Bulgarian Chemical Communications, Volume 49, Number 3, (pp. 711 – 719) 2017

New models of industrial column absorbers. 1. Co-current absorption processes

B. Boyadjiev, Chr. Boyadjiev*

Institute of Chemical Engineering, Bulgarian Academy of Sciences, Acad. St. Angelov str., Bl. 103, 1113 Sofia, Bulgaria

Received July 20, 2016; Revised February 2, 2017

A new approach to modeling the industrial column absorbers is presented. A theoretical analysis of the effect of the velocity radial non-uniformity on the co-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 use of experimental data, for the average concentrations in the gas and liquid phases at the column end, for a concrete process (absorption of an average soluble gas), permits to be obtained the gas and liquid phase 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 co-current columns.

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

INTRODUCTION

In the first paper [1] 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 a co-current column.

CO-CURRENT ABSORPTION PROCESSES

The new approach of the processes modeling in the column apparatuses [2-5] permits to be created the convection-diffusion and average concentration models of the gas absorption process. In the cases of a constant radial non-uniformity of the velocities along the column height $\left(u_j = u_j(r),\ j=1,2\right)$, the convection-diffusion and average concentration models of a chemical absorption (with a pseudo-first-order chemical reaction in the liquid phase) in a co-current column [6] have the forms:

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

$$
\begin{gathered}
\alpha_1(z) \bar{u}_1 \frac{d\bar{c}_1}{dz} + \frac{d\alpha_1}{dz} \bar{u}_1 \bar{c}_1 = D_1 \frac{d^2 \bar{c}_1}{dz^2} - \\
-k\left(\bar{c}_1 - \chi \bar{c}_2\right); \\
\alpha_2(z) \bar{u}_2 \frac{d\bar{c}_2}{dz} + \frac{d\alpha_2}{dz} \bar{u}_2 \bar{c}_2 = D_2 \frac{d^2 \bar{c}_2}{dz^2} + \\
+k\left(\bar{c}_1 - \chi \bar{c}_2\right) - k_0 \bar{c}_2; \\
z=0, \quad \bar{c}_1(0) \equiv c_1^0, \quad \bar{c}_2(0) \equiv 0, \qquad (2) \\
\frac{d\bar{c}_1}{dz} \equiv 0, \quad \frac{d\bar{c}_2}{dz} \equiv 0;
\end{gathered}
$$

$$
\alpha_j(z) = \frac{2}{r_0^2} \int_0^{r_0} r \tilde{u}_j \tilde{c}_j \, dr, \quad \tilde{u}_j(r) = \frac{u_j(r)}{\bar{u}_j},
$$

$$
\tilde{c}_j(r,z) = \frac{c_j(r,z)}{\bar{c}_j(z)}, \quad j=1,2.
$$

---

* To whom all correspondence should be sent:
E-mail: chr.boyadjiev@gmail.com

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

GENERALIZED VARIABLES

In (1), (2) is possible to be introduced the generalized variables:

$$\begin{gathered} r=r_0R, \quad z=lZ, \quad u_j(r)=\bar{u}_jU_j(R), \\ c_1(r,z)=c_1^0C_1(R,Z), \\ c_2(r,z)=\frac{c_1^0}{\chi}C_2(R,Z), \quad \bar{c}_1(z)=c_1^0\bar{C}_1(Z), \\ \bar{c}_2(z)=\frac{c_1^0}{\chi}\bar{C}_2(Z), \end{gathered} \tag{3}$$

and as a result is obtained:

$$\begin{gathered} U_1\frac{\partial C_1}{\partial Z}=\mathrm{Fo}_1\left(\varepsilon\frac{\partial^2 C_1}{\partial Z^2}+\frac{1}{R}\frac{\partial C_1}{\partial R}+\frac{\partial^2 C_1}{\partial R^2}\right)- \\ -K_1(C_1-C_2); \\ U_2\frac{\partial C_2}{\partial Z}=\mathrm{Fo}_2\left(\varepsilon\frac{\partial^2 C_2}{\partial Z^2}+\frac{1}{R}\frac{\partial C_2}{\partial R}+\frac{\partial^2 C_2}{\partial R^2}\right)+ \\ +K_2(C_1-C_2)-\mathrm{Da}\,C_2; \\ R=0, \quad \frac{\partial C_j}{\partial R}\equiv 0; \\ R=1, \quad \frac{\partial C_j}{\partial R}\equiv 0; \quad j=1,2; \\ Z=0, \quad C_1\equiv 1, \quad C_2=0, \\ 1\equiv U_1-\mathrm{Pe}_1^{-1}\frac{\partial C_1}{\partial Z}, \quad \frac{\partial C_2}{\partial Z}\equiv 0. \end{gathered} \tag{4}$$

$$\begin{gathered} A_1(Z)\frac{d\bar{C}_1}{dZ}+\frac{dA_1}{dZ}\bar{C}_1=\mathrm{Pe}_1^{-1}\frac{d^2\bar{C}_1}{dZ^2}- \\ -K_1\left(\bar{C}_1-\bar{C}_2\right); \\ A_2(Z)\frac{d\bar{C}_2}{dZ}+\frac{dA_2}{dZ}\bar{C}_2=\mathrm{Pe}_2^{-1}\frac{d^2\bar{C}_2}{dZ^2}+ \\ +K_2\left(\bar{C}_1-\bar{C}_2\right)-\mathrm{Da}\,\bar{C}_2; \\ Z=0, \quad \bar{C}_1=1, \quad \bar{C}_2=0, \\ \frac{d\bar{C}_1}{dZ}=0, \quad \frac{d\bar{C}_2}{dZ}=0, \end{gathered} \tag{5}$$

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

$$\begin{gathered} \mathrm{Fo}_j=\frac{D_jl}{\bar{u}_jr_0^2}, \quad \mathrm{Pe}_j=\frac{\bar{u}_jl}{D_j}, \quad \mathrm{Da}=\frac{k_0l}{\bar{u}_2}, \\ \varepsilon=\mathrm{Fo}_j^{-1}\mathrm{Pe}_j^{-1}, \\ K_1=\frac{kl}{\bar{u}_1}, \quad K_2=\omega K_1, \quad \omega=\frac{\bar{u}_1\chi}{\bar{u}_2}, \quad j=1,2. \end{gathered} \tag{6}$$

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

In (5) are used the expressions:

$$\begin{gathered} \bar{C}_j(Z)=2\int_0^1 RC_j(R,Z)\,dR, \\ \tilde{c}_j(r,z)=\frac{c_j(r,z)}{\bar{c}_j(z)}=\frac{C_j(R,Z)}{\bar{C}_j(Z)}, \\ \alpha_j(z)=\alpha_j(lZ)=A_j(Z)= \\ =2\int_0^1 RU_j(R)\frac{C_j(R,Z)}{\bar{C}_j(Z)}dR, \quad j=1,2 \end{gathered} \tag{7}$$

The convection-diffusion model (4) permits to be made [2-6] 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.

PHYSICAL ABSORPTION OF AVERAGE SOLUBLE GAS

Let’s consider the physical absorption ($\mathrm{Da}=0$) of an average soluble gas ($\omega \approx 1$)? in an industrial absorption column ($l>1$ [m]), in the cases of down co-current gas-liquid drops flow. The average gas velocity and the average liquid drops velocity are $\bar{u}_1>1, \bar{u}_2>1$ [m.s^{-1}], the diffusivities in the gas (air) and the liquid (water) are $D_1<10^{-4}, D_2<10^{-9}$ [m^2.s^{-1}] . In these conditions is possible to be obtained the order of magnitude of the parameters values:

$$\begin{gathered} \mathrm{Pe}_1^{-1}<10^{-4}, \quad \frac{r_0}{l}>10^{-1}, \quad \mathrm{Fo}_1<10^{-2}, \\ \mathrm{Pe}_2^{-1}<10^{-9}, \quad \mathrm{Fo}_2<10^{-7}, \end{gathered} \tag{8}$$

and the model (4) has a convective form:

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

In the conditions (8) the average concentration model (5) has the form:

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

The theoretical analysis of the model (9) shows [2-6], that the functions $A_j(Z),\ j = 1,2$ is possible to be presented as linear approximations:

$$
A_j = \alpha_{j0} + \alpha_{j1}Z, \quad j = 1,2, \tag{11}
$$

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

The theoretical analysis [6] shows, that the basic approximations of the convection-diffusion models (1) and average concentration models (2) are $\partial\tilde{u}_j / \partial z \equiv 0,\ j = 1,2.$.

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

The radial non-uniformity of the axial velocity components in a co-current column apparatus is the result of the fluid hydrodynamics at the column inlet, where it is a maximum and decreases along the column height as a result of the fluid viscosity. For a theoretical analysis of the effect of the axial modification of the radial non-uniformities of the velocities in a two phases co-current column, this difficulty can be circumvented by appropriate hydrodynamic model, where the average velocities in the phases at the cross section of the column are constants, while the maximal velocities (and as a result the radial non-uniformity of the axial velocities components too) decrease along the column height.

Let's considers [1, 7] the velocity distributions

$$
u_{jn}\left(r, z_n\right) = \bar{u}_j \tilde{u}_{jn}\left(r, z_n\right), \quad j = 1,2 \tag{12}
$$

and an axial step change of the radial non-uniformity of the axial velocity component in a column:

$$
\begin{aligned}
&\tilde{u}_{jn}\left(r, z_n\right) = \tilde{u}_{jn}\left(r_0 R, l Z_n\right) =\\
&= U_{jn}\left(R, Z_n\right) = a_{jn} - b_{jn}R^2,\\
&a_{jn} = 2 - 0.1n, \quad b_{jn} = 2\left(1 - 0.1n\right),\\
&0.1n \le Z_n \le 0.1\left(n+1\right),\\
&n = 0,1,\ldots,9, \quad j = 1,2,
\end{aligned} \tag{13}
$$

where $\tilde{u}_{jn}\left(r, z_n\right),\ j = 1,2$ satisfy the equations:

$$
\frac{2}{r_0^{\,2}} \int\limits_0^{r_0} r\tilde{u}_{jn}\left(r, z_n\right) dr = 1, \quad j = 1,2, \tag{14}
$$

i.e. $\bar{u}_j = const,\ j = 1.2.$

If put (13) in (9), the convection-diffusion model has the form:

$$
\begin{aligned}
&U_{1n} \frac{dC_{1n}}{dZ_n} = -K_1\left(C_{1n} - C_{2n}\right);\\
&U_{2n} \frac{dC_{2n}}{dZ_n} = \omega K_1\left(C_{1n} - C_{2n}\right);\\
&0.1n \le Z_n \le 0.1\left(n+1\right);\\
&Z_n = 0.1n, \quad \mathrm{C}_{jn}\left(R, Z_n\right) = C_{j(n-1)}\left(R, Z_n\right);\\
&n = 0,1,\ldots,9; \quad j = 1,2;\\
&Z_0 = 0, \quad \mathrm{C}_{10}\left(R, Z_0\right) \equiv 1, \quad C_{20}\left(R, Z_0\right) = 0.
\end{aligned} \tag{15}
$$

The parameter ω in (15) is known beforehand. The solution of (15), for concrete process $\left(\omega = 1\right)$ and "theoretical" value of $K_1 = 1$, permits to be obtained the concentration distributions $C_{jn}\left(R, Z_n\right),\ j = 1,2$ for different $Z_n = 0.1\left(n+1\right),\ n = 0,1,\ldots,9$ (Fig. 1).

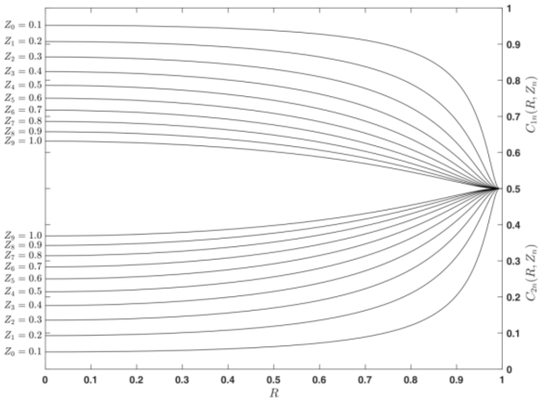

Fig. 1. Concentration distributions $C_{jn}\left(R, Z_n\right),\ j = 1,2$ in the case $\omega = K_1 = 1$ for different $Z_n = 0.1\left(n+1\right),\ n = 0,1,\ldots,9.$

The solution of (15) (Fig. 1) and (7) permit to be obtained the "theoretical" average concentration distributions $\bar{C}_{jn}\left(Z_n\right),\ j = 1,2$ (the points in the Fig. 2) and the functions $A_{jn}\left(Z_n\right),\ j = 1,2$ (the points in the Fig. 3) for different $Z_n = 0.1(n+1),\ n = 0,1,...,9.$

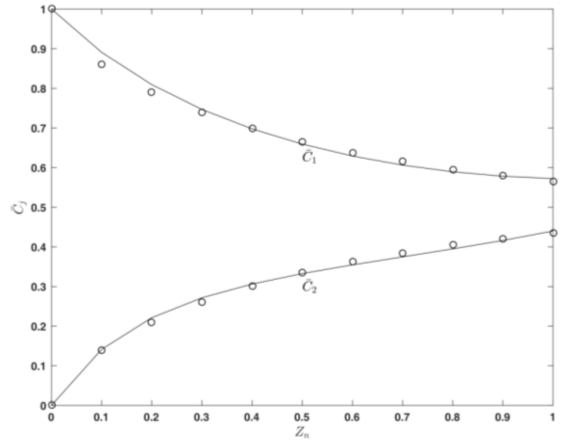

Fig. 2. Average concentration $\bar{C}_j(Z),\ j=1,2$ in the case $\omega = K_1 = 1$: "theoretical" values $\bar{C}_j(Z) = \bar{C}_{jn}(Z_n),\ j=1,2$ as solutions of (15) and (7) for different $Z_n = 0.1(n+1),\ n = 0,1,...,9$ (points); $\bar{C}_j(Z),\ j=1,2$ as a solution of (17), using the "experimental" parameter values $a_{j0}, a_{j1}, a_{j2},\ j=1,2,K_1$ (lines).

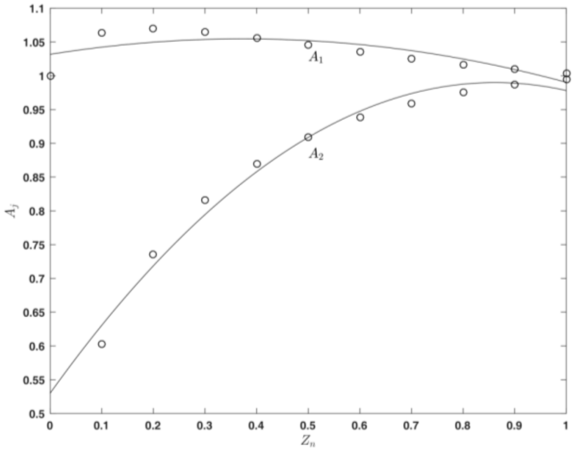

Fig. 3. Function $A_{jn}(Z_n),\ j=1,2$ in the case $\omega = K_1 = 1$: as a solution of (15) and (7) for different $Z_n = 0.1(n+1),\ n = 0,1,...,9$ (points); $A_j(Z),\ j=1,2$ as a quadratic approximation (16) (lines).

From Fig. 3 is seen, that the functions $A_{jn}(Z_n), n = 0,1,...,4,\ j=1,2$ are possible to be presented as quadratic approximations:

$$A_1(Z) = a_{10} + a_{11}Z + a_{12}Z^2, \qquad (16)$$
$$A_2(Z) = a_{20} + a_{21}Z + a_{22}Z^2,$$

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:

$$\begin{gathered}
\left(a_{10} + a_{11}Z + a_{12}Z^2\right)\frac{d\bar{C}_1}{dZ} + \\
+\left(a_{11} + 2a_{12}Z\right)\bar{C}_1 = -K_1\left(\bar{C}_1 - \bar{C}_2\right); \\
\left(a_{20} + a_{21}Z + a_{22}Z^2\right)\frac{d\bar{C}_2}{dZ} + \\
+\left(a_{21} + 2a_{22}Z\right)\bar{C}_2 = \omega K_1\left(\bar{C}_1 - \bar{C}_2\right); \\
Z = 0, \quad \bar{C}_1 = 1, \quad \bar{C}_2 = 0.
\end{gathered} \qquad (17)$$

where, at an unknown velocity distribution in the two phases, ω is known beforehand for a concrete process, while the parameters $K_1, a_{j0}, a_{j1}, a_{j2},\ j=1,2$ must be obtained, using experimental data.

PARAMETERS IDENTIFICATION

The obtained the values of the functions $\bar{C}_{jn}(Z_n),\ j=1,2,$ for a concrete process $(\omega=1)$, "theoretical" value of $K_1 = 1$ and different $Z_n = 0.1(n+1),\ n = 0,1,...,9$ (Fig. 2), permit to be obtained the values of $\bar{C}_j(1) = \bar{C}_{j9}(Z_9), Z_9 = 1,\ j=1,2$ and the artificial experimental data:

$$\begin{gathered}
\bar{C}^m_{j\exp}(1) = \left(0.95 + 0.1B_m\right)\bar{C}_j(1), \\
j = 1,2, \quad m = 1,...,10,
\end{gathered} \qquad (18)$$

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

The obtained artificial experimental data (18) are used for the illustration of the parameters ($K_1, a_{j0}, a_{j1}, a_{j2},\ j=1,2$ $a_{j0}, a_{j1}, a_{j2},\ j=1,2, K_1$) identification in the average concentrations model (17) by the minimization of the least-squares function with respect to $K_1, a_{j0}, a_{j1}, a_{j2},\ j=1,2$:

$$\begin{gathered}
Q\left(1, K_1, a_{j0}, a_{j1}, a_{j2}, j=1,2\right) = \\
= \sum_{m=1}^{10}\left[\begin{matrix}\bar{C}_1\left(1, K_1, a_{j0}, a_{j1}, a_{j2}, j=1,2\right) - \\ -\bar{C}^m_{1\exp}(1)\end{matrix}\right]^2 + \\
+ \sum_{m=1}^{10}\left[\begin{matrix}\bar{C}_2\left(1, K_1, a_{j0}, a_{j1}, a_{j2}, j=1,2\right) - \\ -\bar{C}^m_{2\exp}(1)\end{matrix}\right]^2,
\end{gathered} \qquad (19)$$

where the values of $\bar{C}_i\left(1, K_1, a_{j0}, a_{j1}, a_{j2}, j=1,2\right),\ i=1,2$ are obtained as solutions of (17). The obtained (after the minimization) “experimental” parameter values $K_1, a_{j0}, a_{j1}, a_{j2},\ j=1,2$ are compared with the “theoretical” values on the Table 1.

Table 1. Parameters $K_1, a_{j0}, a_{j1}, a_{j2},\ j=1,2$ (physical absorption).

Parameters	“Theoretical” values	“Experimental” values
a_{10}	1.0318	0.9348
a_{11}	0.1226	0.1286
a_{12}	−0.1640	−0.1616
a_{20}	0.5301	0.5547
a_{21}	1.0671	1.0267
a_{22}	−0.6190	−0.6300
K_1	1	1.0637

The obtained (“experimental”) parameter values $K_1, a_{j0}, a_{j1}, a_{j2},\ j=1,2$ are used for the solution of (17) and the results (the lines) are compared with the “theoretical” average concentration values on the Fig. 2.

The obtained “experimental” value of K_1 permits to be obtained the “experimental” value of the interphase mass transfer coefficient $k = K_1 \bar{u}_1 / l$.

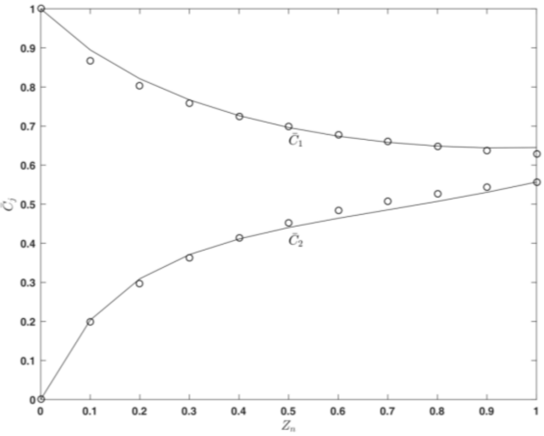

Fig. 4. Average concentration distribution $\bar{C}_j(Z),\ j=1,2$ in the case $\omega = 1.5$: “theoretical” values as solutions of (15) and (7) for different $Z_n = 0.1(n+1),\ n = 0,1,...,9$ (points); as a solution of (17), using the “experimental” parameter values $K_1, a_{j0}, a_{j1}, a_{j2},\ j=1,2$ (lines).

In the same velocities distribution in the phases (the same “experimental” values of $K_1, a_{j0}, a_{j1}, a_{j2},\ j=1,2$ in the Table 1), for other concrete process ($\omega = 1.5$), the solution of (15) and (7) permit to be obtained the “theoretical” average concentrations $\bar{C}_j(Z),\ j=1,2$, which are compared (Fig. 4), with the solution of (17), using the “experimental” values of $K_1, a_{j0}, a_{j1}, a_{j2},\ j=1,2$ in the Table 1.

CHEMICAL ABSORPTION

In the case of chemical absorption, from (4, 5, 8, 16) follow the models:

$$\begin{gathered}
U_{1n}\frac{dC_{1n}}{dZ_n} = -K_1\left(C_{1n} - C_{2n}\right);\\
U_{2n}\frac{dC_{2n}}{dZ_n} = \omega K_1\left(C_{1n} - C_{2n}\right) - \mathrm{Da}\, C_{2n};\\
0.1n \le Z_n \le 0.1(n+1);\\
Z_n = 0.1n,\quad C_{jn}\left(R, Z_n\right) = C_{j(n-1)}\left(R, Z_n\right);\\
n = 0,1,...,4;\quad j = 1,2;\\
Z_0 = 0,\quad C_{10}\left(R, Z_0\right) \equiv 1,\quad C_{20}\left(R, Z_0\right) = 0.
\end{gathered} \tag{20}$$

$$\begin{gathered}
\left(a_{10} + a_{11}Z + a_{12}Z^2\right)\frac{d\bar{C}_1}{dZ} +\\
+\left(a_{11} + 2a_{12}Z\right)\bar{C}_1 = -K_1\left(\bar{C}_1 - \bar{C}_2\right);\\
\left(a_{10} + a_{21}Z + a_{22}Z^2\right)\frac{d\bar{C}_2}{dZ} +\\
+\left(a_{21} + 2a_{22}Z\right)\bar{C}_2 = \omega K_1\left(\bar{C}_1 - \bar{C}_2\right) - \mathrm{Da}\,\bar{C}_2;\\
Z = 0,\quad \bar{C}_1 = 1,\quad \bar{C}_2 = 0.
\end{gathered} \tag{21}$$

The parameters ω, Da in (20), (21) are known beforehand. The solution of (20) for a concrete process ($\omega = 1, \mathrm{Da} = 1$) and a “theoretical” value of $K_1 = 1$ permits to be obtained the concentration distributions $C_{jn}(R, Z_n),\ j=1,2$ for different $Z_n = 0.1(n+1),\ n = 0,1,...,9$ (Fig. 5).

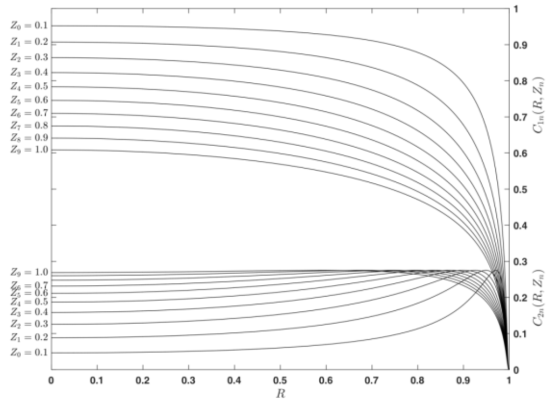

Fig. 5. Concentration distributions $C_{jn}(R, Z_n),\ j=1,2$ in the case $\omega = \mathrm{Da} = K_1 = 1$ for different $Z_n = 0.1(n+1),\ n = 0,1,...,9$ (chemical absorption).

The solution of (20) (Fig. 5) and (7) permit to be obtained the "theoretical" average concentration $\bar{C}_{jn}\left(Z_n\right),\ j=1,2$ (the points in the Fig. 6) and the functions $A_{jn}\left(Z_n\right),\ j=1,2$ (the points in the Fig. 7) for different $Z_n=0.1(n+1),\ n=0,1,...,9$.

From Fig. 7 is seen, that the functions $A_{jn}\left(Z_n\right),\ Z_n=0.1(n+1),\ n=0,1,...,9$ are possible to be presented as quadratic approximations (16) and the "theoretical" values of $a_{j0}, a_{j1}, a_{j2},\ j=1,2,$ are presented in the Table 2.

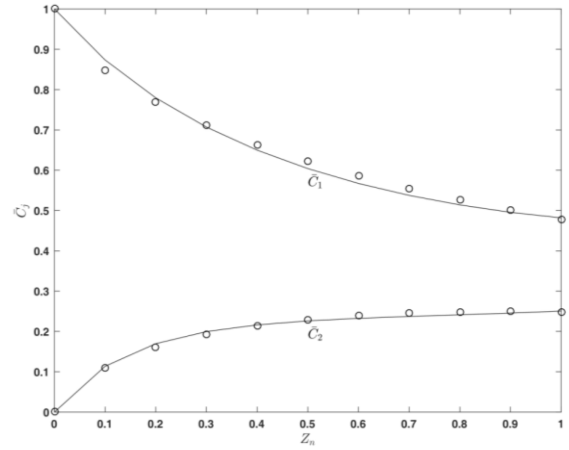

Fig. 6. Average concentration distributions $\bar{C}_{jn}\left(Z_n\right),\ j=1,2$ in the case $\omega=\mathrm{Da}=K_1=1$: "theoretical" values as solutions of (20) and (7) for different $Z_n=0.1(n+1),\ n=0,1,...,9$ (points); as a solution of (21), using the "experimental" parameter values $K_1, a_{j0}, a_{j1}, a_{j2},\ j=1,2$ (lines).

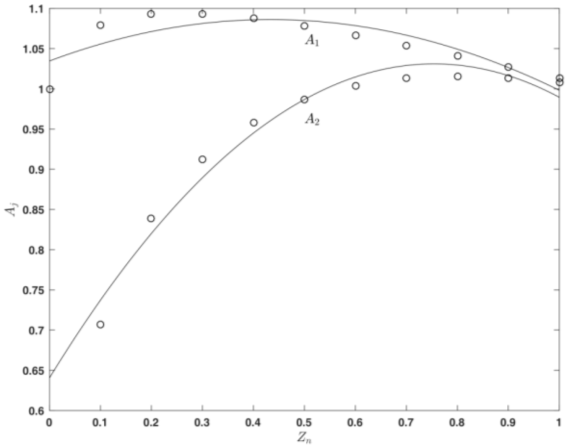

Fig. 7. Function $A_{jn}\left(Z_n\right),\ j=1,2$ in the case $\omega=\mathrm{Da}=K_1=1$: as a solution of (20) and (7) for different $Z_n=0.1(n+1),\ n=0,1,...,9$ (points); $A_j(Z),\ j=1,2$ as a quadratic approximation (16) (line).

The "theoretical" average concentration values $\bar{C}_j(1)=\bar{C}_{j9}\left(Z_9\right),\ Z_9=1,\ j=1,2$ (Fig. 6) are used for to be obtained and the artificial experimental data (18). As a result, the minimization of the least-squares function (19) with respect to $K_1, a_{j0}, a_{j1}, a_{j2},\ j=1,2$ permits to be obtained the "experimental" values of the parameters $K_1, a_{j0}, a_{j1}, a_{j2},\ j=1,2$, presented in the Table 2.

The "theoretical" average concentration as solutions of (20) and (7) for different $Z_n=0.1(n+1),\ n=0,1,...,9$ (points) are compared (Fig. 5) with the solution of (21) for the same case ($\omega=1,\ \mathrm{Da}=1$) (the line), where the "experimental" values of the parameters $K_1, a_{j0}, a_{j1}, a_{j2},\ j=1,2$ in the Table 2 are used.

Table 2. Parameters $K_1, a_{j0}, a_{j1}, a_{j2},\ j=1,2$ (chemical absorption).

Parameters	"Theoretical" values	"Experimental" values
a_{10}	1.0346	0.8825
a_{11}	0.2378	0.2423
a_{12}	−0.2742	−0.2771
a_{20}	0.6405	0.6586
a_{21}	1.0359	1.1074
a_{22}	−0.6869	−0.6794
K_1	1	1.0684

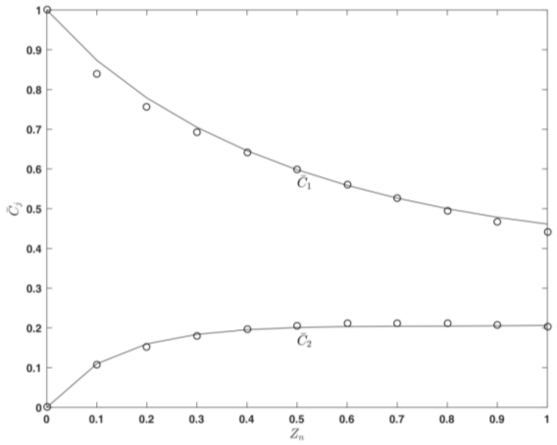

Fig. 8. Average concentration distribution $\bar{C}_j(Z),\ j=1,2$ in the case $\omega=1,\ \mathrm{Da}=1.5$: "theoretical" values as solutions of (20) and (7) for different $Z_n=0.1(n+1),\ n=0,1,...,9$ (points); as a solution of (21) (lines), using the "experimental" parameter values $K_1, a_{j0}, a_{j1}, a_{j2},\ j=1,2$ in the Table 2.

In the same velocities distribution in the phases (the same "experimental" values of $K_1, a_{j0}, a_{j1}, a_{j2},\ j=1,2$ in the Table 2), for other concrete process ($\omega=1, \mathrm{Da}=1.5$), the solution of (20) and (7) permit to be obtained the “theoretical” average concentrations $\bar{C}_j(Z), j=1,2$, which are compared (Fig. 8), with the solution of (17), using the “experimental” values of $K_1, a_{j0}, a_{j1}, a_{j2}, j=1,2$ in the Table 2.

PHYSICAL ABSORPTION OF HIGHLY SOLUBLE GAS (ω = Da = 0)

In the cases of physical absorption of highly soluble gas ($\omega=\mathrm{Da}=0$), from (15), (17) follows $C_{2n}=\bar{C}_{2n}\equiv 0, n=0,1,...,9$, and as a result the models (15), (17) have the forms:

$$U_{1n}\frac{dC_{1n}}{dZ_n}=-K_1C_{1n}; \quad 0.1n\le Z_n\le 0.1(n+1);$$

$$Z_n=0.1n, \quad \mathrm{C}_{1n}(R,Z_n)=C_{1(n-1)}(R,Z_n); \qquad (22)$$

$$n=0,1,...,4; \quad Z_0=0, \quad \mathrm{C}_{10}(R,Z_0)\equiv 1.$$

$$\left(a_{10}+a_{11}Z+a_{12}Z^2\right)\frac{d\bar{C}_1}{dZ}+$$

$$+\left(a_{11}+2a_{12}Z\right)\bar{C}_1=-K_1\bar{C}_1; \quad Z=0, \quad \bar{C}_1=1. \qquad (23)$$

The solution of (22) for “theoretical” value of $K_1=1$ (dimensionless interphase mass transfer coefficient in the gas phase) permits to be obtained the “theoretical” concentration distributions $C_{1n}(R,Z_n)$ for different $Z_n=0.1(n+1), n=0,1,...,9$. This solution of (22) and (7) permit to be obtained the “theoretical” average concentrations $\bar{C}_{1n}(Z_n)$ for different $Z_n=0.1(n+1), \ n=0,1,...,9$ (the points on the Fig. 9), which are compared with the solution of (23) (the line on the Fig. 9), where the “experimental” values of the parameters $a_{10}, a_{11}, a_{12}, K_1$ in the Table 1 are used.

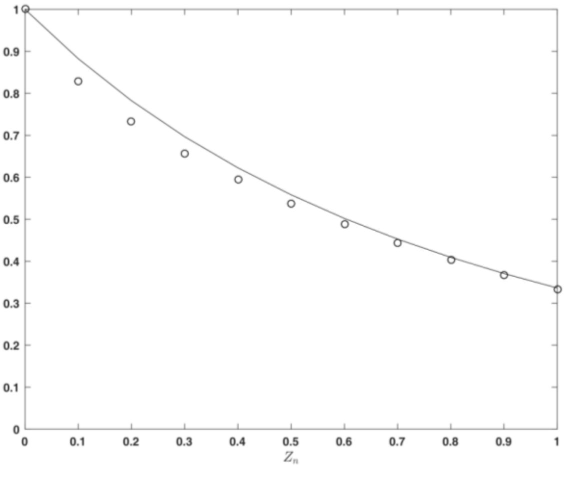

Fig. 9. Average concentration distribution $\bar{C}_1(Z)$ in the case $\omega=\mathrm{Da}=0$: “theoretical” values of $\bar{C}_{1n}(Z_n)$ for different $Z_n=0.1(n+1), \quad n=0,1,...,9$ (points); $\bar{C}_1(Z)$ as solutions of (23) for “experimental” values of $a_{10}, a_{11}, a_{12}, K_1$ (line).

PHYSICAL ABSORPTION OF LIGHTLY SOLUBLE GAS (ω^{-1} = 0)

The model (15), (17) is possible to be presented as

$$U_{1n}\frac{dC_{1n}}{dZ_n}=-\omega^{-1}K_2\left(C_{1n}-C_{2n}\right);$$

$$U_{2n}\frac{dC_{2n}}{dZ_n}=K_2\left(C_{1n}-C_{2n}\right);$$

$$0.1n\le Z_n\le 0.1(n+1); \qquad (24)$$

$$Z_n=0.1n, \quad \mathrm{C}_{jn}(R,Z_n)=C_{j(n-1)}(R,Z_n);$$

$$n=0,1,...,9; \quad j=1,2;$$

$$Z_0=0, \quad \mathrm{C}_{10}(R,Z_0)\equiv 1, \quad C_{20}(R,Z_0)=0.$$

$$\left(a_{10}+a_{11}Z+a_{12}Z^2\right)\frac{d\bar{C}_1}{dZ}+$$

$$+\left(a_{11}+2a_{12}Z\right)\bar{C}_1=-\omega^{-1}K_2\left(\bar{C}_1-\bar{C}_2\right);$$

$$\left(a_{20}+a_{21}Z+a_{22}Z^2\right)\frac{d\bar{C}_2}{dZ}+ \qquad (25)$$

$$+\left(a_{21}+2a_{22}Z\right)\bar{C}_2=K_2\left(\bar{C}_1-\bar{C}_2\right);$$

$$Z=0, \quad \bar{C}_1=1, \quad \bar{C}_2=0.$$

In (24), (25) $K_2=\omega K_1=1$ in the case $\omega=K_1=1$.

In the case of physical absorption of lightly soluble gas ($\omega^{-1}=0$), from (24), (25) follows $C_{1n}\equiv 1, n=0,1,...,9$ and as a result from (24) and (25) is possible to be obtained

$$U_{2n}\frac{dC_{2n}}{dZ_n}=K_2\left(1-C_{2n}\right);$$

$$0.1n\le Z_n\le 0.1(n+1);$$

$$Z_n=0.1n, \quad \mathrm{C}_{2n}(R,Z_n)=C_{2(n-1)}(R,Z_n); \qquad (26)$$

$$n=0,1,...,9;$$

$$Z_0=0, \quad C_{20}(R,Z_0)=0.$$

$$\left(a_{20}+a_{21}Z+a_{22}Z^2\right)\frac{d\bar{C}_2}{dZ}+$$

$$+\left(a_{21}+2a_{22}Z\right)\bar{C}_2=K_2\left(1-\bar{C}_2\right); \qquad (27)$$

$$Z=0, \quad \bar{C}_2=0.$$

The solution of (26) for "theoretical" value of $K_2 = 1$ (dimensionless interphase mass transfer coefficient in the liquid phase) permits to be obtained the "theoretical" concentration distributions $C_{2n}\left(R, Z_n\right)$ for different $Z_n = 0.1(n+1)$, $n = 0,1,...,9$. This solution of (26) and (7) permit to be obtained the "theoretical" average concentration values $\bar{C}_{2n}\left(Z_n\right)$ for different $Z_n = 0.1(n+1)$, $n = 0,1,...,9$ (the points on the Fig. 10), where are compared with the solution of (27) (the line), where the "experimental" values of the parameters $a_{20}, a_{21}, a_{22}, K_2 = K_1$ in the Table 1 are used.

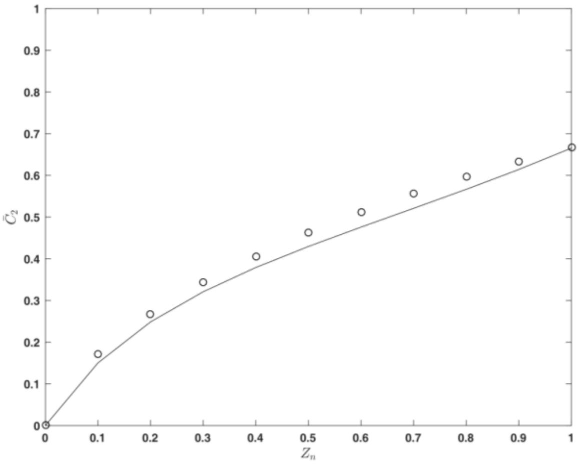

Fig. 10. Average concentration distribution $\bar{C}_2\left(Z\right)$ in the case $\omega^{-1} = 0$: "theoretical" values $\bar{C}_{2n}\left(Z_n\right)$ for different $Z_n = 0.1(n+1)$, $n = 0,1,...,9$ (points); $\bar{C}_2\left(Z\right)$ as solutions of (27) for "experimental" values of $a_{20}, a_{21}, a_{22}, K_2 = K_1$ in the Table 1 (line).

The comparison of the Figs. 2, 9, 10 shows that the obtained parameters in the cases of highly and lightly soluble gases can be used at average soluble gases, where is necessary an experimental determination of the interphase mass transfer coefficient, only.

CONCLUSIONS

The presented numerical analysis of a co-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 at column end, for a concrete process, permits to be obtained the model parameters ($K_1, a_{j0}, a_{j1}, a_{j2}, j = 1,2$), related with the radial non-uniformities of the velocities in the gas and liquid phases. These parameter values permit to be used the average concentration model for modeling of physical and chemical absorption, absorption of highly and lightly soluble gases (different values of the parameters ω, Da, i.e. different values of the column height, average velocities, chemical reaction rate constant and gas solubility).

REFERENCES

1. B. Boyadjiev, Chr. Boyadjiev, Chr., New Models of Industrial Column Chemical Reactors, *Bulg. Chem. Communications*, **49**(3), 2017 (in press).
2. Chr. Boyadjiev, *Int. J. Heat Mass Transfer*, **49**, 796 (2006).
3. Chr. Boyadjiev, Theoretical Chemical Engineering. Modeling and Simulation, Springer-Verlag, Berlin Heidelberg, 2010.
4. M. Doichinova, Chr. Boyadjiev, *Int. J. Heat Mass Transfer*, **55**, 6705 (2012).
5. Chr. Boyadjiev, *J. Pure Appl. Mathematics: Advances and Applications*, **10**(2), 131 (2013).
6. Chr. Boyadjiev, M. Doichinova, B. Boyadjiev, P. Popova-Krumova, Modeling of Column Apparatus Processes, Springer-Verlag, Berlin Heidelberg, 2016.

НОВИ МОДЕЛИ НА ИНДУСТРИАЛНИ КОЛОННИ АБСОРБЕРИ. 1. ПРАВОТОЧНИ АБСОРБЦИОННИ ПРОЦЕСИ

Б. Бояджиев, Хр. Бояджиев

Институт по инженерна химия, Българска академия на науките, ул. „Акад. Г. Бончев“, бл. 103, 1113, София България

Получена на 20 юли, 2016 г.; приета на 2 февруари, 2017 г.

(Резюме)

Представен е нов подход за моделиране на индустриални колонни абсорбери. Предложен е теоретичен анализ на ефекта на радиалната неравномерност на скоростта при правоточни 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. Използването на експериментални данни за средните концентрации в газовата и течната фази на изхода им от колоната за конкретен процес (абсорбция на средно разтворим газ), позволява намирането на моделните параметри в газовата и течната фази, свързани с радиалната неравномерност на скоростите. Тези стойности на параметрите позволяват използването на моделите на средните концентрации за моделиране на различни абсорбционни процеси в правоточни колони.