

## Convective type models of co-current absorption processes in column apparatuses

B. Boyadjiev, Chr. Boyadjiev, P. Popova-Krumova\*

Institute of Chemical Engineering at the Bulgarian Academy of Sciences, Acad. G. Bonchev Str. Bl.103, Sofia 1113, Bulgaria

Received: August 12, 2020; Accepted: August 21, 2020

A new approach for the absorption processes modeling in co-current column apparatuses is presented in the cases of industrial conditions, where the models are convective type form. The use of experimental data for the average concentration at the column end, in the cases of highly soluble and lightly soluble gases, permits to obtain the model parameters related to the radial non-uniformity of the velocity in the gas and liquid phases. These experimental parameter values permit to obtain the mass transfer coefficient in the cases of physical and chemical absorption of the average-soluble gases.

**Keywords:** Mathematical modeling, column apparatuses, co-current absorption, chemical engineering processes

### INTRODUCTION

The modeling and simulation of the mass transfer processes in column apparatuses is possible using the new approach [1-3] on the basis of the physical approximations of the mechanics of continua, where the mathematical point (in the phase volume or on the surface between the phases) 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. On this base are presented [4] convection-diffusion and average-concentration type models.

The convection-diffusion type models permit the qualitative analysis of the processes. These models are the base of the average-concentration models which allow a quantitative analysis of the processes in column apparatuses.

In the industrial processes the diffusion mass transfer is negligible compared to the convective mass transfer and the models are convective type [5].

In the case of the absorption processes in the co-current columns, the effect of the radial component of velocity is not negligible and must be taken into account in the convection and average-concentration type models.

### Convection-diffusion model

A theoretical analysis of the effect of the radial non-uniformity of the axial velocity components in the industrial column will be presented in the case of co-current absorption processes in a cylindrical coordinate system  $(r, z)$  [m], when the radial velocity component is not equal to zero. In the stationary case, the convection-diffusion model [3, 4] of the co-current chemical absorption process, with a pseudo-first-order chemical reaction in the liquid phase, has the form:

$$u_j \frac{\partial c_j}{\partial z} + v_j \frac{\partial c_j}{\partial r} = D_j \left( \frac{\partial^2 c_j}{\partial z^2} + \frac{1}{r} \frac{\partial c_j}{\partial r} + \frac{\partial^2 c_j}{\partial r^2} \right) + (-1)^{(2-j)} k (c_1 - \chi c_2) - (j-1) k_0 c_2;$$

$$r = 0, \quad \frac{\partial c_j}{\partial r} \equiv 0; \quad r = r_0, \quad \frac{\partial c_j}{\partial r} \equiv 0; \quad j = 1, 2; \quad (1)$$

$$z = 0, \quad c_1 \equiv c_1^0, \quad c_2 \equiv 0, \quad u_1^0 c_1^0 \equiv u_1 c_1^0 - D_1 \left( \frac{\partial c_1}{\partial z} \right)_{z=0}, \quad \left( \frac{\partial c_2}{\partial z} \right)_{z=0} = 0.$$

$$\frac{\partial u_j}{\partial z} + \frac{\partial v_j}{\partial r} + \frac{v_j}{r} = 0;$$

$$r = r_0, \quad v_j(r_0, z) = 0; \quad z = 0, \quad u_j = u_j(r, 0); \quad j = 1, 2. \quad (2)$$

\* To whom all correspondence should be sent:

E-mail: [petyabs@yahoo.com](mailto:petyabs@yahoo.com)

In (1, 2)  $u_j = u_j(r, z)$ ,  $v_j = v_j(r, z)$  [m.s<sup>-1</sup>] and  $c_j = c_j(r, z)$  [kg.mol.m<sup>-3</sup>] are the axial and radial velocity components and transferred substance concentrations in the gas ( $j = 1$ ) and liquid ( $j = 2$ ) phases,  $D_j$  [m<sup>2</sup>.s<sup>-1</sup>] are the diffusivities in the phases,  $u_j^0$  and  $v_j^0$  are the inlet velocities and the concentrations in the phases,  $k$  [s<sup>-1</sup>] is the interphase mass transfer coefficient,  $\chi$  - the Henry's number,  $k_0$  [s<sup>-1</sup>] - the chemical reaction rate constant. The concentrations of the transferred substance in the phases are presented as kg-mol of the transferred substance in 1 m<sup>3</sup> of the phase volume. The inlet velocities  $u_j^0$  ( $j = 1, 2$ ) [m.s<sup>-1</sup>] of the gas and liquid phases are equal to the average velocities  $\bar{u}_j$  ( $j = 1, 2$ ) of the phases in the column.

In (1, 2) the generalized variables can be introduced [1]:

$$\begin{aligned} r &= r_0 R, \quad z = lZ, \quad u_j(r, z) = u_j(r_0 R, lZ) = u_j^0 U_j(R, Z), \\ v_j(r, z) &= v_j(r_0 R, lZ) = v_j^0 V_j(R, Z), \quad j = 1, 2, \\ c_1(r, z) &= c_1(r_0 R, lZ) = c_1^0 C_1(R, Z), \\ c_2(r, z) &= c_2(r_0 R, lZ) = \frac{c_1^0}{\chi} C_2(R, Z) \end{aligned} \quad (3)$$

and as a result is obtained:

$$\begin{aligned} U_j \frac{\partial C_j}{\partial Z} + V_j \frac{\partial C_j}{\partial R} &= \text{Fo}_j \left( \varepsilon^2 \frac{\partial^2 C_j}{\partial Z^2} + \frac{1}{R} \frac{\partial C_j}{\partial R} + \frac{\partial^2 C_j}{\partial R^2} \right) + \\ &+ (-1)^{(2-j)} K_j (C_1 - C_2) - (j-1) \text{Da} C_j; \\ R=0, \quad \frac{\partial C_j}{\partial R} &\equiv 0; \quad R=1, \quad \frac{\partial C_j}{\partial R} \equiv 0; \quad j=1, 2; \\ Z=0, \quad C_1 &\equiv 1, \quad C_2 \equiv 0, \quad 1 \equiv U_1 - \varepsilon^2 \text{Fo}_1 \frac{\partial C_1}{\partial Z}, \quad \frac{\partial C_2}{\partial Z} \equiv 0. \end{aligned} \quad (4)$$

$$\frac{\partial U_j}{\partial Z} + \frac{\partial V_j}{\partial R} + \frac{V_j}{R} = 0; \quad R=1, \quad V_j(1, Z) = 0; \quad Z=0, \quad U_j = U_j(R, 0), \quad j=1, 2. \quad (5)$$

The parameters in (4) are

$$\begin{aligned} \text{Fo}_j &= \frac{D_j l}{u_j^0 r_0^2}, \quad j=1, 2, \quad \text{Da} = \frac{k_0 l}{u_2^0}, \quad \varepsilon^2 = \frac{r_0^2}{l^2}, \\ K_1 &= \frac{kl}{u_1^0}, \quad K_2 = \omega K_1, \quad \omega = \frac{u_1^0 \chi}{u_2^0}, \end{aligned} \quad (6)$$

where Fo and Da are the Fourier and Damkohler numbers, respectively.

In the cases of physical absorption  $\text{Da} = 0$ . In industrial conditions  $\text{Fo}_j = \frac{D_j l}{u_j^0 r_0^2} \ll 1$ ,  $j=1, 2$ ,

and the model (4) has a convective form:

$$\begin{aligned} U_j \frac{\partial C_j}{\partial Z} + V_j \frac{\partial C_j}{\partial R} &= (-1)^{(2-j)} K_j (C_1 - C_2); \quad j=1, 2; \\ R=1, \quad \frac{\partial C_j}{\partial R} &\equiv 0; \quad Z=0, \quad C_1 \equiv 1, \quad C_2 \equiv 0. \end{aligned} \quad (7)$$

#### Axial and radial velocity components

The radial non-uniformity of the gas and liquid axial velocity components in the absorption columns is a result of the fluid hydrodynamics at the column inlet and decreases along the column height as a result of the fluid viscosities. As a result radial velocity components are initiated. The theoretical analysis of the change in the radial non-uniformity of the axial velocity components (effect of the radial velocity components) in a column can be made by an appropriate hydrodynamic model, where the average velocities at the cross section of the column are constants (inlet average axial velocity components). In generalized variables [1], as an example, the following velocity distributions can be used, where the difference between the gas and liquid flows is in the average (inlet) velocities only:

$$U_j = (2 - 0.4Z) - 2(1 - 0.4Z)R^2, \quad V_j = 0.2(R - R^3), \quad j=1, 2. \quad (8)$$

The velocity components (8) satisfy the equation (5) and the average velocities are constants:

$$\bar{u}_j = \frac{2}{r_0^2} \int_0^{r_0} r u_j(r, z) dr = u_j^0, \quad \bar{V}_j = 2 \int_0^1 R U_j dR = 1, \quad j=1, 2. \quad (9)$$

#### Average-concentration model

The average values of the velocity and the concentrations at the column cross-sectional area are [3]:

$$\bar{u}_j(z) = \frac{2}{r_0^2} \int_0^{r_0} r u_j(r, z) dr, \quad \bar{c}_j(z) = \frac{2}{r_0^2} \int_0^{r_0} r c_j(r, z) dr, \quad j=1, 2. \quad (10)$$

The functions  $u_j(r, z)$ ,  $v_j(r, z)$ ,  $c_j(r, z)$ ,  $j=1, 2$  in (1, 2) can be presented with the help of the average functions (10):

$$\begin{aligned} u_j(r, z) &= \bar{u}_j U_j(R, Z), \quad v_j(r, z) = \varepsilon \bar{u}_j V_j(R, Z), \\ c_j(r, z) &= \bar{c}_j(z) \tilde{c}_j(r, z), \quad j=1, 2, \end{aligned} \quad (11)$$

where  $\tilde{c}_j(r, z)$ ,  $j=1,2$  present the radial non-uniformity of the concentrations and satisfy the following conditions:

$$\frac{2}{r_0^2} \int_0^{r_0} r \tilde{c}_j(r, z) dr = 1, \quad j=1,2. \quad (12)$$

The average concentration model may be obtained when putting (11) into (1), multiplying by  $r$  and integrating over  $r$  in the interval  $(0, r_0)$ . As a result, the following is obtained:

$$\begin{aligned} \alpha_j(z) \bar{u}_j \frac{d\bar{c}_j}{dz} + [\beta_j(z) + \varepsilon\gamma_j(z)] \bar{u}_j \bar{c}_j &= \\ = D_j \frac{d^2\bar{c}_j}{dz^2} + (-1)^{(2-j)} k(\bar{c}_1 - \chi\bar{c}_2) - (j-1)k_0\bar{c}_2; \\ z=0, \quad \bar{c}_j(0) &\equiv (2-j)c_j^0, \quad \frac{d\bar{c}_j}{dz} \equiv 0; \quad j=1,2. \end{aligned} \quad (13)$$

where

$$\begin{aligned} \alpha_j(z) &= \frac{2}{r_0^2} \int_0^{r_0} r U_j \tilde{c}_j dr, \quad \beta_j(z) = \frac{2}{r_0^2} \int_0^{r_0} r U_j \frac{\partial \tilde{c}_j}{\partial z} dr, \quad \gamma_j(z) = \frac{2}{r_0^2} \int_0^{r_0} r V_j \frac{\partial \tilde{c}_j}{\partial r} dr, \\ U_j &= U_j(R, Z), \quad V_j = V_j(R), \quad \tilde{c}_j(r, z) = \tilde{C}_j(R, Z), \quad j=1,2. \end{aligned} \quad (14)$$

The theoretical analysis of the model (13) will be made using the following generalized variables and functions:

$$\begin{aligned} r &= r_0 R, \quad z = lZ, \quad \bar{c}_j(z) = c_j^0 \bar{C}_j(Z), \quad c_2^0 = \frac{c_1^0}{\chi}, \\ \bar{C}_j(Z) &= 2 \int_0^1 R C_j(R, Z) dR, \quad \tilde{c}_j(r, z) = \frac{c_j(r, z)}{\bar{c}_j(z)} = \frac{C_j(R, Z)}{\bar{C}_j(Z)} = \tilde{C}_j(R, Z), \\ \alpha_j(z) &= \alpha_j(lZ) = A_j(Z) = 2 \int_0^1 R U_j(R, Z) \tilde{C}_j(R, Z) dR, \\ \beta_j(z) &= \beta_j(lZ) = B_j(Z) = 2 \int_0^1 R U_j(R, Z) \frac{\partial \tilde{C}_j}{\partial Z} dR, \\ \gamma_j(z) &= \gamma_j(lZ) = G_j(Z) = 2 \int_0^1 R V_j(R) \frac{\partial \tilde{C}_j}{\partial R} dR, \quad j=1,2. \end{aligned} \quad (15)$$

As a result, the model (13) has the form:

$$\begin{aligned} A_j(Z) \frac{d\bar{C}_j}{dZ} + [B_j(Z) + G_j(Z)] \bar{C}_j &= \\ = \varepsilon^2 \text{Fo}_j \frac{d^2\bar{C}_j}{dZ^2} + (-1)^{(2-j)} K_j (\bar{C}_1 - \bar{C}_2) - (j-1) \text{Da} \bar{C}_j; \\ Z=0, \quad \bar{C}_1 &= 1, \quad \bar{C}_2 = 0, \quad \frac{d\bar{C}_j}{dZ} = 0; \quad j=1,2. \end{aligned} \quad (16)$$

In industrial conditions  $\text{Fo}_j \ll 1$ ,  $j=1,2$ , and the model (16) has a convective form:

$$\begin{aligned} A_j(Z) \frac{d\bar{C}_j}{dZ} + [B_j(Z) + G_j(Z)] \bar{C}_j &= (-1)^{(2-j)} K_j (\bar{C}_1 - \bar{C}_2) - (j-1) \text{Da} \bar{C}_j; \\ Z=0, \quad \bar{C}_1 &= 1, \quad \bar{C}_2 = 0; \quad j=1,2. \end{aligned} \quad (17)$$

The presented models (7, 17) permit to analyze the physical absorption ( $0 = \text{Da} \leq 10^{-2}$ ) of highly soluble ( $0 = \omega \leq 10^{-2}$ ), lightly soluble ( $0 = \omega^{-1} \leq 10^{-2}$ ) or average-soluble ( $10^{-1} < \omega < 10$ ) gases.

#### Physical absorption of highly soluble gas

In the cases of physical absorption of a highly soluble gas ( $\omega = K_2 = \text{Da} = 0$ ) and from (7, 17) follows  $C_2 = \bar{C}_2 \equiv 0$ .

$$\begin{aligned} U_1 \frac{\partial C_1}{\partial Z} + V_1 \frac{\partial C_1}{\partial R} &= -K_1 C_1; \\ R=1, \quad \frac{\partial C_1}{\partial R} &\equiv 0; \quad Z=0, \quad C_1 \equiv 1. \end{aligned} \quad (18)$$

Eq. (18) is solved (similar to [5]), using the Method of Lines [6], by discretizing it in respect to  $R_i = i/n$ ,  $i=0, \dots, n$  (transformation of the partial differential equation (18) to a system of ordinary differential equations in respect to  $Z$ ):

$$R_0 = 0, \quad R_n = 1, \quad 0 < R_i = \frac{i}{n} < 1, \quad i=1, 2, \dots, (n-1) \quad (19)$$

From (8, 18, 19) follows:

$$V_1(R_0) = V_1(R_n) = 0, \quad \left( \frac{\partial C_{1n}}{\partial R} \right)_{R=R_n} = 0. \quad (20)$$

As a result from (18) follows:

$$\begin{aligned} U_1(R_0, Z) \frac{dC_{10}}{dZ} &= -K_1 C_{10}; \\ U_1(R_i, Z) \frac{dC_{1i}}{dZ} &= -V_1(R_i) \left( \frac{\partial C_{1i}}{\partial R} \right)_{R=R_i} - K_1 C_{1i}; \\ U_1(R_n, Z) \frac{dC_{1n}}{dZ} &= -K_1 C_{1n}; \\ Z=0, \quad C_{10} &= 1, \quad C_{1i} = 1, \quad C_{1n} = 1, \quad i=1, \dots, n-1. \end{aligned} \quad (21)$$

As a result, from (21) follows the next equations system, where 2 points finite difference scheme is used:

$$U_1(R_0, Z) \frac{dC_{10}}{dZ} = -K_1 C_{10};$$

$$U_1(R_i, Z) \frac{dC_{1i}}{dZ} = -V_1(R_i) \frac{C_{1i} - C_{1(i-1)}}{R_i - R_{i-1}} - K_1 C_{1i};$$

$$U_1(R_n, Z) \frac{dC_{1n}}{dZ} = -K_1 C_{1n};$$

$$Z = 0, \quad C_0 = 1, \quad C_i = 1, \quad C_n = 1; \quad i = 1, \dots, n-1. \quad (22)$$

As a result:

$$C_1(R, Z) = C_{10}(0, Z), C_{11}(R_1, Z), C_{12}(R_2, Z), \dots, C_{1(n-1)}(R_{(n-1)}, Z), C_{1n}(1, Z) = 0 \quad (23)$$

The solution of (18) permits to obtain the concentration distribution in the gas phase  $C_1(R, Z)$ . In the case  $K_1 = 1$ , the result is presented on Fig. 1.

The concentration distribution  $C_1(R, Z)$  and (15) permit to obtain the average concentrations  $\bar{C}_1(Z_n)$  (“theoretical” values, points in Fig. 2) and functions

$A_1(Z_n), B_1(Z_n), G_1(Z_n)$  in (15), which are presented on Fig. 3 (points).

The functions  $A_1(Z), B_1(Z), G_1(Z)$  in Fig. 3 (points) can be presented as the following approximations:

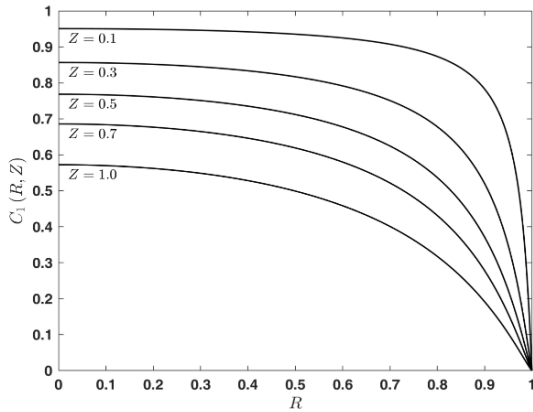
$$A_1(Z) = 1 + a_{11}Z + a_{12}Z^2, \quad B_1(Z) = b_{11}Z^{b_{12}}, \quad G_1(Z) = g_{11}Z. \quad (24)$$

where the “theoretical” values of  $a_{11}, a_{12}, b_{11}, b_{12}, g_{11}$  are presented in Table 1.

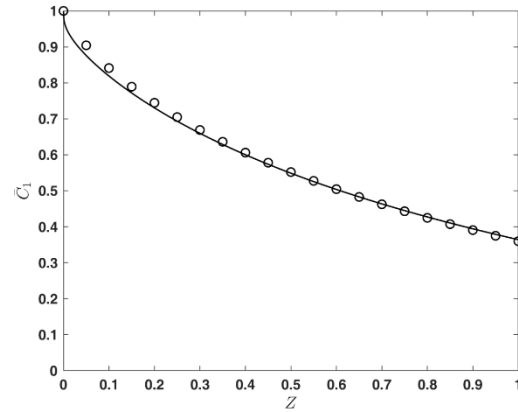
The average-concentration model in the cases of physical absorption of highly soluble gas ( $\omega = K_2 = Da = \bar{C}_2 \equiv 0$ ) follows from (17):

$$A_1(Z) \frac{d\bar{C}_1}{dZ} + [B_1(Z) + G_1(Z)] \bar{C}_1 = -K_1 \bar{C}_1; \quad (25)$$

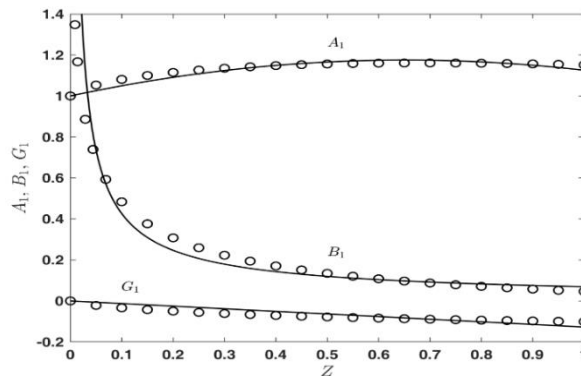
$$Z = 0, \quad \bar{C}_1 \equiv 1.$$



**Fig. 1.** Concentration distributions  $C_1(R, Z)$ , for different  $Z = 0.1, 0.3, 0.5, 0.7, 1.0$ .



**Fig. 2.** Average concentrations  $\bar{C}_1(Z)$ : “theoretical” values (points); solution of (25), using the “experimental” parameter values  $P_1, K_1$  in Table 1 (line).



**Fig. 3.** Functions  $A_1(Z_n), B_1(Z_n), G_1(Z_n)$  (points); approximations (24) (lines).

In (25), the parameters  $P_1(a_{11}, a_{12}, b_{11}, b_{12}, g_{11})$  in the functions  $A_1(Z), B_1(Z), G_1(Z)$  and  $K_1$  must be obtained using experimental data.

The obtained values of the function  $\bar{C}_1(Z_n)$  in the cases of physical absorption of a highly soluble gas ( $\omega = K_2 = Da = 0$ ), “theoretical” value of  $K_1 = 1$  and different  $Z_n$  (Fig. 2), permit to obtain the value of  $\bar{C}_1(1)$  and the artificial experimental data (for  $j = 1$ ):

$$\bar{C}_{j\text{exp}}^m(1) = (0.95 + 0.1B_m)\bar{C}_j(1), \quad j = 1, 2, \quad m = 1, \dots, 10, \quad (26)$$

where  $0 \leq B_m \leq 1, m = 1, \dots, 10$  are obtained by a generator of random numbers. The obtained artificial experimental data (26) for  $j = 1$  are used for the parameters  $P_1, K_1$  identification in the average concentrations model (25), by the minimization of the least-squares function  $Q^{(1)}$  with respect to  $P_1, K_1$ :

$$Q^{(1)}(P_1, K_1) = \sum_{m=1}^{10} [\bar{C}_1(1, P_1, K_1) - \bar{C}_{1\text{exp}}^m(1)]^2, \quad (27)$$

where the values of  $\bar{C}_1(1, P_1, K_1)$  are obtained as solutions of (25). The obtained (after the minimization) “experimental” parameter values  $P_1, K_1$  are compared with the “theoretical” values on Table 1. They are used for the solution of (25) and the result (the line) is compared with the “theoretical” average concentration values on Fig. 2.

A comparison of (18) and (28) shows that in the case  $K_1 = K_2 = 1$  is possible to obtain  $C_1 + C_2 = 1$ , i.e. the solution of (28) is  $C_2(R, Z) = 1 - C_1(R, Z)$  and is presented on Fig. 4.

#### Physical absorption of a lightly soluble gas

In the cases of physical absorption of a lightly soluble gas ( $\omega^{-1} = K_1 = Da = 0$ ), from (7, 17) follows:  $C_1 = \bar{C}_1 \equiv 1$ .

From convection type model (7) follows:

$$U_2 \frac{\partial C_2}{\partial Z} + V_2 \frac{\partial C_2}{\partial R} = K_2(1 - C_2); \quad (28)$$

$$R = 1, \quad \frac{\partial C_2}{\partial R} \equiv 0; \quad Z = 0, \quad C_2 \equiv 0.$$

**Table 1.** Parameters  $P_j, K_j, j = 1, 2, K_1 = K, K_2 = \omega K$  (physical absorption).

Parameters	“Theoretical” values	“Experimental” values
$a_{11}$	0.537	0.578
$a_{12}$	-0.412	-0.415
$b_{11}$	0.069	0.070
$b_{12}$	-0.788	-0.680
$g_{11}$	-0.127	-0.134
$K_1 (\omega = 0)$	1	0.991
$a_{21}$	0.925	0.921
$a_{22}$	0.204	0.207
$b_2$	10.297	10.465
$g_{21}$	12.957	13.061
$g_{22}$	4.113	4.112
$K_2$	1	1.007
$K$	1	0.921

The average concentration distribution can be obtained directly  $\bar{C}_2(Z) = 1 - \bar{C}_1(Z)$  and the “theoretical” values  $\bar{C}_2(Z_n)$  are presented on Fig. 5 (points).

The obtained result for  $C_2(R, Z), \bar{C}_2(Z)$ , and (15) permit to obtain the functions  $A_2(Z_n), B_2(Z_n), G_2(Z_n)$  in (15), which are presented on Figs. 6, 7 (points).

The functions  $A_2(Z), B_2(Z), G_2(Z)$  in Figs. 6, 7 (points) can be presented as the approximations:

$$A_2(Z) = a_{21}Z^{a_{22}}, \quad B_2(Z) = \frac{1}{b_2Z}, \quad G_2(Z) = \frac{1}{g_{21}Z + g_{22}}. \quad (29)$$

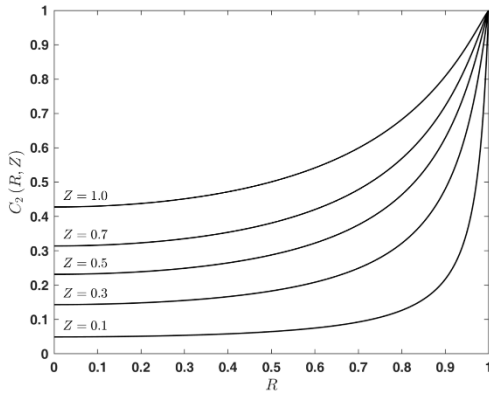
where the “theoretical” values of  $a_{21}, a_{22}, b_2, g_{21}, g_{22}$  are presented in Table 1.

In the cases of physical absorption of a lightly soluble gas ( $\omega^{-1} = K_1 = Da = 0, C_1 = \bar{C}_1 \equiv 1$ ) from (16) follows:

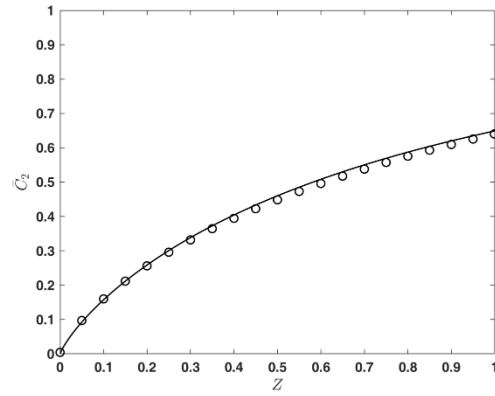
$$A_2(Z) \frac{d\bar{C}_2}{dZ} + [B_2(Z) + G_2(Z)]\bar{C}_2 = K_2(1 - \bar{C}_2); \quad (30)$$

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

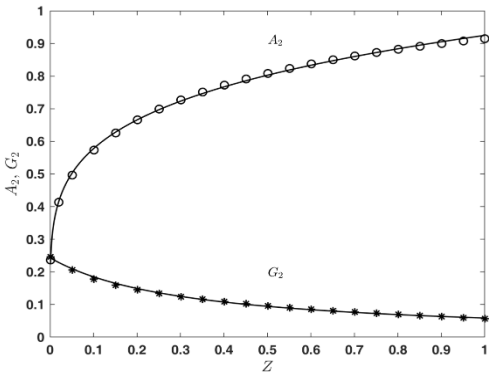
The solution of (30) is similar to the solution of (25), where the parameters  $P_2(a_{21}, a_{22}, b_2, g_{21}, g_{22})$  in the functions  $A_2(Z), B_2(Z), G_2(Z)$  and  $K_2$  must be obtained using experimental data.



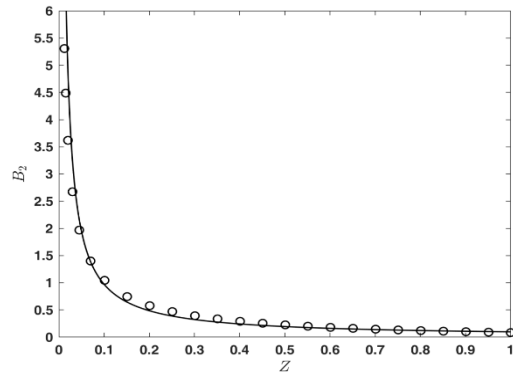
**Fig. 4.** Concentration distributions  $C_2(R, Z)$ , for different  $Z = 0.1, 0.3, 0.5, 0.7, 1.0$ .



**Fig. 5.** Average concentration distributions  $\bar{C}_2(Z)$ , for different  $Z$  (points); solution of (30), using the “experimental” parameter values  $P_2, K_2$  in Table 1 (line).



**Fig. 6.** Functions  $A_2(Z_n), G_2(Z_n)$  (points); approximations (29) (lines).



**Fig. 7.** Function  $B_2(Z_n)$  (points); approximation (29) (lines).

The obtained values of the function  $\bar{C}_2(Z_n)$  in the cases of physical absorption of lightly soluble gas ( $\omega^{-1} = K_1 = Da = 0$ ), “theoretical” value of  $K_2 = 1$  and different  $Z_n$  (Fig. 5), permit to obtain the value of  $\bar{C}_2(1)$  and the artificial experimental data (26) for  $j=2$ . They are used for the parameters  $P_2, K_2$  identification in the average concentrations model (30), by the minimization of the least-squares function  $Q^{(2)}$  with respect to  $P_2, K_2$ :

$$Q^{(2)}(P_2, K_2) = \sum_{m=1}^{10} \left[ \bar{C}_2(1, P_2, K_2) - \bar{C}_{2\text{exp}}^m(1) \right]^2, \quad (31)$$

where the values of  $\bar{C}_2(1, P_2, K_2)$  are obtained as solutions of (30). The obtained (after the minimization) “experimental” parameter values  $P_2, K_2$  are compared with the “theoretical” values on Table 1. They are used for the solution of (30)

and the result (the line) is compared with the “theoretical” average concentration values (points) on Fig. 5.

#### Physical absorption of average-soluble gas

In the cases of physical absorption of an average-soluble gas ( $\omega \sim 1, K_1 = K, K_2 = \omega K, Da = 0$ ), the convection type model can be obtained from (7):

$$\begin{aligned} U_1 \frac{\partial C_1}{\partial Z} + V_1 \frac{\partial C_1}{\partial R} &= -K(C_1 - C_2); \\ R=1, \quad \frac{\partial C_1}{\partial R} &\equiv 0, \quad Z=0, \quad C_1 \equiv 1. \\ U_2 \frac{\partial C_2}{\partial Z} + V_2 \frac{\partial C_2}{\partial R} &= \omega K(C_1 - C_2); \\ R=1, \quad \frac{\partial C_2}{\partial R} &\equiv 0; \quad Z=0, \quad C_2 \equiv 0. \end{aligned} \quad (32)$$

The problem (32) is solved using the Method of Lines [6]:

$$\begin{aligned}
 U_1(R_0, Z) \frac{dC_{10}}{dZ} &= -K(C_{10} - C_{20}); \\
 U_1(R_i, Z) \frac{dC_{1i}}{dZ} &= -V_1(R_i) \frac{C_{1i} - C_{1(i-1)}}{R_i - R_{i-1}} - K(C_{1i} - C_{2i}); \\
 U_1(R_n, Z) \frac{dC_{1n}}{dZ} &= -K(C_{1n} - C_{2n}); \\
 Z=0, \quad C_{10} &= 1, \quad C_{1i} = 1, \quad C_{1n} = 1; \quad i=1, \dots, n-1.
 \end{aligned} \tag{33}$$

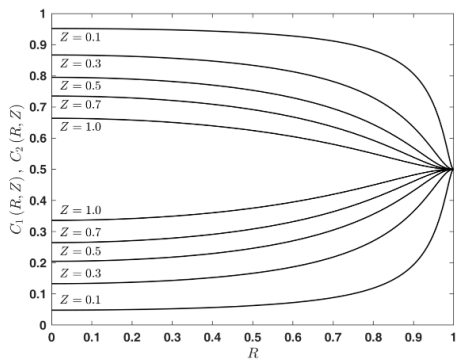
$$\begin{aligned}
 U_2(R_0, Z) \frac{dC_{20}}{dZ} &= \omega K(C_{10} - C_{20}); \\
 U_2(R_i, Z) \frac{dC_{2i}}{dZ} &= -V_2(R_i) \frac{C_{2i} - C_{2(i-1)}}{R_i - R_{i-1}} + \omega K(C_{1i} - C_{2i}); \\
 U_2(R_n, Z) \frac{dC_{2n}}{dZ} &= \omega K(C_{1n} - C_{2n}); \\
 Z=0, \quad C_{20} &= 0, \quad C_{2i} = 0, \quad C_{2n} = 0; \quad i=1, \dots, n-1.
 \end{aligned} \tag{34}$$

The solution of (33, 34) permits to obtain the concentrations  $C_j(R, Z)$ ,  $j=1, 2$  in the case  $\omega=1, K=1$ , which are presented on Fig. 8 for different  $Z$  (points). This solution and (15) permit to obtain the average concentrations  $\bar{C}_j(Z_n)$ ,  $j=1, 2$  for different  $Z_n$  (Fig. 9),  $\bar{C}_j(1)$ ,  $j=1, 2$  and the artificial experimental data (26). They are used to obtain the mass transfer coefficient  $K$  by the minimization of the least-squares function  $Q$  with respect to  $K$ :

$$Q(K) = \sum_{m=1}^{10} [\bar{C}_1(1, K) - \bar{C}_{1\text{exp}}^m(1)]^2 + \sum_{m=1}^{10} [\bar{C}_2(1, K) - \bar{C}_{2\text{exp}}^m(1)]^2 \tag{35}$$

where  $\bar{C}_1(1, K), \bar{C}_2(1, K)$  are solutions of the average-concentration model:

$$\begin{aligned}
 A_1(Z) \frac{d\bar{C}_1}{dZ} + [B_1(Z) + G_1(Z)] \bar{C}_1 &= -K(\bar{C}_1 - \bar{C}_2); \quad Z=0, \quad \bar{C}_1 = 1. \\
 A_2(Z) \frac{d\bar{C}_2}{dZ} + [B_2(Z) + G_2(Z)] \bar{C}_2 &= \omega K(\bar{C}_1 - \bar{C}_2); \quad Z=0, \quad \bar{C}_2 = 0.
 \end{aligned} \tag{36}$$



**Fig. 8.** Concentration distributions  $C_j(R, Z)$ ,  $j=1, 2$  for different  $Z=0.1, 0.3, 0.5, 0.7, 1.0$ .

The “experimental” parameter value  $K$  and the “experimental” values of the parameters  $P_1, P_2$  in Table 1 obtained (after the minimization) are used for the solution of the average-concentration model (36). The solution of (36), using the “experimental” parameter values  $P_1, P_2, K$ , is presented (lines) on Fig. 9.

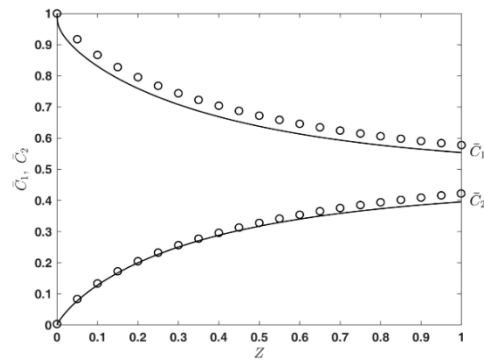
### Chemical absorption

In the cases of chemical absorption of the average-soluble gas, the convection type model can be obtained from (7), where  $\omega \sim 1$ ,  $K_1 = K, K_2 = \omega K, Da \neq 0$  and  $K$  is the “experimental” value in Table 1:

$$\begin{aligned}
 U_1 \frac{\partial C_1}{\partial Z} + V_1 \frac{\partial C_1}{\partial R} &= -K(C_1 - C_2); \\
 R=1, \quad \frac{\partial C_1}{\partial R} &\equiv 0; \quad Z=0, \quad C_1 \equiv 1. \\
 U_2 \frac{\partial C_2}{\partial Z} + V_2 \frac{\partial C_2}{\partial R} &= \omega K(C_1 - C_2) - Da C_2; \\
 R=1, \quad \frac{\partial C_2}{\partial R} &\equiv 0; \quad Z=0, \quad C_2 \equiv 0.
 \end{aligned} \tag{37}$$

The solution of (37) is similar to (32), where (34) must be presented as:

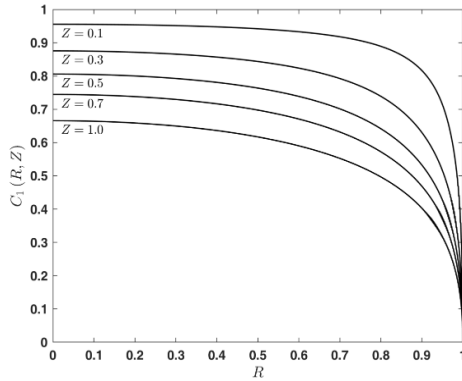
$$\begin{aligned}
 U_1(R_0, Z) \frac{dC_{10}}{dZ} &= -K(C_{10} - C_{20}); \\
 U_1(R_i, Z) \frac{dC_{1i}}{dZ} &= -V_1(R_i) \frac{C_{1i} - C_{1(i-1)}}{R_i - R_{i-1}} - K(C_{1i} - C_{2i}); \\
 U_1(R_n, Z) \frac{dC_{1n}}{dZ} &= -K(C_{1n} - C_{2n}); \\
 Z=0, \quad C_{10} &= 1, \quad C_{1i} = 1, \quad C_{1n} = 1; \quad i=1, \dots, n-1.
 \end{aligned} \tag{38}$$



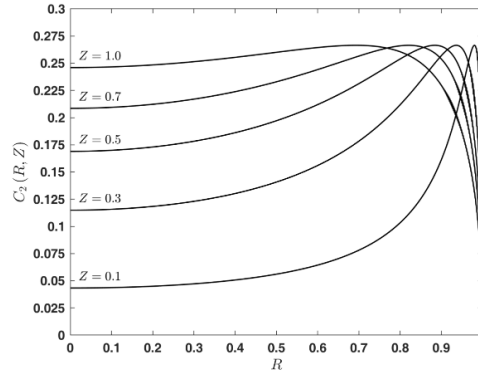
**Fig. 9.** Average concentrations  $\bar{C}_j(Z)$ ,  $j=1, 2$ : “theoretical” values (points); solution of (36) using the “experimental” parameter values  $P_1, P_2, K$  in Table 1 (line).

$$\begin{aligned}
 U_2(R_0, Z) \frac{dC_{20}}{dZ} &= \omega K(C_{10} - C_{20}) - Da C_{20}; \\
 U_2(R_i, Z) \frac{dC_{2i}}{dZ} &= -V_2(R_i) \frac{C_{2i} - C_{2(i-1)}}{R_i - R_{i-1}} + \omega K(C_{1i} - C_{2i}) - Da C_{2i}; \\
 U_2(R_n, Z) \frac{dC_{2n}}{dZ} &= \omega K(C_{1n} - C_{2n}) - Da C_{2n}; \\
 Z=0, \quad C_{20} &= 0, \quad C_{2i} = 0, \quad C_{2i} = 0; \quad i=1, \dots, n-1.
 \end{aligned}
 \tag{39}$$

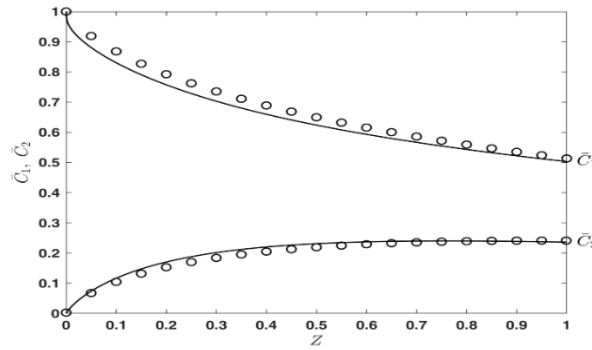
The obtained concentrations  $C_j(Z)$ ,  $j=1,2$  in the case  $\omega=1, Da=1$  are presented on Figs. 10, 11. The solution of (37) and (15) permits to be obtained average concentrations  $\bar{C}_j(Z_n)$ ,  $j=1,2$  for different  $Z$ , which are presented on Fig. 12 (points).



**Fig. 10.** Concentration distributions  $C_1(R, Z)$  for different  $Z=0.1, 0.3, 0.5, 0.7, 1.0$ .



**Fig. 11.** Concentration distributions  $C_2(R, Z)$  for different  $Z=0.1, 0.3, 0.5, 0.7, 1.0$ .



**Fig. 12.** Average concentrations  $\bar{C}_j(Z)$ ,  $j=1,2$ : “theoretical” values (points); solution of (39), using the “experimental” parameter values  $P_2, K$  in Table 1 and  $Da=1$  (line).

The obtained “experimental” values of the parameters  $P_1, P_2, K$  in Table 1 are used for the solution of the average-concentration model of the chemical absorption ( $Da \neq 0$ ) of the average-soluble gases ( $\omega \sim 1$ ), obtained from (17):

$$\begin{aligned}
 A_1(Z) \frac{d\bar{C}_1}{dZ} + [B_1(Z) + G_1(Z)] \bar{C}_1 &= -K(\bar{C}_1 - \bar{C}_2); \quad Z=0, \quad \bar{C}_1=1. \\
 A_2(Z) \frac{d\bar{C}_2}{dZ} + [B_2(Z) + G_2(Z)] \bar{C}_2 &= \omega K(\bar{C}_1 - \bar{C}_2) - Da \bar{C}_2; \quad Z=0, \quad \bar{C}_2=0.
 \end{aligned}
 \tag{40}$$

The obtained solution of (39) is presented on Fig. 12 (line).

## CONCLUSIONS

A new approach for the absorption processes modeling in co-current column apparatuses, is

presented in the cases of industrial conditions, where the models are convective type form. The use of experimental data, for the average concentration at the column end, in the cases of highly soluble and lightly soluble gases, permits to obtain the model parameters, related with the radial non-uniformity of the velocity in the gas and liquid phases. These experimental parameter values permit to obtain the mass transfer coefficient in the cases of physical and chemical absorption of the average-soluble gases.

**Acknowledgements:** This work is supported by Project of Fundamental Scientific Research 19-58-18004, conducted by RFBR and the National Science Fund of Bulgaria under contract No KP 06 RUSIA-3 from 27 Sep. 2019, “Modeling, simulation



*and experimental investigations of the interphase mass transfer and separation in distillation, absorption, adsorption and catalytic processes in industrial column apparatuses”.*

#### REFERENCES

1. Chr. Boyadjiev, Theoretical Chemical Engineering. Modelling and simulation, Berlin, Heidelberg, Springer-Verlag, 2010.
2. Chr. Boyadjiev, M. Doichinova, B. Boyadjiev, P. Popova-Krumova, Modeling of Column Apparatus Processes, Berlin, Heidelberg, Springer-Verlag, 2016.
3. Chr. Boyadjiev, M. Doichinova, B. Boyadjiev, P. Popova-Krumova, Modeling of Column Apparatus Processes, Second edn., Berlin, Heidelberg, Springer-Verlag, 2018.
4. B. Boyadjiev, Chr. Boyadjiev, *Bulg. Chem. Commun.*, **49**(3), 711 (2017).
5. B. Boyadjiev, Chr. Boyadjiev, *J. Eng. Thermophysics*, **29**(1), 186 (2020).
6. W. E. Schiesser, The Numerical Method of Lines, Academic Press, San Diego, 1991.