes modeling in counter-current columns (different values of the parameters ω, Da, i.e. different values of the column height, average velocities, chemical reaction rate constant and gas solubility).

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НОВИ МОДЕЛИ НА ИНДУСТРИАЛНИ КОЛОННИ АБСОРБЕРИ.
2. ПРОТИВОТОЧНИ АБСОРБЦИОННИ ПРОЦЕСИ

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(Резюме)

Представен е теоретичен анализ на ефекта на радиалната неравномерност на скоростта при противоточни абсорбционни процеси в колонни апарати. Моделът на средните концентрации, където радиалната компонента на скоростта е нула (в случаите на постоянна радиална неравномерност на скоростта по височината на колоната), е използван в случаите на аксиално изменение на радиалната неравномерност на аксиалните компоненти на скоростите в газовата и течната фази. Проблемът на моделирането при противоточните потоци е усложнен, защото моделните уравнения трябва да се представят в две координатни системи (в една координатна система уравненията нямат решение поради отрицателната стойност на Лапласиана).

Използването на експериментални данни за средните концентрации в газовата и течната фази на изхода им от колоната, в случаите на силно и слабо разтворими газове, позволява да се намерят моделните параметри, свързани с радиалната неравномерност на скоростите. Стойностите на тези параметри са използвани за намиране на моделите на средните концентрации за моделиране на различни адсорбционни процеси в противоочни колони.