

**Тема 3.10.7. МОДЕЛИРАНЕ И СИМУЛИРАНЕ НА АБСОРБЦИОННИ И  
АДСОРБЦИОННИ ПРОЦЕСИ В ИНДУСТРИАЛНИ АПАРАТИ**

***MODELING AND SIMULATION OF ABSORPTION AND ADSORPTION  
PROCESSES IN INDUSTRIAL COLUMN APPARATUSES***

**Лектор:**

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**Хорариум:**

30 учебни часа

**Анотация:**

В курса се предлагат методите за моделиране и симулиране на абсорбционни и адсорбционни процеси в колонни промишлени апарати, развити в монографиите:

Chr. Boyadjiev, “Theoretical Chemical Engineering. Modeling and simulation”, Springer-Verlag, Berlin Heidelberg, 2010, pp. 594.

Chr. Boyadjiev, M. Doichinova, B. Boyadjiev, P. Popova-Krumova, “Modeling of Column Apparatus Processes”, Springer-Verlag, Berlin Heidelberg, 2016, pp. 313.

Ще бъдат разгледани конвективно-дифузионни и средно-концентрационни модели в приближенията на механиката на непрекъснатите среди в случаите на физична и химична абсорбция в системи газ-течност и физична и химична адсорбция в системи газ (течност)-твърдо. Разглежданите модели дават възможност за качествен и количествен анализ на абсорбционни и адсорбционни процеси в колонни промишлени апарати. Ще бъдат разгледани и изчислителните проблеми при симулирането на разглежданите процеси.

**Annotation:**

In the course are presented the methods for modeling and simulation of absorption and adsorption processes in column industrial apparatuses, developed in the monographs:

Chr. Boyadjiev, "Theoretical Chemical Engineering. Modeling and simulation", Springer-Verlag, Berlin Heidelberg, 2010, pp. 594.

Chr. Boyadjiev, M. Doichinova, B. Boyadjiev, P. Popova-Krumova, "Modeling of Column Apparatus Processes", Springer-Verlag, Berlin Heidelberg, 2016, pp. 313.

Will be discussed the convective-diffusion and average-concentration models in approximations of Mechanics of Continua in cases of physical and chemical absorption in gas-liquid systems and physical and chemical adsorption in gas (liquid)-solid systems. The models considered are suitable for qualitative and quantitative analysis of the absorption and adsorption processes in industrial column apparatuses. Will be discussed the calculation problems in process simulations.

#### Литература:

Chr. Boyadjiev, M. Doichinova, B. Boyadjiev, P. Popova-Krumova, "Modeling of Column Apparatus Processes", Springer-Verlag, Berlin Heidelberg, 2016, pp. 313.

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#### Пълнен текст

The modeling of two-phase gas-liquid ( $j=1,2$ ), gas-solid ( $j=1,3$ ) and liquid-solid ( $j=2,3$ ) interphase mass transfer processes in column apparatuses is possible to be used in the case of absorption, adsorption and heterogeneous (catalytic) chemical reactions. For the modeling of two-phase processes [1–5] the model equations (I.3–I.5) have to be used, i.e. components mass balances ( $i=1,2,\dots,i_0$ ) in the phases, where according (2.1.10) the radial velocity components are equal to zero ( $v_j \equiv 0, j=1,2,3$ ):

$$\begin{aligned}
 u_j \frac{\partial c_{ij}}{\partial z_j} &= D_{ij} \left( \frac{\partial^2 c_{ij}}{\partial z_j^2} + \frac{1}{r} \frac{\partial c_{ij}}{\partial r} + \frac{\partial^2 c_{ij}}{\partial r^2} \right) + Q_{ij}(c_{ij}); \\
 r=0, \quad \frac{\partial c_{ij}}{\partial r} &\equiv 0; \quad r=r_0, \quad \frac{\partial c_{ij}}{\partial r} \equiv 0; \\
 z_j=0, \quad c_{ij} &\equiv c_{ij}^0, \quad u_j^0 c_{ij}^0 \equiv u_j c_{ij}^0 - D_{ij} \left( \frac{\partial c_{ij}}{\partial z_j} \right)_{z_j=0}; \\
 i=1,2,\dots,i_0, \quad j &= 1,2=1,3=2,3.
 \end{aligned} \tag{0.0.1}$$

In (2.0.1)  $u_j = u_j(r)$  [ $\text{m}\cdot\text{s}^{-1}$ ] and  $c_{ij} = c_{ij}(r, z_j)$  [ $\text{kg}\cdot\text{mol}\cdot\text{m}^{-3}$ ] are the axial velocity components and transferred substance concentrations in the phases,  $D_{ij}$  [ $\text{m}^2\cdot\text{s}^{-1}$ ] are the diffusivities in the phases,  $u_j^0$  and  $c_{ij}^0$  are the inlet velocities and the concentrations in the phases. The concentrations of the transferred substance in the phases are presented as kg-mol of the

transferred substance in  $1 \text{ m}^3$  of the phase volume. The hold-up coefficients ( $\text{m}^3$  of the phase volume in  $1 \text{ m}^3$  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 phase flow rates [ $\text{m}^3 \cdot \text{s}^{-1}$ ] in the column,  $j=1,2,3$ , and  $F_0 = \sum_{j=1}^3 F_j$  [ $\text{m}^3 \cdot \text{s}^{-1}$ ] is the total flow rate of the fluids in the column. The volume reactions terms  $Q_{ij}$ ,  $j=1,2,3$  [ $\text{kg} \cdot \text{mol} \cdot \text{m}^{-3} \cdot \text{s}^{-1}$ ] are the rates of the chemical reactions and interphase mass transfer, as volume sources ( $Q_{ij} > 0$ ) or sinks ( $Q_{ij} < 0$ ), in the phase parts of the elementary column volume and participate in the mass balance in the elementary phase volumes.

The model (2.0.1) is possible to be used for co-current two-phase flows ( $z_1 = z_2 = z$ ) or for counter-current ones ( $z_1 + z_2 = l$ , where  $l$  is the active zone height [m] of the column). In the counter-current flows the mass transfer process models has to be presented in a two-coordinate systems [1] because in a one-coordinate system one of the equations has no solution due to the negative Laplacian value. The solution method of the equation set in two-coordinate systems will be presented in Chap. 8.

### 1. Absorption processes

The convection-diffusion type models of the absorption processes [5, 6] in the gas-liquid systems is possible to be obtained from (3.0.1) if  $j=1,2$  ( $1 = \varepsilon_1 + \varepsilon_2$ ),  $i=1,2$ . The kinetic terms  $Q_j$ ,  $j=1,2$  are the inter-phase mass transfer rates  $(-1)^j k_0 (c_{11} - \chi c_{12})$ ,  $j=1,2$  in the gas and liquid phases and the chemical reaction rate ( $-k c_{22}$ ) in the liquid phase, as volume sources or sinks of the substances in the phase parts of the elementary (column) volume [ $\text{kg} \cdot \text{mol} \cdot \text{m}^{-3} \cdot \text{s}^{-1}$ ], where  $k_0$  [ $\text{s}^{-1}$ ] is the interphase mass transfer coefficient,  $\chi$  - the Henry's number,  $k$  - the chemical reaction rate constant. The same models is possible to be used for modeling of the extraction processes if  $\chi$  is the redistribution factor.

The concentration of the transferred substance ( $i=1$ ) in the gas (liquid) phase is  $c_{11}$  ( $c_{12}$ ) [ $\text{kg} \cdot \text{mol} \cdot \text{m}^{-3}$ ], i.e. kg-mol of the transferred substance in the gas (liquid) phase in  $1 \text{ m}^3$  of the phase (elementary) volume, while the concentration of the reagent ( $i=2$ ) in the liquid phase is  $c_{22}$  [ $\text{kg} \cdot \text{mol} \cdot \text{m}^{-3}$ ] (in  $1 \text{ m}^3$  of the phase elementary volume).

The inlet concentration of the transferred substance in the gas (liquid) phase is  $c_{11}^0$  ( $c_{12}^0$ ). In the cases of absorption (desorption)  $c_{12}^0 = 0$  ( $c_{11}^0 = 0$ ) practically. The input velocities  $u_j^0$  ( $j=1,2$ ) [ $\text{m} \cdot \text{s}^{-1}$ ] of the gas and liquid phases are equal to the average velocities  $\bar{u}_j$  ( $j=1,2$ ) of the phases in the column, which are defined as

$$u_j^0 = \frac{F_j}{\varepsilon_j \pi r_0^2} = \bar{u}_j = \frac{2}{r_0^2} \int_0^{r_0} r u_j(r) dr, \quad j=1,2, \quad (0.1.1)$$

where  $F_j$ ,  $j=1,2$  are the gas and liquid phase flow rates [ $\text{m}^3 \cdot \text{s}^{-1}$ ] in the column volume.

#### 1.1 Physical absorption

The physical absorption is an interphase mass transfer of one substance from the gas to the liquid phase. The opposite is desorption. In these cases  $i_0 = 1$  and the substance index  $i$  is

possible to be ignored, i.e., the concentrations will be designated as  $c_j, j=1,2$ . As a result the convection-diffusion type model for the steady-state physical absorption in the column apparatuses has the form:

$$u_j \frac{\partial c_j}{\partial z_j} = D_j \left( \frac{\partial^2 c_j}{\partial z_j^2} + \frac{1}{r} \frac{\partial c_j}{\partial r} + \frac{\partial^2 c_j}{\partial r^2} \right) + (-1)^j k_0 (c_1 - \chi c_2), \quad j=1,2, \quad (0.1.2)$$

where  $u_j$  [m.s<sup>-1</sup>],  $D_j$  [m<sup>2</sup>.s<sup>-1</sup>] and  $\varepsilon_j$  ( $j=1,2$ ) are the velocities, the diffusivities and the hold-up coefficients in the gas and liquid phases. The boundary conditions of (2.1.2) are different in the cases of co-current and counter-current gas-liquid flows.

Let us consider a counter-current gas-liquid bubble column with an active zone height  $l$ , where  $c_1(r, z_1)$  and  $c_2(r, z_2)$  are the concentrations of the absorbed substance in the gas and the liquid phase ( $z_1 + z_2 = l$ ). The boundary conditions of (2.1.2) have the form:

$$\begin{aligned} r = 0, \quad \frac{\partial c_1}{\partial r} = \frac{\partial c_2}{\partial r} \equiv 0; \quad r = r_0, \quad \frac{\partial c_1}{\partial r} = \frac{\partial c_2}{\partial r} \equiv 0; \\ z_1 = 0, \quad c_1(r, 0) \equiv c_1^0, \quad u_1^0 c_1^0 \equiv u_1(r) c_1^0 - D_1 \left( \frac{\partial c_1}{\partial z_1} \right)_{z_1=0}; \\ z_2 = 0, \quad c_2(r, 0) \equiv c_2^0, \quad u_2^0 c_2^0 \equiv u_2(r) c_2^0 - D_2 \left( \frac{\partial c_2}{\partial z_2} \right)_{z_2=0}, \end{aligned} \quad (0.1.3)$$

where  $u_j^0, j=1,2$  are the inlet (average) velocities in the gas and the liquid phase. In the case of gas absorption  $c_2^0 = 0$  is practically valid. In the cases of co-current flows  $z_1 = z_2 = z$ . The presented convection-diffusion type model (2.1.2), (2.1.3) permits a qualitative analysis of the physical absorption processes [5, 6] to be made using dimensionless (generalized) variables:

$$R = \frac{r}{r_0}, \quad Z_1 = \frac{z_1}{l}, \quad Z_2 = \frac{z_2}{l}, \quad U_1 = \frac{u_1}{u_1^0}, \quad U_2 = \frac{u_2}{u_2^0}, \quad C_1 = \frac{c_1}{c_1^0}, \quad C_2 = \frac{c_2 \chi}{c_1^0}. \quad (0.1.4)$$

If (2.1.4) is put into (2.1.2), (2.1.3) the model in generalized variables assumes the form:

$$\begin{aligned} U_1(R) \frac{\partial C_1}{\partial Z_1} = \text{Fo}_{11} \left( \varepsilon \frac{\partial^2 C_1}{\partial Z_1^2} + \frac{1}{R} \frac{\partial C_1}{\partial R} + \frac{\partial^2 C_1}{\partial R^2} \right) - K_0 (C_1 - C_2); \\ U_2(R) \frac{\partial C_2}{\partial Z_2} = \text{Fo}_{12} \left( \varepsilon \frac{\partial^2 C_2}{\partial Z_2^2} + \frac{1}{R} \frac{\partial C_2}{\partial R} + \frac{\partial^2 C_2}{\partial R^2} \right) + K_0 \frac{u_1^0 \chi}{u_2^0} (C_1 - C_2); \\ R = 0, \quad \frac{\partial C_j}{\partial R} \equiv 0; \quad R = 1, \quad \frac{\partial C_j}{\partial R} \equiv 0; \quad j = 1, 2; \\ Z_1 = 0, \quad C_1 \equiv 1, \quad 1 \equiv U_1(R) - \text{Pe}_{11}^{-1} \left( \frac{\partial C_1}{\partial Z_1} \right)_{z_1=0}; \\ Z_2 = 0, \quad C_2 \equiv 0, \quad \left( \frac{\partial C_2}{\partial Z_2} \right)_{z_2=0} \equiv 0, \end{aligned} \quad (0.1.5)$$

where

$$K_0 = \frac{k_0 l}{u_1^0}, \quad \text{Fo}_{1j} = \frac{D_{1j} l}{u_j^0 r_0^2}, \quad \text{Pe}_{11} = \frac{u_1^0 l}{D_{11}}, \quad j = 1, 2. \quad (0.1.6)$$

From (2.1.5) it is possible to obtain directly the models of the physical absorption in the cases of highly ( $\chi \rightarrow 0, C_2 \equiv 0$ ) and slightly ( $\chi \rightarrow \infty, C_1 \equiv 1$ ) soluble gases.

The approximations of the film theory and the boundary layer theory of the mass transfer are not valid for the interphase mass transfer in the column apparatuses and the expressions for the distribution of the interphase mass transfer resistance between the gas and liquid phases (0.4.5, 0.4.12) are not possible to be used.

From (2.1.5) it follows that  $0 = K_0 = \frac{k_0 l}{u_1^0} \leq 10^{-2}$ ,  $C_1 \equiv 1$  in the cases of a big average gas velocity  $\bar{u}_1 = u_1^0$ , i.e. the solution of the first equation in (2.1.5) is equal to unity. The concentration gradient in the gas phase is equal to zero as a result of the very big convective mass transfer rate in the gas phase, i.e. the mass transfer resistance in the gas phase is very small and the process is limited by the mass transfer in the liquid phase.

In the cases  $0 = K_0 \frac{u_1^0 \chi}{u_2^0} \leq 10^{-2}$ ,  $C_2 \equiv 0$ , i.e. the solution of the second equation in (2.1.5) is equal to zero. The concentration gradient in the liquid phase is equal to zero as a result of the very big convective mass transfer rate (big average liquid velocity  $\bar{u}_2 = u_2^0$ ), i.e. the mass transfer resistance in the liquid phase is equal to zero and the process is limited by the mass transfer in the gas phase.

These results show that the convection-diffusion type model permits to be obtained the dimensionless mass transfer resistances in the gas ( $\rho_1$ ) and liquid ( $\rho_2$ ) phases:

$$\rho_1 = K_0, \quad \rho_2 = \rho_0 \rho_1, \quad \rho_0 = \frac{u_1^0 \chi}{u_2^0},$$

$$\rho_1 + \rho_2 = 1, \quad \rho_1 = \frac{1}{1 + \rho_0}, \quad \rho_2 = \frac{\rho_0}{1 + \rho_0}. \quad (0.1.7)$$

From (2.1.7) it is possible to obtain directly models of the physical absorption in the cases of highly ( $\chi \rightarrow 0, \rho_0 \rightarrow 0, \rho_2 \rightarrow 0, C_2 \equiv 0$ ) and slightly ( $\chi \rightarrow \infty, \rho_0 \rightarrow \infty, \rho_1 \rightarrow 0, C_1 \equiv 1$ ) soluble gases.

The intensification of the absorption processes is possible to be realized by intensification of the mass transfer in the limiting phase (practically by increasing of the convective mass transfer), i.e. phase with the higher mass transfer resistance. The increasing of the convective transfer in the liquid drops and gas bubbles has a limit, i.e. the optimal organization of the absorption process is the absorption in gas-liquid drops systems, when the resistance is in the gas phase ( $\rho_2 \leq 10^{-2}, \rho_0 \leq 10^{-2}$ ), or absorption in liquid-gas bubbles systems, when the resistance is in the liquid phase ( $\rho_1 \leq 10^{-2}, \rho_0 \geq 10^2$ ).

For high columns the parameter  $\varepsilon$  is very small ( $0 = \varepsilon \leq 10^{-2}$ ) and the problem (2.1.5) is possible to be solved in zero approximation with respect to  $\varepsilon$ :

$$U_1(R) \frac{\partial C_1}{\partial Z_1} = Fo_1 \left( \frac{1}{R} \frac{\partial C_1}{\partial R} + \frac{\partial^2 C_1}{\partial R^2} \right) - K_0 (C_1 - C_2);$$

$$U_2(R) \frac{\partial C_2}{\partial Z_2} = Fo_2 \left( \frac{1}{R} \frac{\partial C_2}{\partial R} + \frac{\partial^2 C_2}{\partial R^2} \right) + K_0 \frac{u_1^0 \chi}{u_2^0} (C_1 - C_2);$$

$$R = 0, \quad \frac{\partial C_i}{\partial R} \equiv 0; \quad R = 1, \quad \frac{\partial C_i}{\partial R} \equiv 0; \quad i = 1, 2;$$

$$Z_1 = 0, \quad \frac{\partial R}{\partial Z_1} \equiv 1; \quad Z_2 = 0, \quad \frac{\partial R}{\partial Z_2} \equiv 0. \quad (0.1.8)$$

For big values of the average velocities  $0 = Fo_1 \leq 10^{-2}, 0 = Fo_2 \leq 10^{-2}$  and from (2.1.5) follows the convective type model

$$\begin{aligned}
U_1(R) \frac{dC_1}{dZ_1} &= -K_0 (C_1 - C_2); \\
U_2(R) \frac{dC_2}{dZ_2} &= K_0 \frac{u_1^0 \chi}{u_2^0} (C_1 - C_2); \\
Z_1 = 0, \quad C_1 &\equiv 1; \quad Z_2 = 0, \quad C_2 \equiv 0. \quad (0.1.9)
\end{aligned}$$

For small values of the average velocities  $0 = K_0^{-1} \leq 10^{-2}$ ,  $0 = \left( K_0 \frac{u_1^0 \chi}{u_2^0} \right)^{-1} \leq 10^{-2}$  from (2.1.5) follows the diffusion type model:

$$\begin{aligned}
0 &= K_0^{-1} \text{Fo}_1 \left( \varepsilon \frac{\partial^2 C_1}{\partial Z_1^2} + \frac{1}{R} \frac{\partial C_1}{\partial R} + \frac{\partial^2 C_1}{\partial R^2} \right) - (C_1 - C_2); \\
0 &= \left( K_0 \frac{u_1^0 \chi}{u_2^0} \right)^{-1} \text{Fo}_2 \left( \varepsilon \frac{\partial^2 C_2}{\partial Z_2^2} + \frac{1}{R} \frac{\partial C_2}{\partial R} + \frac{\partial^2 C_2}{\partial R^2} \right) + (C_1 - C_2); \\
R = 0, \quad \frac{\partial C_i}{\partial R} &\equiv 0; \quad R = 1, \quad \frac{\partial C_i}{\partial R} \equiv 0; \quad i = 1, 2; \\
Z_1 = 0, \quad C_1 &\equiv 1, \quad 1 \equiv U_1(R) - \text{Pe}_1^{-1} \left( \frac{\partial C_1}{\partial Z_1} \right)_{Z_1=0}; \\
Z_2 = 0, \quad C_2 &\equiv 0, \quad \left( \frac{\partial C_2}{\partial Z_2} \right)_{Z_2=0} \equiv 0.
\end{aligned} \quad (0.1.10)$$

The solution of the model equations of a counter-current physical absorption in two-coordinate systems are presented in Chap. 8 and [6].

### 1.2 Chemical absorption

Two reagents ( $i_0 = 2$ ) participate in the chemical absorption. The first is in the gas phase ( $i = 1, j = 1$ ) and the second is in the liquid phase ( $i = 2, j = 2$ ). The chemical absorption will be presented in a co-current column ( $z_1 = z_2 = z$ ). Considering that  $c_{11}$  ( $c_{12}$ ) is the concentration of the first reagent in the gas (liquid) phase and  $c_{22}$  is the concentration of the second reagent in the absorbent, the mass sources (sinks) in the medium elementary volume (in the physical approximations of the mechanics of continua) are equal to the chemical reaction rate -  $k c_{12} c_{22}$  and the inter-phase mass transfer rate -  $k_0 (c_{11} - \chi c_{12})$ . As a result, the convection-diffusion model in a column has the form:

$$\begin{aligned}
u_1 \frac{\partial c_{11}}{\partial z} &= D_{11} \left( \frac{\partial^2 c_{11}}{\partial z^2} + \frac{1}{r} \frac{\partial c_{11}}{\partial r} + \frac{\partial^2 c_{11}}{\partial r^2} \right) - k_0 (c_{11} - \chi c_{12}), \\
u_2 \frac{\partial c_{12}}{\partial z} &= D_{12} \left( \frac{\partial^2 c_{12}}{\partial z^2} + \frac{1}{r} \frac{\partial c_{12}}{\partial r} + \frac{\partial^2 c_{12}}{\partial r^2} \right) + k_0 (c_{11} - \chi c_{12}) - k c_{12} c_{22}, \\
u_2 \frac{\partial c_{22}}{\partial z} &= D_{22} \left( \frac{\partial^2 c_{22}}{\partial z^2} + \frac{1}{r} \frac{\partial c_{22}}{\partial r} + \frac{\partial^2 c_{22}}{\partial r^2} \right) - k c_{12} c_{22},
\end{aligned} \quad (0.1.11)$$

where  $u_1(r)$ ,  $u_2(r)$  are the velocity distributions in the gas and liquid phases,  $c_{ij}(r, z)$  and  $D_{ij}$  ( $i = 1, 2; j = 1, 2$ ) are the concentration distributions and the diffusivities of the first reagent in the gas and liquid phases and of the second reagent in the liquid phase.

Let us consider a co-current liquid-gas bubble column with a radius  $r_0$  and working zone height  $l$ . The boundary conditions of the model equations (2.1.11) have the form:

$$\begin{aligned}
r=0, \quad \frac{\partial c_{11}}{\partial r} = \frac{\partial c_{12}}{\partial r} = \frac{\partial c_{22}}{\partial r} \equiv 0; \quad r=r_0, \quad \frac{\partial c_{11}}{\partial r} = \frac{\partial c_{12}}{\partial r} = \frac{\partial c_{22}}{\partial r} \equiv 0; \\
z=0, \quad c_{11} \equiv c_{11}^0, \quad u_1^0 c_{11}^0 \equiv u_1(r) c_{11}^0 - D_{11} \left( \frac{\partial c_{11}}{\partial z} \right)_{z=0}; \\
z=0, \quad c_{12} \equiv c_{12}^0, \quad u_2^0 c_{12}^0 \equiv u_2(r) c_{12}^0 - D_{12} \left( \frac{\partial c_{12}}{\partial z} \right)_{z=0}; \\
z=0, \quad c_{22} \equiv c_{22}^0, \quad u_2^0 c_{22}^0 \equiv u_2(r) c_{22}^0 - D_{22} \left( \frac{\partial c_{22}}{\partial z} \right)_{z=0},
\end{aligned} \tag{0.1.12}$$

where  $u_j^0, c_{ij}^0, i=1,2, j=1,2$  are the inlet velocities and concentrations in the gas and liquid phases. In the cases of gas absorption  $c_{12}^0 = 0$  is practically valid.

A qualitative analysis of the model is possible to be made using dimensionless (generalized) variables:

$$R = \frac{r}{r_0}, \quad Z = \frac{z}{l}, \quad U_1 = \frac{u_1}{u_1^0}, \quad U_2 = \frac{u_2}{u_2^0}, \quad C_{11} = \frac{c_{11}}{c_{11}^0}, \quad C_{12} = \frac{c_{12} \chi}{c_{11}^0}, \quad C_{22} = \frac{c_{22}}{c_{22}^0}. \tag{0.1.13}$$

The model (2.1.11), (2.1.12) in generalized variables (2.1.13) has the form:

$$\begin{aligned}
U_1(R) \frac{\partial C_{11}}{\partial Z} &= \text{Fo}_{11} \left( \varepsilon \frac{\partial^2 C_{11}}{\partial Z^2} + \frac{1}{R} \frac{\partial C_{11}}{\partial R} + \frac{\partial^2 C_{11}}{\partial R^2} \right) - K_0 (C_{11} - C_{12}); \\
U_2(R) \frac{\partial C_{12}}{\partial Z} &= \text{Fo}_{12} \left( \varepsilon \frac{\partial^2 C_{12}}{\partial Z^2} + \frac{1}{R} \frac{\partial C_{12}}{\partial R} + \frac{\partial^2 C_{12}}{\partial R^2} \right) + \\
&\quad + K_0 \frac{u_1^0 \chi}{u_2^0} (C_{11} - C_{12}) - \text{Da} \frac{c_{22}^0 \chi}{c_{11}^0} C_{12} C_{22}; \\
U_2(R) \frac{\partial C_{22}}{\partial Z} &= \text{Fo}_{22} \left( \varepsilon \frac{\partial^2 C_{22}}{\partial Z^2} + \frac{1}{R} \frac{\partial C_{22}}{\partial R} + \frac{\partial^2 C_{22}}{\partial R^2} \right) - \text{Da} C_{12} C_{22}; \\
R=0, \quad \frac{\partial C_s}{\partial R} &\equiv 0; \quad R=1, \quad \frac{\partial C_s}{\partial R} \equiv 0; \quad s=11,12,22;
\end{aligned} \tag{0.1.14}$$

$$\begin{aligned}
Z=0, \quad C_{11} &\equiv 1, \quad 1 \equiv U_1(R) - \text{Pe}_{11}^{-1} \left( \frac{\partial C_{11}}{\partial Z} \right)_{Z=0}; \\
Z=0, \quad C_{12} &\equiv 0, \quad \left( \frac{\partial C_{12}}{\partial Z} \right)_{Z=0} \equiv 0; \\
Z=0, \quad C_{22} &\equiv 1, \quad 1 \equiv U_2(R) - \text{Pe}_{22}^{-1} \left( \frac{\partial C_{22}}{\partial Z} \right)_{Z=0},
\end{aligned}$$

where

$$\begin{aligned}
K_0 &= \frac{k_0 l}{u_1^0}, \quad \text{Fo}_{11} = \frac{D_{11} l}{u_1^0 r_0^2}, \quad \text{Fo}_{12} = \frac{D_{12} l}{u_2^0 r_0^2}, \quad \text{Fo}_{22} = \frac{D_{22} l}{u_2^0 r_0^2}, \\
\text{Da} &= \frac{k l c_{11}^0}{u_2^0 \chi}, \quad \text{Pe}_{11} = \frac{u_1^0 l}{D_{11}}, \quad \text{Pe}_{22} = \frac{u_2^0 l}{D_{22}}.
\end{aligned} \tag{0.1.15}$$

From (2.1.14) follows that the absence of a chemical reaction in liquid phase -  $k=0$  (or  $c_3^0=0$ ) leads to  $\text{Da}=0, C_{22} \equiv 1$ , (or  $C_{22} \equiv 0$ ) and as a result the model of the physical absorption is obtained (2.1.5). The same result is possible to be obtained in the cases

$0 = \text{Da} \frac{c_{22}^0 \chi}{c_{11}^0} \leq 10^{-2}$ , i.e. the chemical reaction effect is negligible (it is not possible to be measured experimentally).

In the cases, when the interphase mass transfer is a result of the chemical reaction in the

liquid phase (  $\text{Da} \frac{c_{22}^0 \chi}{c_{11}^0} \geq 1$  ), the second equation in (2.1.14) should be divided by  $\text{Da} \frac{c_{22}^0 \chi}{c_{11}^0} \geq 1$ ,  
i.e.

$$\begin{aligned}
 U_1(R) \frac{\partial C_{11}}{\partial Z} &= \text{Fo}_{11} \left( \varepsilon \frac{\partial^2 C_{11}}{\partial Z^2} + \frac{1}{R} \frac{\partial C_{11}}{\partial R} + \frac{\partial^2 C_{11}}{\partial R^2} \right) - K_0 (C_{11} - C_{12}); \\
 \text{Da}^{-1} \frac{c_{11}^0}{c_{22}^0 \chi} U_2(R) \frac{\partial C_{12}}{\partial Z} &= \frac{\text{Fo}_{12} c_{11}^0}{\text{Da} c_{22}^0 \chi} \left( \varepsilon \frac{\partial^2 C_{12}}{\partial Z^2} + \frac{1}{R} \frac{\partial C_{12}}{\partial R} + \frac{\partial^2 C_{12}}{\partial R^2} \right) + \\
 &\quad + K_0 \frac{u_1^0 c_{11}^0}{\text{Da} u_2^0 c_{22}^0} (C_{11} - C_{12}) - C_{12} C_{22}; \\
 \text{Da}^{-1} U_2(R) \frac{\partial C_{22}}{\partial Z} &= \text{Da}^{-1} \text{Fo}_{22} \left( \varepsilon \frac{\partial^2 C_{22}}{\partial Z^2} + \frac{1}{R} \frac{\partial C_{22}}{\partial R} + \frac{\partial^2 C_{22}}{\partial R^2} \right) - C_{12} C_{22}; \\
 R=0, \quad \frac{\partial C_s}{\partial R} &\equiv 0; \quad R=1, \quad \frac{\partial C_s}{\partial R} \equiv 0; \quad s=11,12,22; \\
 Z=0, \quad C_{11} &\equiv 1, \quad 1 \equiv U_1(R) - \text{Pe}_{11}^{-1} \left( \frac{\partial C_{11}}{\partial Z} \right)_{Z=0}, \quad C_{12} \equiv 0, \quad \left( \frac{\partial C_{12}}{\partial Z} \right)_{Z=0} \equiv 0, \\
 C_{22} &\equiv 1, \quad 1 \equiv U_2(R) - \text{Pe}_{22}^{-1} \left( \frac{\partial C_{22}}{\partial Z} \right)_{Z=0}.
 \end{aligned} \tag{0.1.16}$$

In the cases of very fast chemical reactions (  $\text{Da} \frac{c_{22}^0 \chi}{c_{11}^0} \geq 10^2$  ) from (2.1.14) is possible to obtain

$$\begin{aligned}
 U_1(R) \frac{\partial C_{11}}{\partial Z} &= \text{Fo}_{11} \left( \varepsilon \frac{\partial^2 C_{11}}{\partial Z^2} + \frac{1}{R} \frac{\partial C_{11}}{\partial R} + \frac{\partial^2 C_{11}}{\partial R^2} \right) - K_0 (C_{11} - C_{12}); \\
 0 &= \frac{\text{Fo}_{12} c_{11}^0}{\text{Da} c_{22}^0 \chi} \left( \varepsilon \frac{\partial^2 C_{12}}{\partial Z^2} + \frac{1}{R} \frac{\partial C_{12}}{\partial R} + \frac{\partial^2 C_{12}}{\partial R^2} \right) + \\
 &\quad + K_0 \frac{u_1^0 c_{11}^0}{\text{Da} u_2^0 c_{22}^0} (C_{11} - C_{12}) - C_{12} C_{22}; \\
 U_2(R) \frac{\partial C_{22}}{\partial Z} &= \text{Fo}_{22} \left( \varepsilon \frac{\partial^2 C_{22}}{\partial Z^2} + \frac{1}{R} \frac{\partial C_{22}}{\partial R} + \frac{\partial^2 C_{22}}{\partial R^2} \right) - \text{Da} C_{12} C_{22}; \\
 R=0, \quad \frac{\partial C_s}{\partial R} &\equiv 0; \quad R=1, \quad \frac{\partial C_s}{\partial R} \equiv 0; \quad s=11,12,22; \\
 Z=0, \quad C_{11} &\equiv 1, \quad 1 \equiv U_1(R) - \text{Pe}_{11}^{-1} \left( \frac{\partial C_{11}}{\partial Z} \right)_{Z=0}; \\
 Z=0, \quad C_{12} &\equiv 0, \quad \left( \frac{\partial C_{12}}{\partial Z} \right)_{Z=0} \equiv 0; \\
 Z=0, \quad C_{22} &\equiv 1, \quad 1 \equiv U_2(R) - \text{Pe}_{22}^{-1} \left( \frac{\partial C_{22}}{\partial Z} \right)_{Z=0}.
 \end{aligned} \tag{0.1.17}$$

For big values of the average velocities  $0 = \text{Fo}_s \leq 10^{-2}$ ,  $s=1,2,3$  from (2.1.14) follows the convective type model



$$\begin{aligned}
U_1(R) \frac{dC_{11}}{dZ} &= -K_0 (C_{11} - C_{12}); \\
U_2(R) \frac{dC_{12}}{dZ} &= K_0 \frac{u_1^0 \chi}{u_2^0} (C_{11} - C_{12}) - \text{Da} \frac{c_{22}^0 \chi}{c_{11}^0} C_{12} C_{22}; \\
U_2(R) \frac{dC_{22}}{dZ} &= -\text{Da} C_{12} C_{22}; \\
Z=0, \quad C_s &\equiv 1, \quad s=11,22; \quad Z=1, \quad C_{12} \equiv 0.
\end{aligned} \tag{0.1.18}$$

The concentration distribution in the chemical absorption case will be obtained for high columns, where the parameter  $\varepsilon$  in (2.1.14) is very small ( $0 = \varepsilon \leq 10^{-2}$ ). The velocity distributions in the phases will be Poiseuille type and the difference between the velocities of the phases will be in the average velocities only:

$$U_1 = U_2 = 2 - 2R^2. \tag{0.1.19}$$

As a result, the problem (2.1.14) takes the form:

$$\begin{aligned}
(2 - 2R^2) \frac{\partial C_{11}}{\partial Z} &= \text{Fo}_{11} \left( \frac{1}{R} \frac{\partial C_{11}}{\partial R} + \frac{\partial^2 C_{11}}{\partial R^2} \right) - K_0 (C_{11} - C_{12}); \\
(2 - 2R^2) \frac{\partial C_{12}}{\partial Z} &= \text{Fo}_{12} \left( \frac{1}{R} \frac{\partial C_{12}}{\partial R} + \frac{\partial^2 C_{12}}{\partial R^2} \right) + \\
&+ K_0 \frac{u_1^0 \chi}{u_2^0} (C_{11} - C_{12}) - \text{Da} \frac{c_{22}^0 \chi}{c_{11}^0} C_{12} C_{22}; \\
(2 - 2R^2) \frac{\partial C_{22}}{\partial Z} &= \text{Fo}_{22} \left( \frac{1}{R} \frac{\partial C_{22}}{\partial R} + \frac{\partial^2 C_{22}}{\partial R^2} \right) - \text{Da} C_{12} C_{22}; \\
R=0, \quad \frac{\partial C_s}{\partial R} &\equiv 0; \quad R=1, \quad \frac{\partial C_s}{\partial R} \equiv 0; \quad s=11,12,22; \\
Z=0, \quad C_{11} &\equiv 1, \quad C_{12} \equiv 0, \quad C_{22} \equiv 1.
\end{aligned} \tag{0.1.20}$$

The solution of (2.1.20) is obtained in the case  $\text{Fo}_{11} = \text{Fo}_{12} = \text{Fo}_{22} = 0.1$ ,

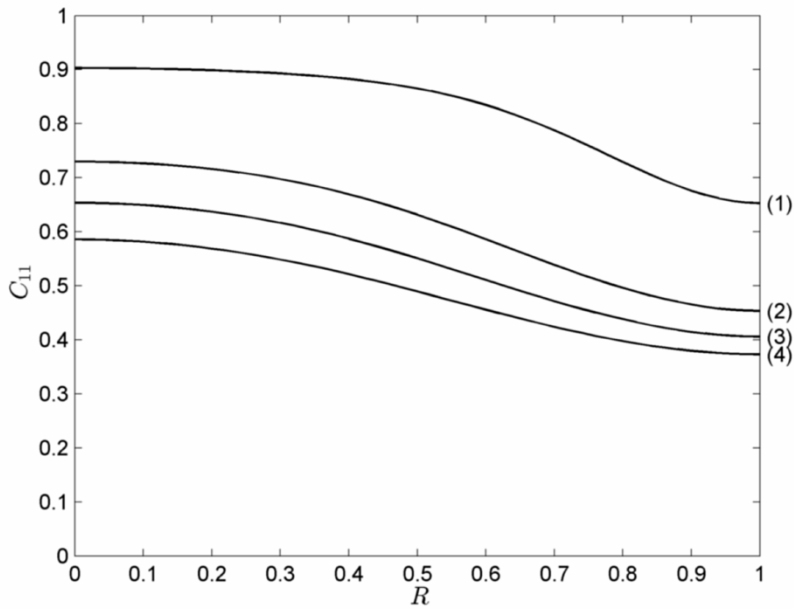
$$K_0 = \text{Da} = 1, \quad \frac{u_1^0 \chi}{u_2^0} = 1, \quad \frac{c_{22}^0 \chi}{c_{11}^0} = 2$$

and the results are presented on Figs. 3.1 and 3.2.

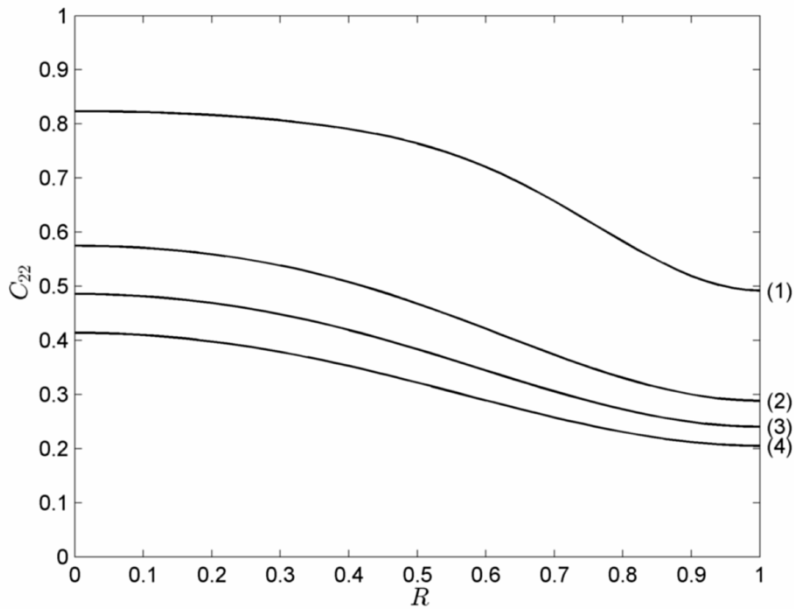
In the chemical absorption case the model (2.1.14) permits to obtain (similar to (2.1.17)) the inter-phase mass transfer resistance distribution between the gas and liquid phases:

$$\begin{aligned}
\rho_1 &= K, \quad \rho_2 = \rho_0 \rho_1, \quad \rho_0 = \frac{u_1^0 c_{11}^0}{\text{Da} u_2^0 c_{22}^0}, \\
\rho_1 + \rho_2 &= 1, \quad \rho_1 = \frac{1}{1 + \rho_0}, \quad \rho_2 = \frac{\rho_0}{1 + \rho_0},
\end{aligned} \tag{0.1.21}$$

where the parameters  $\rho_1$  and  $\rho_2$  can be considered as mass transfer resistances in the gas and liquid phases. Very often the big values of  $\text{Da}$  lead to small values of  $\rho_0$  and as a result  $\rho_1 \ll \rho_2$ , i.e. the gas is the limiting phase and the optimal organization of the absorption process is the absorption in gas-liquid drops systems.



**Fig. 3.1** Concentration distribution  $C_{11}(R,Z)$ : (1) -  $Z=0.2$ ; (2) -  $Z=0.4$ ; (3) -  $Z = 0.8$ ; (4) -  $Z = 1$



**Fig. 3.2** Concentration distribution  $C_{22}(R,Z)$ : (1) -  $Z = 0.2$ ; (2) -  $Z = 0.4$ ; (3) -  $Z = 0.8$ ; (4) -  $Z = 1$

The theoretical procedure (II.5–II.15) presented in Part II will be used for the creation of average concentration models of absorption, adsorption and catalytic processes in two-phase systems.

The convection-diffusion model of the two-phase systems [1–3] has the form (3.0.1):

$$\begin{aligned}
u_j \frac{\partial c_{ij}}{\partial z_j} &= D_{ij} \left( \frac{\partial^2 c_{ij}}{\partial z_j^2} + \frac{1}{r} \frac{\partial c_{ij}}{\partial r} + \frac{\partial^2 c_{ij}}{\partial r^2} \right) + Q_{ij}(c_{ij}); \\
r=0, \quad \frac{\partial c_{ij}}{\partial r} &\equiv 0; \quad r=r_0, \quad \frac{\partial c_{ij}}{\partial r} \equiv 0; \\
z_j=0, \quad c_{ij} &\equiv c_{ij}^0, \quad u_j c_{ij}^0 \equiv u_j c_{ij}^0 - D_{ij} \left( \frac{\partial c_{ij}}{\partial z_j} \right)_{z_j=0}; \\
i=1,2,\dots,i_0; \quad j=1,2=1,3=2,3. & \quad (0.1.22)
\end{aligned}$$

The average values of the velocities and concentrations at the column cross-sectional area in two phase systems follow from (II.3):

$$\begin{aligned}
\bar{u}_j &= \frac{2}{r_0^2} \int_0^{r_0} r u_j(r) dr, \quad \bar{c}_{ij}(z) = \frac{2}{r_0^2} \int_0^{r_0} r c_{ij}(r, z) dr, \\
i=1,2,\dots,i_0, \quad j=1,2=1,3=2,3. & \quad (0.1.23)
\end{aligned}$$

The functions  $u_j(r), c_{ij}(r, z)$  in (6.0.1) can be presented by the average functions (6.0.2):

$$\begin{aligned}
u_j(r) &= \bar{u}_j \tilde{u}_j(r), \quad c_{ij}(r, z) = \bar{c}_{ij}(z) \tilde{c}_{ij}(r, z), \\
i=1,2,\dots,i_0, \quad j=1,2=1,3=2,3, & \quad (0.1.24)
\end{aligned}$$

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

$$\frac{2}{r_0^2} \int_0^{r_0} r \tilde{u}_j(r) dr = 1, \quad \frac{2}{r_0^2} \int_0^{r_0} r \tilde{c}_{ij}(r, z) dr = 1, \quad i=1,2,\dots,i_0, \quad j=1,2=1,3=2,3. \quad (0.1.25)$$

The average concentration model may be obtained when putting (6.0.3) into (6.0.1), multiplying by  $r$  and integrating over  $r$  in the interval  $[0, r_0]$ . As a result, the average concentration model has the form:

$$\begin{aligned}
\alpha_{ij} \bar{u}_j \frac{d \bar{c}_{ij}}{dz_j} + \frac{d \alpha_{ij}}{dz_j} \bar{u}_j \bar{c}_{ij} &= D_{ij} \frac{d^2 \bar{c}_{ij}}{dz_j^2} + \frac{2}{r_0^2} \int_0^{r_0} r Q_{ij} dr; \\
z_j=0, \quad \bar{c}_{ij} &= c_{ij}^0, \quad \left( \frac{d \bar{c}_{ij}}{dz_j} \right)_{z_j=0} = 0; \\
i=1,2,\dots,i_0, \quad j=1,2=1,3=2,3, & \quad (0.1.26)
\end{aligned}$$

where

$$\alpha_{ij}(z) = \frac{2}{r_0^2} \int_0^{r_0} r \tilde{u}_j(r) \tilde{c}_{ij}(r, z) dr, \quad i=1,2,\dots,i_0, \quad j=1,2=1,3=2,3. \quad (0.1.27)$$

## 1 Absorption processes modeling

### 1.1 Physical absorption

The convection-diffusion model of the physical absorption ( $i_0=1$  and the substance index  $i$  is possible to be ignored,  $j=1,2$ ) in a counter-current column [4, 5] has the form (3.1.2, 3.1.3):

$$\begin{aligned}
u_j \frac{\partial c_j}{\partial z_j} &= D_j \left( \frac{\partial^2 c_j}{\partial z_j^2} + \frac{1}{r} \frac{\partial c_j}{\partial r} + \frac{\partial^2 c_j}{\partial r^2} \right) + (-1)^j k_0 (c_1 - \chi c_2); \quad j=1,2; \\
r=0, \quad \frac{\partial c_1}{\partial r} = \frac{\partial c_2}{\partial r} &\equiv 0; \quad r=r_0, \quad \frac{\partial c_1}{\partial r} = \frac{\partial c_2}{\partial r} \equiv 0; \\
z_1=0, \quad c_1(r,0) &\equiv c_1^0, \quad u_1^0 c_1^0 \equiv u_1(r) c_1^0 - D_1 \left( \frac{\partial c_1}{\partial z_1} \right)_{z_1=0}; \\
z_2=0, \quad c_2(r,0) &\equiv c_2^0, \quad u_2^0 c_2^0 \equiv u_2(r) c_2^0 - D_2 \left( \frac{\partial c_2}{\partial z_2} \right)_{z_2=0},
\end{aligned} \tag{0.2.1}$$

where  $z_1 + z_2 = l$  ( $l$  is the column active zone height in the co-current column  $z_1 = z_2 = z$ ) and  $c_2^0 = 0$ , practically.

The use of the averaging procedure (6.0.1)–(6.0.5) leads to the average concentration model of the physical absorption:

$$\begin{aligned}
\alpha_j \bar{u}_j \frac{d\bar{c}_j}{dz_j} + \frac{d\alpha_j}{dz_j} \bar{u}_j \bar{c}_j &= D_j \frac{d^2 \bar{c}_j}{dz_j^2} + (-1)^j k_0 (\bar{c}_1 - \chi \bar{c}_2); \quad j=1,2; \\
z_1=0, \quad \bar{c}_1(r,0) &= c_1^0, \quad \left( \frac{d\bar{c}_1}{dz_1} \right)_{z_1=0} = 0; \quad z_2=0, \quad \bar{c}_2(r,0) = 0, \quad \left( \frac{d\bar{c}_2}{dz_2} \right)_{z_2=0} = 0;
\end{aligned} \tag{0.2.2}$$

where

$$\alpha_j(z_j) = \frac{2}{r_0^2} \int_0^{r_0} r \tilde{u}_j(r) \tilde{c}_j(r, z_j) dr, \quad j=1,2. \tag{0.2.3}$$

For a theoretical analysis of the physical absorption the following dimensionless (generalized) variables have to be used:

$$Z_1 = \frac{z_1}{l}, \quad Z_2 = \frac{z_2}{l}, \quad \bar{C}_1 = \frac{\bar{c}_1}{c_1^0}, \quad \bar{C}_2 = \frac{\bar{c}_2 \chi}{c_1^0}. \tag{0.2.4}$$

If (6.1.4) is put into (6.1.2) the model in generalized variables takes the form:

$$\begin{aligned}
A_j \frac{d\bar{C}_j}{dZ_j} + \frac{dA_j}{dZ_j} \bar{C}_j &= \text{Pe}_j^{-1} \frac{d^2 \bar{C}_j}{dZ_j^2} - (-1)^{j-1} K_{0j} (\bar{C}_1 - \bar{C}_2); \\
Z_1=0, \quad \bar{C}_1 &= 1, \quad \left( \frac{d\bar{C}_1}{dZ_1} \right)_{Z_1=0} = 0; \quad Z_2=0, \quad \bar{C}_2 = 0, \quad \left( \frac{d\bar{C}_2}{dZ_2} \right)_{Z_2=0} = 0,
\end{aligned} \tag{0.2.5}$$

where

$$\text{Pe}_j = \frac{\bar{u}_j l}{D_j}, \quad K_{0j} = \frac{k_0 l}{\bar{u}_j} \chi^{j-1}, \quad j=1,2. \tag{0.2.6}$$

From (6.0.2), (6.0.3), (6.0.6), (6.1.3) and (6.1.4) follow the expressions:

$$\tilde{u}_j(r) = \frac{u_j(r_0 R)}{\bar{u}_j} = U_j(R), \quad \tilde{c}_j(r, z_j) = \frac{c_j(r_0 R, l Z_j)}{\bar{c}_j(l Z_j)} = \frac{C_j(R, Z_j)}{\bar{C}_j(Z_j)}, \tag{0.2.7}$$

$$\bar{C}_j(Z_j) = 2 \int_0^1 R C_j(R, Z_j) dR,$$

$$\alpha_j(z_j) = \alpha_j(l Z_j) = A_j(Z_j) = 2 \int_0^1 R U_j(R) \frac{C_j(R, Z_j)}{\bar{C}_j(Z_j)} dR, \quad j=1,2.$$

As an example will be considered the case of parabolic velocity distribution (Poiseuille flow), where the difference between the phase velocities lies in the average velocities only:

$$U_1 = U_2 = 2 - 2R^2. \quad (0.2.8)$$

The solution of the model equations (2.1.8) for a high column ( $0 = \varepsilon \leq 10^{-2}$ ,  $0 = \text{Pe}_j^{-1} = \varepsilon \text{Fo}_j \leq 10^{-2}$  for  $\text{Fo}_j \leq 1$ ,  $j=1,2$ ,  $\text{Fo}_1 = 0.1$ ,  $\text{Fo}_2 = 0.01$ ,  $K_{01} = 1$ ,  $K_{02} = 0.1$ ), using the iterative algorithm [5] in Chapter 8 and (6.1.7) permits to obtain the average concentrations  $\bar{C}_j(Z_j)$  (Figs. 6.1 and 6.2) and the functions  $A_j(Z_j)$ ,  $j=1,2$  (Figs. 6.3 and 6.4).

The functions  $A_j = A_j(Z_j)$ ,  $j=1,2$  presented on Figs. 6.3 and 6.4 show that linear approximations are possible to be used:

$$A_j = a_{0j} + a_{1j}Z_j, \quad j=1,2. \quad (0.2.9)$$

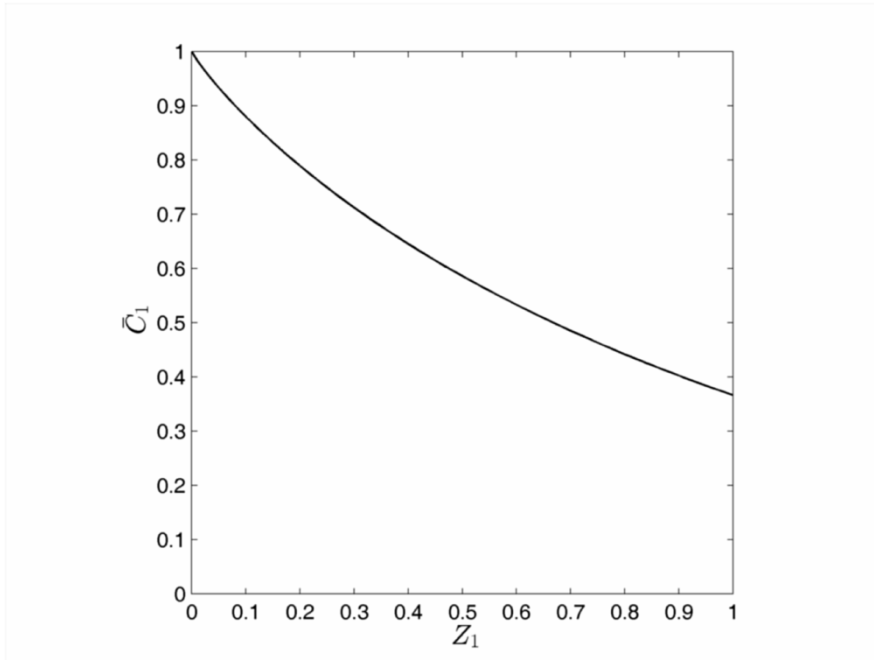
The obtained (“theoretical”) parameters’ values are presented in Table 6.1.

In the case of high columns ( $\text{Pe}_j^{-1} = \varepsilon = 0$ ) the average concentration model of a counter-current physical absorption process has the form:

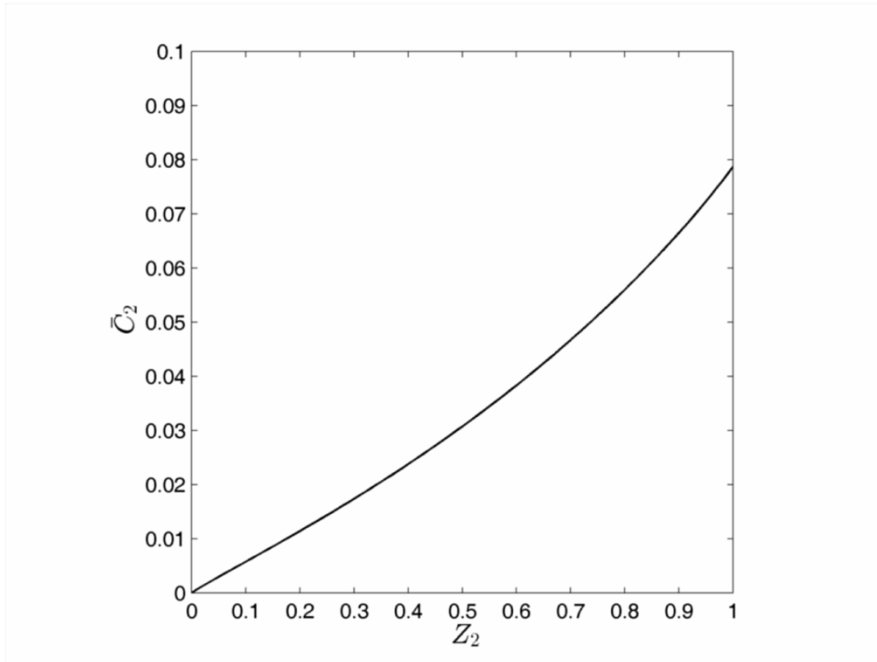
$$\begin{aligned} (a_{01} + a_{11}Z_1) \frac{d\bar{C}_1}{dZ_1} + a_{11}\bar{C}_1 &= -K_{01}(\bar{C}_1 - \bar{C}_2); \quad Z_1 = 0, \quad \bar{C}_1(0) = 1. \\ (a_{02} + a_{12}Z_2) \frac{d\bar{C}_2}{dZ_2} + a_{12}\bar{C}_2 &= K_{02}(\bar{C}_1 - \bar{C}_2); \quad Z_2 = 0, \quad \bar{C}_2(0) = 0. \end{aligned} \quad (0.2.10)$$

The obtained average concentrations  $\bar{C}_j(Z_j)$ ,  $j=1,2$  (Figs. 6.1 and 6.2) permit to obtained “artificial experimental data” for different values of  $Z_j$ ,  $j=1,2$ :

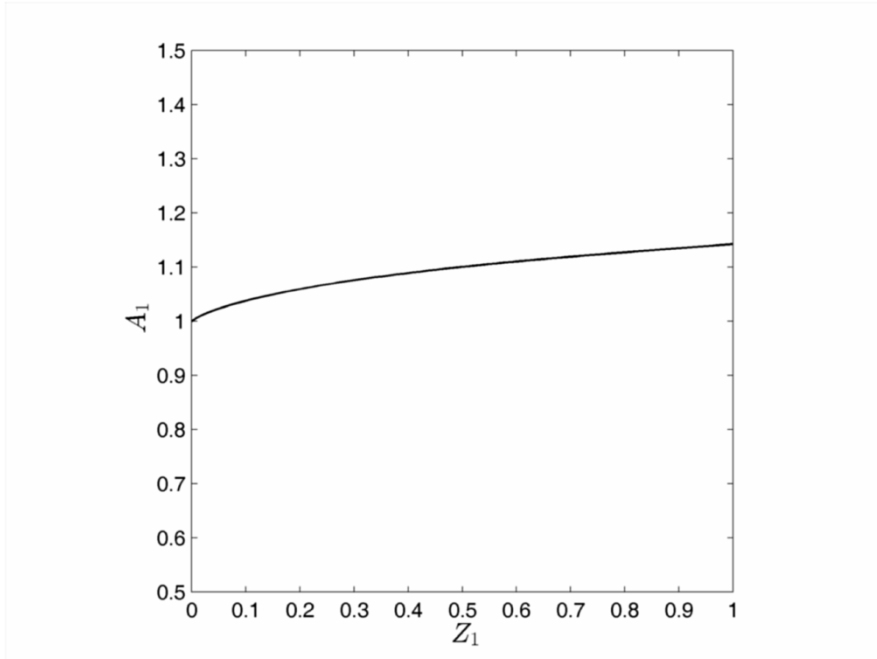
$$\begin{aligned} \bar{C}_{j\text{exp}}^m(Z_{jn}) &= (0.95 + 0.1S_m)\bar{C}_j(Z_{jn}), \quad m=1, \dots, 10, \\ Z_{jn} &= 0.1n, \quad n=1, 2, \dots, 10, \quad j=1, 2, \end{aligned} \quad (0.2.11)$$



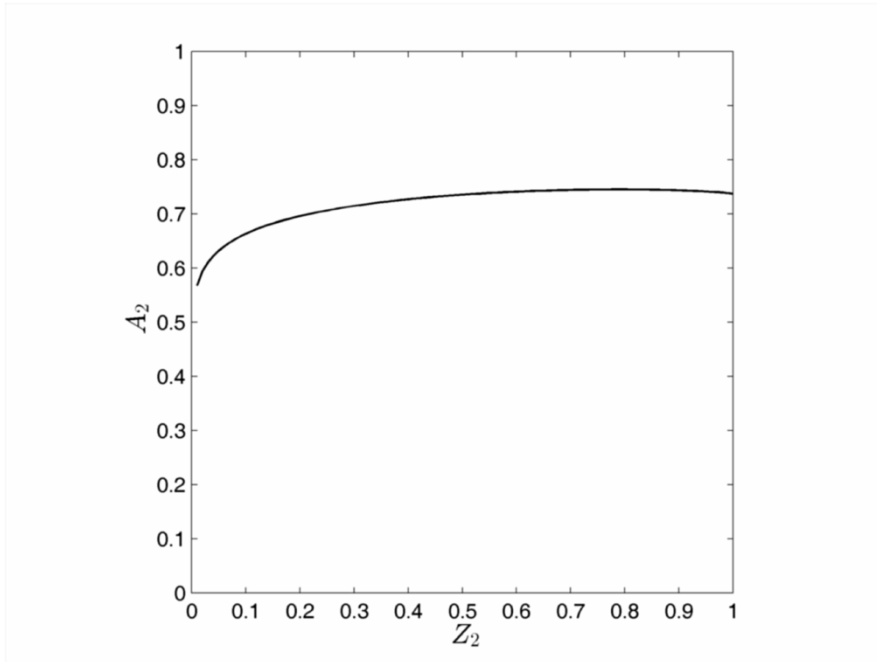
**Fig. 6.1** Average concentration  $\bar{C}_1(Z_1)$  for  $\text{Fo}_1 = 0.1$ ,  $\text{Fo}_2 = 0.01$ ,  $K_{01} = 1$ ,  $K_{02} = 0.1$



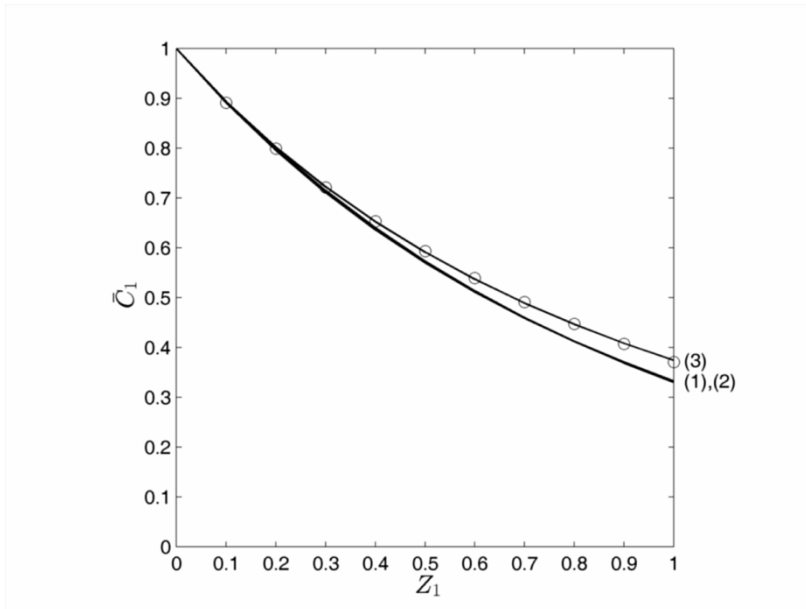
**Fig. 6.2** Average concentration  $\bar{C}_2(Z_2)$  for  $Fo_1 = 0.1$ ,  $Fo_2 = 0.01$ ,  $K_{01} = 1$ ,  $K_{02} = 0.1$



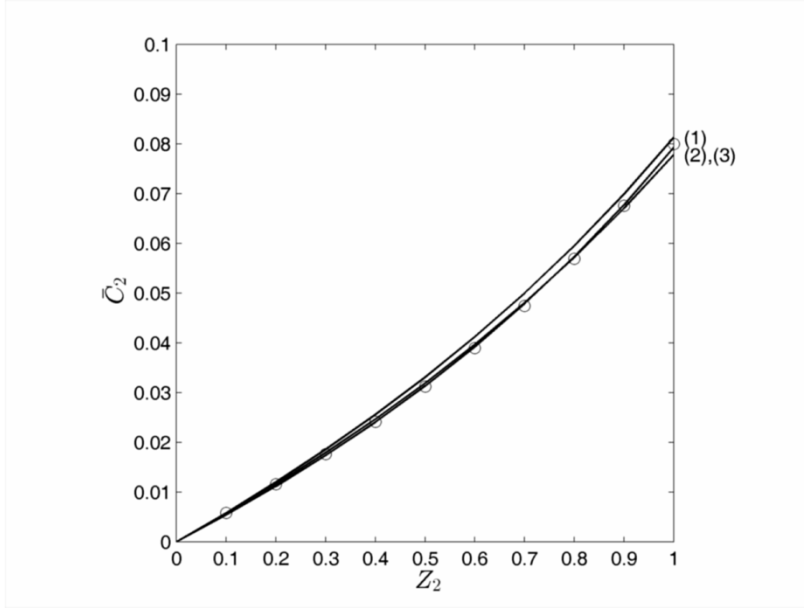
**Fig. 6.3** Function  $A_1(Z_1)$  for  $Fo_1 = 0.1$ ,  $Fo_2 = 0.01$ ,  $K_{01} = 1$ ,  $K_{02} = 0.1$



**Fig. 6.4** Function  $A_2(Z_2)$  for  $Fo_1 = 0.1$ ,  $Fo_2 = 0.01$ ,  $K_{01} = 1$ ,  $K_{02} = 0.1$



**Fig. 6.5** Comparison of concentration distributions (6.1.10): (1)-  $\bar{C}_1^1(Z_1, a_{01}^1, a_{11}^1)$ ; (2)-  $\bar{C}_1^2(Z_1, a_{01}^2, a_{11}^2)$ ; (3)-  $\bar{C}_1^0(Z_1, a_{01}^0, a_{11}^0)$ ;  $\circ$  - “artificial experimental data” (6.1.11).



**Fig. 6.6** Comparison of concentration distributions (6.1.10): (1)-  $\bar{C}_2^1(Z_2, a_{02}^1, a_{12}^1)$ ; (2)-  $\bar{C}_2^2(Z_2, a_{02}^2, a_{12}^2)$ ; (3)-  $\bar{C}_2^0(Z_2, a_{02}^0, a_{12}^0)$ ;  $\circ$  - “artificial experimental data” (6.1.11).

**Table 6.1**  
Parameters values

	“Theoretical” values	“Experimental” values		
of $A_j(Z)$ , $j=1,2$ for	$a_{01} = 1.0316$	$a_{01}^0 = 1.2242$	$a_{01}^1 = 0.9264$	$a_{01}^2 = 0.8888$
$Fo_1 = 0.1$ , $Fo_2 = 0.01$ ,	$a_{11} = 0.1225$	$a_{11}^0 = 0.4759$	$a_{11}^1 = 0.1564$	$a_{11}^2 = 0.0798$
$K_{01} = 1$ , $K_{02} = 0.1$	$a_{02} = 0.6664$	$a_{02}^0 = 0.7191$	$a_{02}^1 = 0.5863$	$a_{02}^2 = 0.6021$
where	$a_{12} = 0.1036$	$a_{12}^0 = 0.0223$	$a_{12}^1 = 0.1096$	$a_{12}^2 = 0.1289$
$0 \leq S_m \leq 1$ , $m = 1, \dots, 10$				

are obtained by means of a generator of random numbers. The obtained “artificial experimental data” (6.1.11) are used as illustration of the parameter identification in the average concentrations models (6.1.10) by minimization of the least-squares functions  $Q_n$ ,  $n = 1, 2, \dots, 10$  and  $Q$ :

$$\begin{aligned}
 Q_n(Z_n, a_{01}^n, a_{11}^n, a_{02}^n, a_{12}^n) &= \sum_{m=1}^{10} [\bar{C}_1(Z_{1n}, a_{01}^n, a_{11}^n) - \bar{C}_{1\text{exp}}^m(Z_{1n})]^2 + \\
 &+ \sum_{m=1}^{10} [\bar{C}_2(Z_{2n}, a_{02}^n, a_{12}^n) - \bar{C}_{2\text{exp}}^m(Z_{2n})]^2, \quad Z_n = Z_{1n} = Z_{2n} = 0.1n, \quad n = 1, 2; \\
 Q(a_{01}^0, a_{11}^0, a_{02}^0, a_{12}^0) &= \sum_{n=1}^{10} Q_n(Z_n, a_{01}^0, a_{11}^0, a_{02}^0, a_{12}^0),
 \end{aligned} \tag{0.2.12}$$

where the values of  $\bar{C}_j(Z_{jn}, a_{01}^n, a_{11}^n, a_{02}^n, a_{12}^n)$  are obtained as solutions of (6.1.10) for different  $Z_{jn} = 0.1n$ ,  $n = 1, 2, \dots, 10$ ,  $j = 1, 2$ . The obtained (“experimental”) values  $(a_{01}^0, a_{11}^0, a_{02}^0, a_{12}^0)$ ,  $(a_{01}^1, a_{11}^1, a_{02}^1, a_{12}^1)$  and  $(a_{01}^2, a_{11}^2, a_{02}^2, a_{12}^2)$  are presented in Table 6.1. They are used for the calculation of the functions  $\bar{C}_1^0(Z_1, a_{01}^0, a_{11}^0)$ ,  $\bar{C}_1^1(Z_1, a_{01}^1, a_{11}^1)$ ,  $\bar{C}_1^2(Z_1, a_{01}^2, a_{11}^2)$ , (the lines in Fig. 6.5) and  $\bar{C}_2^0(Z_2, a_{02}^0, a_{12}^0)$ ,  $\bar{C}_2^1(Z_2, a_{02}^1, a_{12}^1)$ ,  $\bar{C}_2^2(Z_2, a_{02}^2, a_{12}^2)$ , (the lines in Fig. 6.6). The points in Figs. 6.5 and 6.6 are the “artificial experimental data” (6.1.11).



The comparison of the functions (lines) and “artificial experimental data” (points) in Figs. 6.5 and 6.6 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 identification.

### 1.2 Chemical absorption

The chemical absorption ( $i_0 = 2$ ) is a result of the chemical reaction between the absorbed substance in the liquid phase ( $i=1, j=2$ ) and a reagent in the liquid phase ( $i=j=2$ ). If the kinetic model of the chemical reaction is  $k c_{12} c_{22}$ , the convection-diffusion model of the chemical absorption in a co-current column has the form (3.1.11, 3.1.12):

$$\begin{aligned}
u_1 \frac{\partial c_{11}}{\partial z} &= D_{11} \left( \frac{\partial^2 c_{11}}{\partial z^2} + \frac{1}{r} \frac{\partial c_{11}}{\partial r} + \frac{\partial^2 c_{11}}{\partial r^2} \right) - k_0 (c_{11} - \chi c_{12}); \\
u_2 \frac{\partial c_{12}}{\partial z} &= D_{12} \left( \frac{\partial^2 c_{12}}{\partial z^2} + \frac{1}{r} \frac{\partial c_{12}}{\partial r} + \frac{\partial^2 c_{12}}{\partial r^2} \right) + k_0 (c_{11} - \chi c_{12}) - k c_{12} c_{22}; \\
u_2 \frac{\partial c_{22}}{\partial z} &= D_{22} \left( \frac{\partial^2 c_{22}}{\partial z^2} + \frac{1}{r} \frac{\partial c_{22}}{\partial r} + \frac{\partial^2 c_{22}}{\partial r^2} \right) - k c_{12} c_{22}; \\
r = 0, \quad \frac{\partial c_{11}}{\partial r} &= \frac{\partial c_{12}}{\partial r} = \frac{\partial c_{22}}{\partial r} \equiv 0; \quad r = r_0, \quad \frac{\partial c_{11}}{\partial r} = \frac{\partial c_{12}}{\partial r} = \frac{\partial c_{22}}{\partial r} \equiv 0; \\
z = 0, \quad c_{11} &\equiv c_{11}^0, \quad c_{12} \equiv c_{12}^0, \quad c_{22} \equiv c_{22}^0, \quad u_1^0 c_{11}^0 \equiv u_1(r) c_{11}^0 - D_{11} \left( \frac{\partial c_{11}}{\partial z} \right)_{z=0}, \\
u_2^0 c_{12}^0 &\equiv u_2(r) c_{12}^0 - D_{12} \left( \frac{\partial c_{12}}{\partial z} \right)_{z=0}, \quad u_2^0 c_{22}^0 \equiv u_2(r) c_{22}^0 - D_{22} \left( \frac{\partial c_{22}}{\partial z} \right)_{z=0},
\end{aligned} \tag{0.2.13}$$

where  $u_j^0, c_{ij}^0, i=1,2, j=1,2$ , are the inlet velocities and concentrations in the gas and liquid phases ( $c_{12}^0 = 0$ , practically).

From (II.3) follow the average values of the velocity and concentration in (6.1.13) at the column cross-sectional area:

$$\begin{aligned}
\bar{u}_1 &= \frac{2}{r_0^2} \int_0^{r_0} r u_1(r) dr, \quad \bar{u}_2 = \frac{2}{r_0^2} \int_0^{r_0} r u_2(r) dr, \quad \bar{c}_{11}(z) = \frac{2}{r_0^2} \int_0^{r_0} r c_{11}(r, z) dr, \\
\bar{c}_{12}(z) &= \frac{2}{r_0^2} \int_0^{r_0} r c_{12}(r, z) dr, \quad \bar{c}_{22}(z) = \frac{2}{r_0^2} \int_0^{r_0} r c_{22}(r, z) dr.
\end{aligned} \tag{0.2.14}$$

The functions in (6.1.13) can be presented by the average functions (6.1.14):

$$\begin{aligned}
u_1(r) &= \bar{u}_1 \tilde{u}_1(r), \quad u_2(r) = \bar{u}_2 \tilde{u}_2(r), \quad c_{11}(r, z) = \bar{c}_{11}(z) \tilde{c}_{11}(r, z), \\
c_{12}(r, z) &= \bar{c}_{12}(z) \tilde{c}_{12}(r, z), \quad c_{22}(r, z) = \bar{c}_{22}(z) \tilde{c}_{22}(r, z).
\end{aligned} \tag{0.2.15}$$

where

$$\begin{aligned}
\frac{2}{r_0^2} \int_0^{r_0} r \tilde{u}_1(r) dr &= 1, \quad \frac{2}{r_0^2} \int_0^{r_0} r \tilde{u}_2(r) dr = 1, \\
\frac{2}{r_0^2} \int_0^{r_0} r \tilde{c}_{11}(r, z) dr &= 1, \quad \frac{2}{r_0^2} \int_0^{r_0} r \tilde{c}_{12}(r, z) dr = 1, \quad \frac{2}{r_0^2} \int_0^{r_0} r \tilde{c}_{22}(r, z) dr = 1.
\end{aligned} \tag{0.2.16}$$

The use of the averaging procedure (6.0.1)–(6.0.5) leads to the average concentration model of the chemical absorption:

$$\begin{aligned}
\alpha_{11}\bar{u}_1 \frac{d\bar{c}_{11}}{dz} + \frac{d\alpha_{11}}{dz}\bar{u}_1\bar{c}_{11} &= D_{11} \frac{d^2\bar{c}_{11}}{dz^2} - k_0(\bar{c}_{11} - \chi\bar{c}_{12}); \\
\alpha_{12}\bar{u}_2 \frac{d\bar{c}_{12}}{dz} + \frac{d\alpha_{12}}{dz}\bar{u}_2\bar{c}_{12} &= D_{12} \frac{d^2\bar{c}_{12}}{dz^2} + k_0(\bar{c}_{11} - \chi\bar{c}_{12}) - \delta k\bar{c}_{12}\bar{c}_{22}; \\
\alpha_{22}\bar{u}_2 \frac{d\bar{c}_{22}}{dz} + \frac{d\alpha_{22}}{dz}\bar{u}_2\bar{c}_{22} &= D_{22} \frac{d^2\bar{c}_{22}}{dz^2} - \delta k\bar{c}_{12}\bar{c}_{22}; \\
z=0, \quad \bar{c}_{11}(0) &= c_{11}^0, \quad \bar{c}_{12}(0) = 0, \quad \bar{c}_{22}(0) = c_{22}^0, \\
\left(\frac{d\bar{c}_{11}}{dz}\right)_{z=0} &= 0, \quad \left(\frac{d\bar{c}_{12}}{dz}\right)_{z=0} = 0, \quad \left(\frac{d\bar{c}_{22}}{dz}\right)_{z=0} = 0,
\end{aligned} \tag{0.2.17}$$

where

$$\begin{aligned}
\alpha_{11}(z) &= \frac{2}{r_0^2} \int_0^{r_0} r \tilde{u}_1(r) \tilde{c}_{11}(r, z) dr, \quad \alpha_{12}(z) = \frac{2}{r_0^2} \int_0^{r_0} r \tilde{u}_2(r) \tilde{c}_{12}(r, z) dr, \\
\alpha_{22}(z) &= \frac{2}{r_0^2} \int_0^{r_0} r \tilde{u}_2(r) \tilde{c}_{22}(r, z) dr, \quad \delta(z) = \frac{2}{r_0^2} \int_0^{r_0} r \tilde{c}_{12}(r, z) \tilde{c}_{22}(r, z) dr.
\end{aligned} \tag{0.2.18}$$

The use of dimensionless (generalized) variables

$$Z = \frac{z}{l}, \quad \bar{C}_{11} = \frac{\bar{c}_{11}}{c_{11}^0}, \quad \bar{C}_{12} = \frac{\bar{c}_{12}\chi}{c_{11}^0}, \quad \bar{C}_{22} = \frac{\bar{c}_{22}}{c_{22}^0}. \tag{0.2.19}$$

leads to

$$\begin{aligned}
A_{11} \frac{d\bar{C}_{11}}{dZ} + \frac{dA_{11}}{dZ} \bar{C}_{11} &= \text{Pe}_{11}^{-1} \frac{d^2\bar{C}_{11}}{dZ^2} - K_{01}(\bar{C}_{11} - \bar{C}_{12}); \\
A_{12} \frac{d\bar{C}_{12}}{dZ} + \frac{dA_{12}}{dZ} \bar{C}_{12} &= \text{Pe}_{12}^{-1} \frac{d^2\bar{C}_{12}}{dZ^2} + K_{02}(\bar{C}_{11} - \bar{C}_{12}) - \Delta K c_{22}^0 \bar{C}_{12} \bar{C}_{22}; \\
A_{22} \frac{d\bar{C}_{22}}{dZ} + \frac{dA_{22}}{dZ} \bar{C}_{22} &= \text{Pe}_{22}^{-1} \frac{d^2\bar{C}_{22}}{dZ^2} - \Delta K \frac{c_{11}^0}{\chi} \bar{C}_{12} \bar{C}_{22}; \\
Z=0, \quad \bar{C}_{11} &= 1, \quad \bar{C}_{12} = 0, \quad \bar{C}_{22} = 1, \\
\left(\frac{d\bar{C}_{11}}{dZ}\right)_{Z=0} &= 0, \quad \left(\frac{d\bar{C}_{12}}{dZ}\right)_{Z=0} = 0, \quad \left(\frac{d\bar{C}_{22}}{dZ}\right)_{Z=0} = 0;
\end{aligned} \tag{0.2.20}$$

where

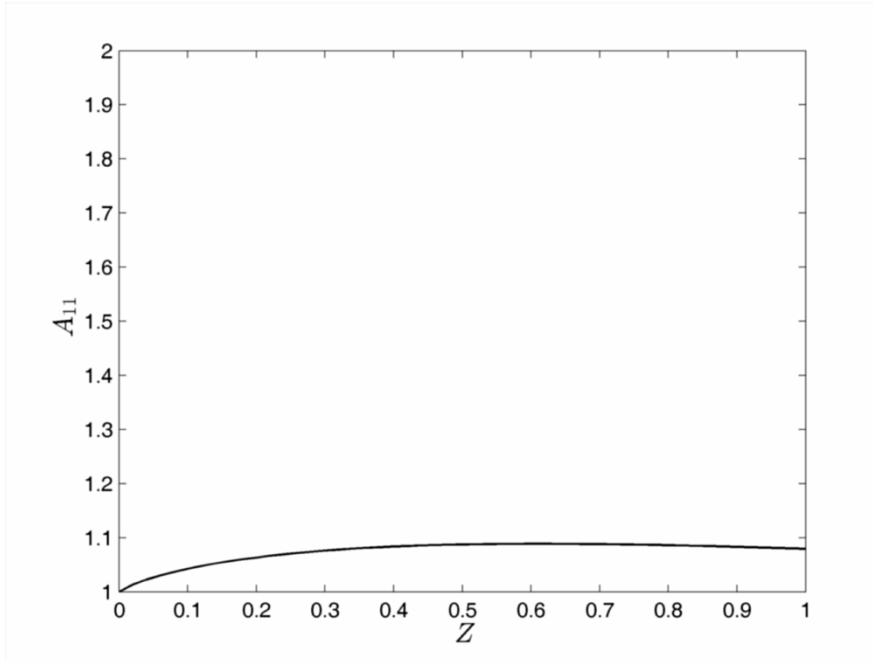
$$\begin{aligned}
\text{Pe}_{11} &= \frac{\bar{u}_1 l}{D_{11}}, \quad \text{Pe}_{12} = \frac{\bar{u}_2 l}{D_{12}}, \quad \text{Pe}_{22} = \frac{\bar{u}_2 l}{D_{22}}, \\
K_{0j} &= \frac{k_0 l}{\bar{u}_j} \chi^{j-1}, \quad j=1, 2, \quad K = \frac{kl}{\bar{u}_2}.
\end{aligned} \tag{0.2.21}$$

From (6.0.2), (6.0.3), (6.0.6), (6.1.3) and (6.1.4) for the co-current flows ( $z_1 = z_2 = z$ ) follow the expressions

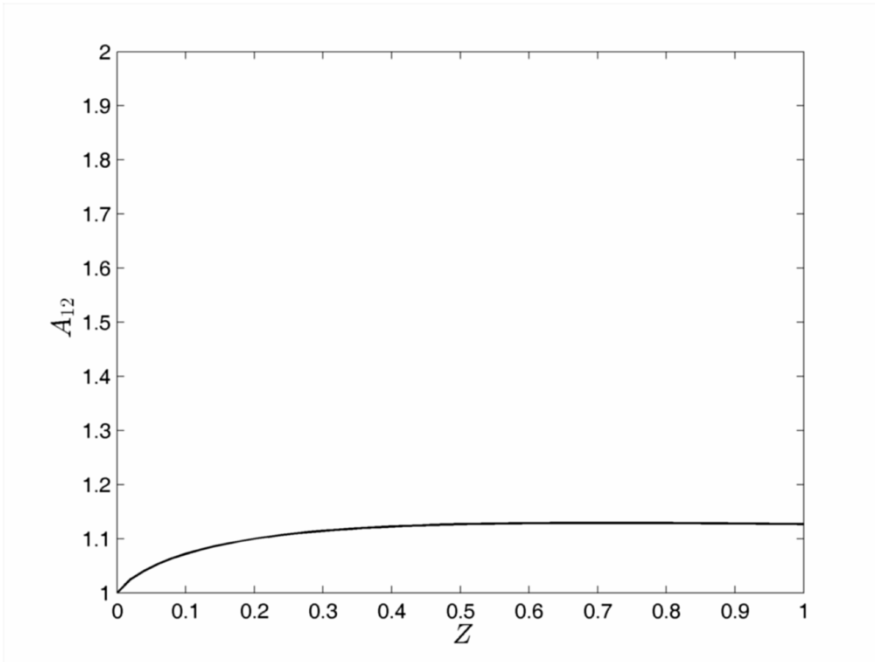
$$\begin{aligned}
\tilde{c}_{1j}(r, z) &= \frac{c_{1j}(r_0 R, lZ)}{\bar{c}_{1j}(lZ)} = \frac{C_{1j}(R, Z)}{\bar{C}_{1j}(Z)}, \quad \bar{C}_{1j}(Z) = 2 \int_0^1 R C_{1j}(R, Z) dR, \quad j = 1, 2, \\
\tilde{c}_{22}(r, z) &= \frac{c_{22}(r_0 R, lZ)}{\bar{c}_{22}(lZ)} = \frac{C_{22}(R, Z)}{\bar{C}_{22}(Z)}, \quad \bar{C}_{22}(Z) = 2 \int_0^1 R C_{22}(R, Z) dR, \\
\alpha_{1j}(z) &= \alpha_{1j}(lZ) = A_{1j}(Z) = 2 \int_0^1 R U_j(R) \frac{C_{1j}(R, Z)}{\bar{C}_{1j}(Z)} dR, \quad j = 1, 2, \\
\delta(z) &= \delta(lZ) = \Delta(Z) = 2 \int_0^1 R \frac{C_{12}(R, Z)}{\bar{C}_{12}(Z)} \frac{C_{22}(R, Z)}{\bar{C}_{22}(Z)} dR.
\end{aligned} \tag{0.2.22}$$

A practical case leads to has the following orders of magnitude of the model parameters in (4.1.14):

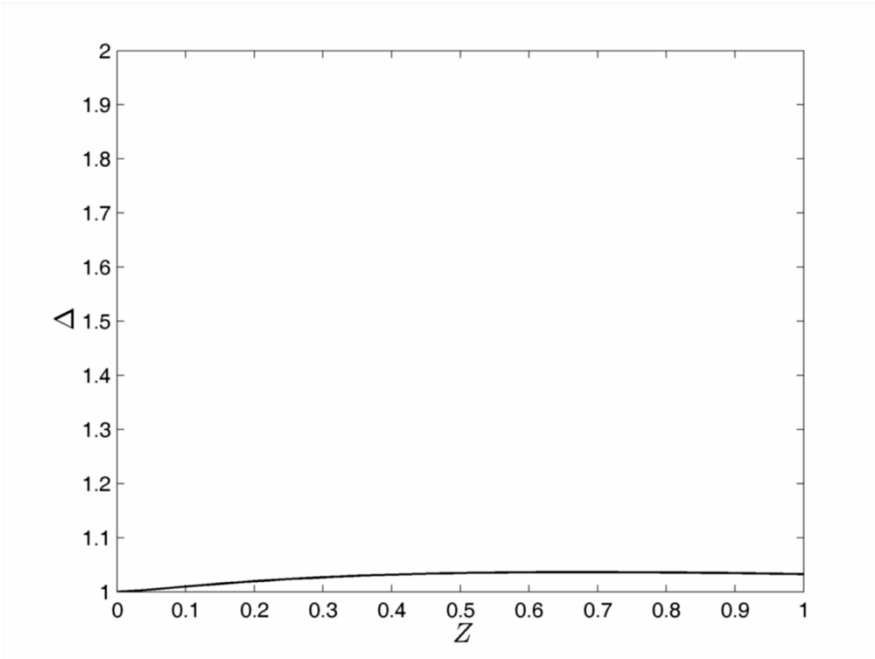
$$\begin{aligned}
\text{Fo}_s &= 0.1, \quad s = 11, 12, 22, \quad K_0 = K_{01} = 1, \quad \text{Da} = K \frac{c_{11}^0}{\chi} = 1, \\
K_{02} &= K_0 \frac{u_1^0 \chi}{u_2^0} = 1, \quad \frac{u_1^0 \chi}{u_2^0} = 1, \quad \frac{c_{22}^0 \chi}{c_{11}^0} = 2.
\end{aligned} \tag{0.2.23}$$



**Fig. 6.7** Function  $A_{11}(Z)$



**Fig. 6.8** Function  $A_{12}(Z)$



**Fig. 6.9** Function  $\Delta(Z)$

The use of the parameter values (6.1.23) for solution of the model equations (3.1.20) permits to be obtained the functions  $C_{11}(R, Z), C_{12}(R, Z), C_{22}(R, Z)$  and after that the functions  $\bar{C}_{11}(Z), \bar{C}_{12}(Z), \bar{C}_{22}(Z), A_{11}(Z), A_{12}(Z), \Delta(Z)$  in (6.1.22) (Figs. 6.7–6.9), where  $U_j = 2 - 2R^2, j = 1, 2$ . From the Figs. 6.7–6.9 it is seen that the functions  $A_{11}(Z), A_{12}(Z), \Delta(Z)$  can be presented as linear approximations

$$A_{11}(Z) = a_{110} + a_{111}Z, \quad A_{12}(Z) = a_{120} + a_{121}Z, \quad \Delta(Z) = \delta_0 + \delta_1Z \quad (0.2.24)$$

with the approximations parameters being

$$a_{110} = 1.04, \quad a_{111} = 0.05, \quad a_{120} = 1.07, \quad a_{121} = 0.08, \quad \delta_0 = 1.01, \quad \delta_1 = 0.03. \quad (0.2.25)$$

From (6.1.25) it is seen that the maximal effect of the velocity non-uniformity on the function  $\Delta(Z)$  is about 4 % and cannot be registered experimentally, i.e.  $\Delta(Z) \equiv 1$ .

The parameters identification in (6.1.24) is possible to be realized similar to the case of the physical absorption.

## 2. Adsorption processes

In the adsorption process [7–10] participate two reagents ( $i_0 = 2$ ), where the first is in the gas or liquid phase ( $i=1, j=1,2$ ) and the second is in the solid phase ( $i=2, j=3$ ). The adsorption is the process of mass transfer of an active component (the substance, which is possible to be adsorbed) from the gas (liquid) volume to the solid interface due to a physical (Van der Waals's) or chemical (valence) force [1]. The rate of the adsorption process determines analogically the chemical reaction rates, where law of mass action is changed by the law of surface action.

The convection-diffusion type models of the adsorption processes in the gas (liquid)-solid systems are possible to be obtained from (2.0.1) if  $j=1,3=2,3$  ( $1 = \varepsilon_1 + \varepsilon_3 = \varepsilon_2 + \varepsilon_3$ ),  $i_0 = 2$ , where  $i=1$  is the active component (AC) in the gas (liquid) phase,  $i=2$  - the active sites (AS) in the adsorbent (solid phase). The volume adsorption rate in the case of a solid adsorbent is  $Q_3 = b_0 Q_{03}$  [kg-mol.m<sup>-3</sup>.s<sup>-1</sup>], where  $b_0$  [m<sup>2</sup>.m<sup>-3</sup>] is m<sup>2</sup> of the inner surface in the solid phase (the surface of the capillaries in the solid phase) in 1 m<sup>3</sup> of the solid phase (adsorbent),  $Q_{03}$  [kg-mol.m<sup>-2</sup>.s<sup>-1</sup>] - the surface adsorption rate. A gas adsorption will be considered for convenience, where  $c_{11}$  [kg-mol.m<sup>-3</sup>] is the volume concentration of the AC in the gas phase (elementary) volume,  $c_{13}$  [kg-mol.m<sup>-3</sup>] - the volume concentration of the AC in the void volume of the solid phase (adsorbent),  $c_{23}$  [kg-eq.m<sup>-3</sup>] - the volume concentration of the AS in the solid phase (elementary) volume (1 kg-eq AS in the adsorbent combine 1 kg-mol AC),  $1 = \varepsilon_1 + \varepsilon_3$ ,  $u_1 = u_1(r)$  - velocity of the gas phase [m.s<sup>-1</sup>],  $u_3 = 0$  (solid phase is immobile). All concentrations are in kg-mol (kg-eq) in 1 m<sup>3</sup> of the phase (elementary) volume. The inlet gas velocity in the column is  $u_1^0 = F_1 / \varepsilon_1 \pi r_0^2$ , where  $r_0$  is the column radius [m] and  $F_1$  - the gas phase flow rates [m<sup>3</sup>.s<sup>-1</sup>]. The average velocities  $\bar{u}_1$  of the gas phases in the column are supposed to be equal to the inlet gas velocity in the column.

### 2.1 Physical adsorption

In the cases of physical adsorption on a solid surface [7] the adsorption rate is proportional to the surface concentration of the free AS (which may be associated with the molecules of the AC) and the volume concentration of the AC:

$$Q_0^1 = k_1 c_{13} \left( 1 - \frac{\Gamma}{\Gamma_\infty} \right), \quad (0.3.1)$$

where  $k_1$  [m.s<sup>-1</sup>] is the adsorption rate constant,  $\Gamma$  [kg-eq.m<sup>-2</sup>] – the surface concentration of the AS, which is linked to the molecules of the AC (the surface concentration of the adsorbed AC),  $\Gamma_\infty$  [kg-eq.m<sup>-2</sup>] – the maximal surface concentration of the free AS. The surface concentration of the free AS is  $(\Gamma_\infty - \Gamma)$ .

The physical adsorption process is reversible and the desorption rate could be obtained by analogical consideration, represented as:

$$Q_0^2 = k_2 \Gamma, \quad (0.3.2)$$

where  $k_2$  [s<sup>-1</sup>] is the desorption rate constant. The resultant adsorption rate is

$$Q_{03} = Q_0^1 - Q_0^2 = k_1 c_{13} \left( 1 - \frac{\Gamma}{\Gamma_\infty} \right) - k_2 \Gamma. \quad (0.3.3)$$

The volume concentration of the free AS in the solid phase (adsorbent)  $c_{23}$  and its maximum value  $c_{23}^0$  [kg-eq.m<sup>-3</sup>] are possible to be obtained immediately:

$$c_{23} = b(\Gamma_\infty - \Gamma), \quad c_{23}^0 = b\Gamma_\infty \quad (0.3.4)$$

and from (2.2.3) and (2.2.4) follows the expression for the surface adsorption rate:

$$Q_{03} = k_1 c_{13} C_{23} - k_2 \frac{c_{23}^0}{b_0} (1 - C_{23}), \quad C_{23} = \frac{c_{23}}{c_{23}^0}. \quad (0.3.5)$$

Let us consider a non-stationary gas adsorption in a column apparatus, where the solid phase (adsorbent) is immobile. The convection-diffusion model of this process is possible to be obtained from (2.0.1), where the diffusivity of the free AS in the solid phase (adsorbent) volume is equal to zero. If the rate of the interphase mass transfer of the AC from the gas phase to the solid phase is  $k_0(c_{11} - c_{13})$  and the process is non-stationary as a result of the free AS concentration decrease, i.e. the convection-diffusion model has the form:

$$\begin{aligned} \frac{\partial c_{11}}{\partial t} + u_1 \frac{\partial c_{11}}{\partial z} &= D_{11} \left( \frac{\partial^2 c_{11}}{\partial z^2} + \frac{1}{r} \frac{\partial c_{11}}{\partial r} + \frac{\partial^2 c_{11}}{\partial r^2} \right) - k_0 (c_{11} - c_{13}); \\ \frac{dc_{13}}{dt} &= k_0 (c_{11} - c_{13}) - b_0 k_1 c_{13} \frac{c_{23}}{c_{23}^0} + k_2 c_{23}^0 \left( 1 - \frac{c_{23}}{c_{23}^0} \right); \\ \frac{dc_{23}}{dt} &= -b_0 k_1 c_{13} \frac{c_{23}}{c_{23}^0} + k_2 c_{23}^0 \left( 1 - \frac{c_{23}}{c_{23}^0} \right); \end{aligned} \quad (0.3.6)$$

where  $t$  is the time,  $D_{11}$  is the diffusivity of the AC in the gas phase and  $k_0$  is the inter-phase mass transfer coefficient [s<sup>-1</sup>]. In (2.2.6)  $c_{11} = c_{11}(t, r, z)$  and  $(r, z)$  are parameters in  $c_{13} = c_{13}(t, r, z)$  and  $c_{23} = c_{23}(t, r, z)$ . The concentration of the adsorbed AC is  $(c_{23}^0 - c_{23})$ .

The model (2.2.6) represents the decrease of the concentration of the AC (free AS) in the part of the elementary volume  $\varepsilon_1$  ( $\varepsilon_3$ ) due to the physical adsorption.

Let us consider an adsorption column with a radius  $r_0$  and a height of the active volume  $l$ . The boundary conditions of (2.2.6) have the form:

$$\begin{aligned}
t = 0, \quad c_{11} &\equiv c_{11}^0, \quad c_{13} \equiv 0, \quad c_{23} \equiv c_{23}^0; \quad r = 0, \quad \frac{\partial c_{11}}{\partial r} \equiv 0; \quad r = r_0, \quad \frac{\partial c_{11}}{\partial r} \equiv 0; \\
z = 0, \quad c_{11} &\equiv c_{11}^0, \quad u_1^0 c_{11}^0 \equiv u_1(r) c_{11}^0 - D_{11} \left( \frac{\partial c_{11}}{\partial z} \right)_{z=0};
\end{aligned} \tag{0.3.7}$$

where  $u_1^0$  is the inlet (average) velocity of the gas phase.

The use of dimensionless (generalized) variables [1] permit a qualitative analysis of the model (2.2.6), (2.2.7) to be made, where as characteristic scales are used the average velocity, the inlet concentrations, the characteristic time  $t_0$  (s) and the column parameters ( $r_0, l$ ):

$$T = \frac{t}{t_0}, \quad R = \frac{r}{r_0}, \quad Z = \frac{z}{h}, \quad U = \frac{u_1}{u_1^0}, \quad C_{11} = \frac{c_{11}}{c_{11}^0}, \quad C_{13} = \frac{c_{13}}{c_{11}^0}, \quad C_{23} = \frac{c_{23}}{c_{23}^0}. \tag{0.3.8}$$

If (2.2.8) is put in (2.2.6), (2.2.7), the model in generalized variables takes the form:

$$\begin{aligned}
\gamma \frac{\partial C_{11}}{\partial T} + U(R) \frac{\partial C_{11}}{\partial Z} &= \text{Fo} \left( \varepsilon \frac{\partial^2 C_{11}}{\partial Z^2} + \frac{1}{R} \frac{\partial C_{11}}{\partial R} + \frac{\partial^2 C_{11}}{\partial R^2} \right) - K_0 (C_{11} - C_{13}); \\
\frac{dC_{13}}{dT} &= K_3 (C - C_1) - K_1 C_{13} C_{23} + K_2 \frac{c_{23}^0}{c_{11}^0} (1 - C_{23}); \\
\frac{dC_{23}}{dT} &= -K_1 \frac{c_{11}^0}{c_{23}^0} C_{13} C_{23} + K_2 (1 - C_{23}); \\
T = 0, \quad C_{11} &\equiv 1, \quad C_{13} \equiv 0, \quad C_{23} \equiv 1; \quad R = 0, \quad \frac{\partial C_{11}}{\partial R} \equiv 0; \quad R = 1, \quad \frac{\partial C_{11}}{\partial R} \equiv 0; \\
Z = 0, \quad C_{11} &\equiv 1, \quad 1 \equiv U(R) - \text{Pe}^{-1} \left( \frac{\partial C_{11}}{\partial Z} \right)_{Z=0},
\end{aligned} \tag{0.3.9}$$

where  $(R, Z)$  are parameters in  $C_{13}(T, R, Z)$ ,  $C_{23}(T, R, Z)$  and

$$\begin{aligned}
\text{Fo} &= \frac{D_{11} l}{u_1^0 r_0^2}, \quad \text{Pe} = \frac{u_1^0 l}{D_{11}}, \quad \gamma = \frac{l}{u_1^0 t_0}, \quad \varepsilon = \frac{r_0^2}{l^2}, \\
K_0 &= \frac{k_0 l}{u_1^0}, \quad K_1 = k_1 t_0 b_0, \quad K_2 = k_2 t_0, \quad K_3 = k_0 t_0.
\end{aligned} \tag{0.3.10}$$

Practically for long duration processes  $0 \leq \gamma \leq 10^{-2}$  and the problem (2.2.9) has the form:

$$\begin{aligned}
U(R) \frac{\partial C_{11}}{\partial Z} &= \text{Fo} \left( \varepsilon \frac{\partial^2 C_{11}}{\partial Z^2} + \frac{1}{R} \frac{\partial C_{11}}{\partial R} + \frac{\partial^2 C_{11}}{\partial R^2} \right) - K_0 (C_{11} - C_{13}); \\
\frac{dC_{13}}{dT} &= K_3 (C_{11} - C_{13}) - K_1 C_{13} C_{23} + K_2 \frac{c_{23}^0}{c_{11}^0} (1 - C_{23}); \\
\frac{dC_{23}}{dT} &= -K_1 \frac{c_{11}^0}{c_{23}^0} C_{13} C_{23} + K_2 (1 - C_{23}); \\
T = 0, \quad C_{13} &\equiv 0, \quad C_{23} \equiv 1; \\
R = 0, \quad \frac{\partial C_{11}}{\partial R} &\equiv 0; \quad R = 1, \quad \frac{\partial C_{11}}{\partial R} \equiv 0; \\
Z = 0, \quad C_{11} &\equiv 1, \quad 1 \equiv U(R) - \text{Pe}^{-1} \left( \frac{\partial C_{11}}{\partial Z} \right)_{Z=0},
\end{aligned} \tag{0.3.11}$$

where  $T$  is a parameter in  $C_{11}(T, R, Z)$ .

For big gas velocity  $0 = \text{Fo} \leq 10^{-2}$ ,  $0 = \gamma \leq 10^{-2}$  and from (2.2.9) follows the convection type model

$$\begin{aligned} U(R) \frac{dC_{11}}{dZ} &= -K_0 (C_{11} - C_{13}); \\ \frac{dC_{13}}{dT} &= K_3 (C_{11} - C_{13}) - K_1 C_{13} C_{23} + K_2 \frac{c_{23}^0}{c_{11}^0} (1 - C_{23}); \\ \frac{dC_{23}}{dT} &= -K_1 \frac{c_{11}^0}{c_{23}^0} C_{13} C_{23} + K_2 (1 - C_{23}); \\ T = 0, \quad C_{13} &\equiv 0, \quad C_{23} \equiv 1; \quad Z = 0, \quad C \equiv 1. \end{aligned} \quad (0.3.12)$$

In the cases of high columns ( $0 = \varepsilon \leq 10^{-2}$ ) the problem (2.2.11) has to be solved in zero approximation with respect to  $\varepsilon$  ( $\varepsilon = 0$ ,  $\text{Pe}^{-1} = \varepsilon \text{Fo} = 0$ ):

$$\begin{aligned} U(R) \frac{\partial C_{11}}{\partial Z} &= \text{Fo} \left( \frac{1}{R} \frac{\partial C_{11}}{\partial R} + \frac{\partial^2 C_{11}}{\partial R^2} \right) - K_0 (C_{11} - C_{13}); \\ R = 0, \quad \frac{\partial C_{11}}{\partial R} &\equiv 0; \quad R = 1, \quad \frac{\partial C_{11}}{\partial R} \equiv 0; \quad Z = 0, \quad C_{11} \equiv 1. \end{aligned} \quad (0.3.13)$$

$$\frac{dC_{13}}{dT} = K_3 (C_{11} - C_{13}) - K_1 C_{13} C_{23} + K_2 \frac{c_{23}^0}{c_{11}^0} (1 - C_{23}); \quad T = 0, \quad C_{13} \equiv 0. \quad (0.3.14)$$

$$\frac{dC_{23}}{dT} = -K_1 \frac{c_{11}^0}{c_{23}^0} C_{13} C_{23} + K_2 (1 - C_{23}); \quad T = 0, \quad C_{23} \equiv 1. \quad (0.3.15)$$

The solution of the model equations (2.2.13), (2.2.14), (2.2.15), using a multi-step algorithm (see Chap. 9 and [10]) is obtained in the case of parabolic velocity distribution (Poiseuille flow) in the gas phase  $U(R) = 2 - 2R^2$  and the parameters values  $\text{Fo} = 10^{-1}$ ,  $K_0 = K_1 = K_3 = c_{23}^0 = 1$ ,  $K_2 = 10^{-3}$ ,  $c_{11}^0 = 10^{-2}$ . The concentration distributions  $C_{11}(0.6, R, Z)$  and  $C_{11}(T, 0.2, Z)$ , for different  $T$  and  $Z$ , are presented in Figs. 3.3 and 3.4.

## 2.2 Chemical adsorption

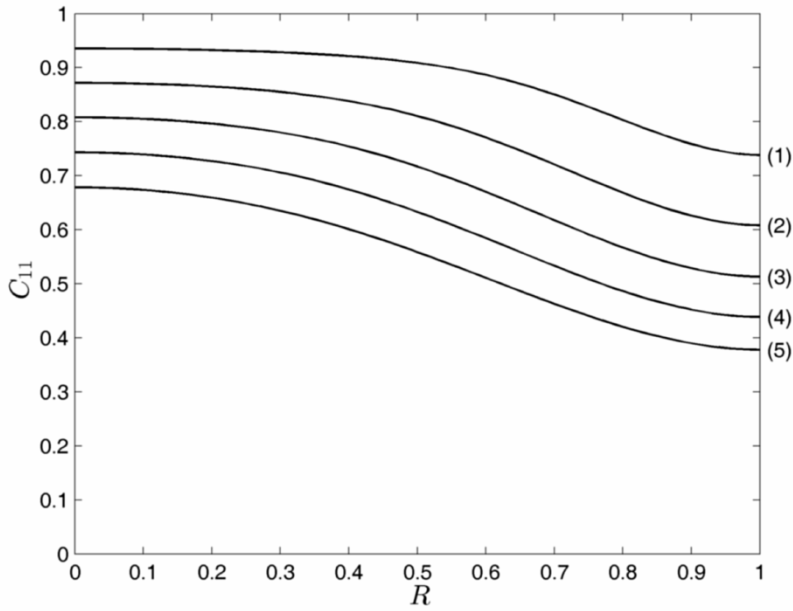
The presence of chemical bonds between the AC and AS at the solid surface leads to the next expression [1] for the adsorption rate:

$$Q = k_0 \exp(-E/RT) \prod_{s=1}^m z_s^{\alpha_s} \prod_{i=1}^n p_i^{\beta_i} z_0^{(m_i - \sum_{s=1}^m \alpha_s)}, \quad (0.3.16)$$

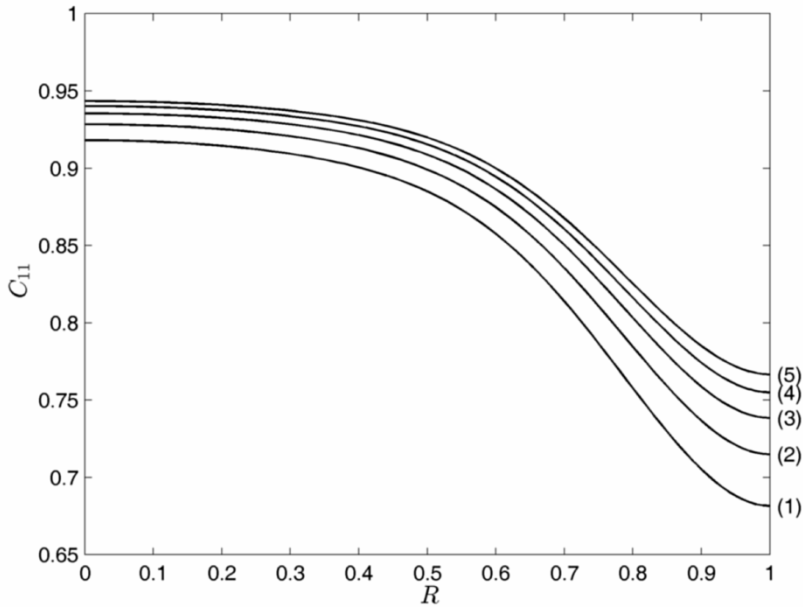
where  $z_s$  is the part of the face interphase occupied by the molecules of the substances  $A_s$  ( $s = 1, \dots, m$ ),  $p_i$  – the partial pressures (volume concentrations) of the substances  $B_i$  ( $i = 1, \dots, n$ ) in the gas (liquid),  $z_0$  – the part of the free surface, which is able to realize physical bonds with the molecules of the substances  $B_i$  ( $j = 1, \dots, n$ ),  $m_i$  – the number of the AS at the interface, which realize the physical bonds.

In (2.2.16) it is assumed that the molecules  $A_s$  ( $s = 1, \dots, m$ ) from the solid surface react chemically with a part of the molecules  $B_i$  ( $i = 1, \dots, n$ ), while the other part realize physical bonds with the active places  $m_i$ . The heterogeneous reaction rate and the reactions orders are  $Q$ ,  $\alpha_s$  ( $s = 1, \dots, m$ ) and  $\beta_i$  ( $i = 1, \dots, n$ ).





**Fig.3.3** Concentration distributions  $C_{11}(0.6,R,Z)$ : (1) $Z=0.2$ ; (2) $Z=0.4$ ; (3) $Z=0.6$ ; (4) $Z=0.8$ ; (5) $Z=1$



**Fig.3.4** Concentration distributions  $C_{11}(T,R,0.2)$ : (1) $T=0.2$ ; (2) $T=0.4$ ; (3) $T=0.6$ ; (4) $T=0.8$ ; (5) $T=1$

In the cases of reversible heterogeneous chemical reactions the equation of adsorption rate follows from (2.2.3) and (2.2.16)

$$Q = k_{pi} \prod_{i=1}^n c_i / \left( 1 + \sum_{i=1}^n k_{pi} c_i \right), \quad (0.3.17)$$

where  $k_{pi}$  are the equilibrium constants of the reagents  $B_i (i = 1, \dots, n)$ .

All equations of the adsorption kinetics [1] are based on the ideal adsorption layer model. Practically the main part of the adsorption processes are related with real adsorption layers, i.e. the adsorbent surfaces are non-homogeneous as a result of the changes of the solid phase structure.

The convection-diffusion model of the chemical adsorption [7] is possible to be obtained on the basis of the two-phase processes model (2.0.1), where  $\varepsilon_1$  and  $\varepsilon_3$  are the parts of the gas phase and sorbent particles (solid) phase ( $\varepsilon_1 + \varepsilon_3 = 1$ ) of the medium elementary volume in the column apparatus, where the solid phase is immobile ( $u_3 = 0$ ). The volume concentrations of the AC in the gas phase and in the void volume of the solid phase (adsorbent) are  $c_{11}$  and  $c_{13}$  [kg-mol.m<sup>-3</sup>]. For the interphase (gas-solid) mass transfer rate it is possible to use  $k_0(c_{11} - c_{13})$ , where  $k_0$  is the interphase mass transfer coefficient. The adsorption rate in the solid phase (similar to two components chemical reaction) is presented as  $k c_{13} c_{23}$ , where  $c_{23}$  [kg-eq.m<sup>-3</sup>] is the volume concentration of the (AS) in the solid phase (particles volume),  $k$  – the chemical reaction rate constant (1 kg-eq AS in the adsorbent combine chemically 1 kg-mol AC in gas phase). All concentrations are in kg-mol (kg-eq) in 1 m<sup>3</sup> of the phase (elementary) volume.

The diffusivity of the AC in the mobile gas phase is  $D_{11}$ . The convective transport of AC and AS in the solid phase is not possible. The diffusion mass transfer of AC in the solid phase (Knudsen diffusion) can be neglected due to the small value of the Knudsen diffusivity. The diffusivity of the AS in the adsorbent phase (particles volume) is equal to zero, too.

If the process is non-stationary as a result of the free AS concentration decrease, the convection-diffusion model of the chemical adsorption has the form:

$$\begin{aligned} \frac{\partial c_{11}}{\partial t} + u_1 \frac{\partial c_{11}}{\partial z} &= D_{11} \left( \frac{\partial^2 c_{11}}{\partial z^2} + \frac{1}{r} \frac{\partial c_{11}}{\partial r} + \frac{\partial^2 c_{11}}{\partial r^2} \right) - k_0 (c_{11} - c_{13}), \\ \frac{dc_{13}}{dt} &= k_0 (c_{11} - c_{13}) - k c_{13} c_{23} = 0, \quad \frac{dc_{23}}{dt} = -k c_{13} c_{23}. \end{aligned} \quad (0.3.18)$$

The initial and boundary conditions of (2.2.18) are:

$$t = 0, \quad c_{11} \equiv c_{11}^0, \quad c_{13} \equiv 0, \quad c_{23} \equiv c_{23}^0; \quad (0.3.19)$$

$$r = 0, \quad \frac{\partial c_{11}}{\partial r} \equiv 0; \quad r = r_0, \quad \frac{\partial c_{11}}{\partial r} \equiv 0;$$

$$z = 0, \quad c_{11} \equiv c_{11}^0, \quad u_1 c_{11}^0 \equiv u_1(r) c_{11}^0 - D_{11} \left( \frac{\partial c_{11}}{\partial z} \right)_{z=0},$$

where  $u_1^0, c_{11}^0$  are the inlet velocity and the concentration of the active component in the gas phase,  $c_{23}^0$  – the initial concentration of AS in the solid phase.

The using of dimensionless (generalized) variables

$$T = \frac{t}{t^0}, \quad R = \frac{r}{r_0}, \quad Z = \frac{z}{l}, \quad U = \frac{u_1}{u_1^0}, \quad C_{11} = \frac{c_{11}}{c_{11}^0}, \quad C_{13} = \frac{c_{13}}{c_{11}^0}, \quad C_{23} = \frac{c_{23}}{c_{23}^0} \quad (0.3.20)$$

leads to:

$$\begin{aligned}
\gamma \frac{\partial C_{11}}{\partial T} + U(R) \frac{\partial C_{11}}{\partial Z} &= \text{Fo} \left( \varepsilon \frac{\partial^2 C_{11}}{\partial Z^2} + \frac{1}{R} \frac{\partial C_{11}}{\partial R} + \frac{\partial^2 C_{11}}{\partial R^2} \right) - K_0 (C_{11} - C_{13}); \\
\frac{dC_{13}}{dT} &= K_3 (C_{11} - C_{13}) - Kc_{23}^0 C_{13} C_{23}; \quad \frac{dC_{23}}{dT} = -Kc_{11}^0 C_{13} C_{23}; \\
T = 0, \quad C_{11} &\equiv 1, \quad C_{13} \equiv 0, \quad C_{23} \equiv 1; \\
R = 0, \quad \frac{\partial C_{11}}{\partial R} &\equiv 0; \quad R = 1, \quad \frac{\partial C_{11}}{\partial R} \equiv 0; \\
Z = 0, \quad C_{11} &\equiv 1, \quad 1 \equiv U(R) - \text{Pe}^{-1} \left( \frac{\partial C_{11}}{\partial Z} \right)_{Z=0},
\end{aligned} \tag{0.3.21}$$

where  $(R, Z)$  are parameters in  $C_{13}(T, R, Z)$ ,  $C_{23}(T, R, Z)$  and

$$\begin{aligned}
\text{Fo} &= \frac{D_{11} l}{u_1^0 r_0^2}, \quad \text{Pe} = \frac{u_1^0 l}{D_{11}}, \quad \gamma = \frac{l}{u_1^0 t^0}, \quad \varepsilon = \left( \frac{r_0}{l} \right)^2, \\
K &= k t^0, \quad K_0 = \frac{k_0 l}{u_1^0}, \quad K_3 = k_0 t^0.
\end{aligned} \tag{0.3.22}$$

For lengthy processes it is possible to use the approximation  $0 = \gamma \leq 10^{-2}$ :

$$\begin{aligned}
U(R) \frac{\partial C_{11}}{\partial Z} &= \text{Fo} \left( \varepsilon \frac{\partial^2 C_{11}}{\partial Z^2} + \frac{1}{R} \frac{\partial C_{11}}{\partial R} + \frac{\partial^2 C_{11}}{\partial R^2} \right) - K_0 (C_{11} - C_{13}); \\
\frac{dC_{13}}{dT} &= K_3 (C_{11} - C_{13}) - Kc_{23}^0 C_{13} C_{23}; \quad \frac{dC_{23}}{dT} = -Kc_{11}^0 C_{13} C_{23}; \\
T = 0, \quad C_{13} &\equiv 0, \quad C_{23} \equiv 1; \\
R = 0, \quad \frac{\partial C_{11}}{\partial R} &\equiv 0; \quad R = 1, \quad \frac{\partial C_{11}}{\partial R} \equiv 0; \\
Z = 0, \quad C_{11} &\equiv 1, \quad 1 \equiv U(R) - \text{Pe}^{-1} \left( \frac{\partial C_{11}}{\partial Z} \right)_{Z=0};
\end{aligned} \tag{0.3.23}$$

where  $T$  is a parameter in  $C_{11}(T, R, Z)$ .

In the cases of high columns ( $\varepsilon \leq 10^{-2}$ ) the problem (2.2.21) has to be solved in zero approximation with respect to  $\varepsilon$  ( $\varepsilon = 0$ ):

$$\begin{aligned}
\gamma \frac{\partial C_{11}}{\partial T} + U(R) \frac{\partial C_{11}}{\partial Z} &= \text{Fo} \left( \frac{1}{R} \frac{\partial C_{11}}{\partial R} + \frac{\partial^2 C_{11}}{\partial R^2} \right) - K_0 (C_{11} - C_{13}); \\
\frac{dC_{13}}{dT} &= K_3 (C_{11} - C_{13}) - Kc_{23}^0 C_{13} C_{23}; \quad \frac{dC_{23}}{dT} = -Kc_{11}^0 C_{13} C_{23}; \\
T = 0, \quad C_{11} &\equiv 1, \quad C_{13} \equiv 0, \quad C_{23} \equiv 1; \\
R = 0, \quad \frac{\partial C_{11}}{\partial R} &\equiv 0; \quad R = 1, \quad \frac{\partial C_{11}}{\partial R} \equiv 0; \\
Z = 0, \quad C_{11} &\equiv 1.
\end{aligned} \tag{0.3.24}$$

For big gas velocity  $0 = \text{Fo} \leq 10^{-2}$ ,  $0 = \gamma \leq 10^{-2}$  and from (2.2.23) follows the convection type model

$$\begin{aligned}
U(R) \frac{dC_{11}}{dZ} &= -K_0 (C_{11} - C_{13}); \\
\frac{dC_{13}}{dT} &= K_3 (C_{11} - C_{13}) - Kc_{23}^0 C_{13} C_{23}; \quad \frac{dC_{23}}{dT} = -Kc_{11}^0 C_{13} C_{23}; \\
T = 0, \quad C_{13} &\equiv 0, \quad C_{23} \equiv 1; \quad Z = 0, \quad C_{11} \equiv 1,
\end{aligned} \tag{0.3.25}$$

where  $T$  is a parameter in  $C_{11}(T, R, Z)$ , while  $R$  and  $Z$  are parameters in  $C_{13}(T, R, Z)$  and  $C_{23}(T, Z, R)$ .

## 2 Adsorption processes modeling

### 2.1 Physical adsorption

The convection-diffusion model of the non-stationary physical adsorption in the column apparatuses [6, 7] has the form (3.2.6, 3.2.7):

$$\begin{aligned} \frac{\partial c_{11}}{\partial t} + u_1 \frac{\partial c_{11}}{\partial z} &= D_{11} \left( \frac{\partial^2 c_{11}}{\partial z^2} + \frac{1}{r} \frac{\partial c_{11}}{\partial r} + \frac{\partial^2 c_{11}}{\partial r^2} \right) - k_0 (c_{11} - c_{13}); \\ \frac{dc_{13}}{dt} &= k_0 (c_{11} - c_{13}) - b_0 k_1 c_{13} \frac{c_{23}}{c_{23}^0} + k_2 c_{23}^0 \left( 1 - \frac{c_{23}}{c_{23}^0} \right); \\ \frac{dc_{23}}{dt} &= -b_0 k_1 c_{13} \frac{c_{23}}{c_{23}^0} + k_2 c_{23}^0 \left( 1 - \frac{c_{23}}{c_{23}^0} \right); \\ t = 0, \quad c_{11} &\equiv c_{11}^0, \quad c_{13} \equiv 0, \quad c_{23} \equiv c_{23}^0; \quad r = 0, \quad \frac{\partial c_{11}}{\partial r} \equiv 0; \quad r = r_0, \quad \frac{\partial c_{11}}{\partial r} \equiv 0; \\ z = 0, \quad c_{11} &\equiv c_{11}^0, \quad u_1^0 c_{11}^0 \equiv u_1(r) c_{11}^0 - D_{11} \left( \frac{\partial c_{11}}{\partial z} \right)_{z=0}. \end{aligned} \quad (0.4.1)$$

From (II.3) follow the average values of the velocity and concentration functions in (6.2.1) at the column cross-sectional area:

$$\begin{aligned} \bar{u}_1 &= \frac{2}{r_0^2} \int_0^{r_0} r u_1(r) dr, \quad \bar{c}_{11}(z) = \frac{2}{r_0^2} \int_0^{r_0} r c_{11}(r, z) dr, \\ \bar{c}_{13}(z) &= \frac{2}{r_0^2} \int_0^{r_0} r c_{13}(r, z) dr, \quad \bar{c}_{23}(z) = \frac{2}{r_0^2} \int_0^{r_0} r c_{23}(r, z) dr. \end{aligned} \quad (0.4.2)$$

The functions in (6.2.1) can be presented by the average functions (6.2.2):

$$\begin{aligned} u_1(r) &= \bar{u}_1 \tilde{u}_1(r), \quad c_{11}(t, r, z) = \bar{c}_{11}(t, z) \tilde{c}_{11}(t, r, z), \\ c_{13}(t, r, z) &= \bar{c}_{13}(t, z) \tilde{c}_{13}(t, r, z), \quad c_{23}(t, r, z) = \bar{c}_{23}(t, z) \tilde{c}_{23}(t, r, z), \end{aligned} \quad (0.4.3)$$

where

$$\frac{2}{r_0^2} \int_0^{r_0} r \tilde{u}_1(r) dr = 1, \quad \frac{2}{r_0^2} \int_0^{r_0} r \tilde{c}_{11}(t, r, z) dr = 1, \quad (0.4.4)$$

$$\frac{2}{r_0^2} \int_0^{r_0} r \tilde{c}_{13}(t, r, z) dr = 1, \quad \frac{2}{r_0^2} \int_0^{r_0} r \tilde{c}_{23}(t, r, z) dr = 1.$$

The use of the averaging procedure (6.0.1)–(6.0.5) leads to the average concentration model of the physical adsorption:

$$\begin{aligned}
\frac{\partial \bar{c}_{11}}{\partial t} + \alpha \bar{u}_1 \frac{\partial \bar{c}_{11}}{\partial z} + \frac{\partial \alpha}{\partial z} \bar{u}_1 \bar{c}_{11} &= D_{11} \frac{\partial^2 \bar{c}_{11}}{\partial z^2} - k_0 (\bar{c}_{11} - \bar{c}_{13}); \\
\frac{d \bar{c}_{13}}{dt} &= k_0 (\bar{c}_{11} - \bar{c}_{13}) - b_0 k_1 \beta \bar{c}_{13} \frac{\bar{c}_{23}}{c_{23}^0} + k_2 c_{23}^0 \left(1 - \frac{\bar{c}_{23}}{c_{23}^0}\right); \\
\frac{d \bar{c}_{23}}{dt} &= -b_0 k_1 \beta \bar{c}_{13} \frac{\bar{c}_{23}}{c_{23}^0} + k_2 c_{23}^0 \left(1 - \frac{\bar{c}_{23}}{c_{23}^0}\right); \\
t = 0, \quad \bar{c}_{11} &\equiv c_{11}^0, \quad \bar{c}_{13} \equiv 0, \quad \bar{c}_{23} \equiv c_{23}^0; \quad z = 0, \quad \bar{c}_{11} \equiv c_{11}^0, \quad \left(\frac{\partial \bar{c}_{11}}{\partial z}\right)_{z=0} \equiv 0.
\end{aligned} \tag{0.4.5}$$

where

$$\begin{aligned}
\alpha &= \alpha(t, z) = \frac{2}{r_0^2} \int_0^{r_0} r \tilde{u}_1(r) \tilde{c}_{11}(t, r, z) dr, \\
\beta &= \beta(t, z) = \frac{2}{r_0^2} \int_0^{r_0} r \tilde{c}_{13}(t, r, z) \tilde{c}_{23}(t, r, z) dr.
\end{aligned} \tag{0.4.6}$$

The use of the generalized variables

$$T = \frac{t}{l^0}, \quad Z = \frac{z}{l}, \quad \bar{C}_{11} = \frac{\bar{c}_{11}}{c_{11}^0}, \quad \bar{C}_{13} = \frac{\bar{c}_{13}}{c_{11}^0}, \quad \bar{C}_{23} = \frac{\bar{c}_{23}}{c_{23}^0}, \tag{0.4.7}$$

leads to:

$$\begin{aligned}
\gamma \frac{\partial \bar{C}_{11}}{\partial T} + A \frac{\partial \bar{C}_{11}}{\partial Z} + \frac{\partial A}{\partial Z} \bar{C}_{11} &= \text{Pe}^{-1} \frac{\partial^2 \bar{C}_{11}}{\partial Z^2} - K_0 (\bar{C}_{11} - \bar{C}_{13}); \\
\frac{d \bar{C}_{13}}{dT} &= K_3 (\bar{C}_{11} - \bar{C}_{13}) - BK_1 \bar{C}_{13} \bar{C}_{23} + K_2 \frac{c_{23}^0}{c_{11}^0} (1 - \bar{C}_{23}); \\
\frac{d \bar{C}_{23}}{dT} &= -BK_1 \frac{c_{11}^0}{c_{23}^0} \bar{C}_{13} \bar{C}_{23} + K_2 (1 - \bar{C}_{23}); \\
T = 0, \quad \bar{C}_{11} &\equiv 1, \quad \bar{C}_{13} \equiv 0, \quad \bar{C}_{23} \equiv 1; \quad Z = 0, \quad \bar{C}_{11} \equiv 1, \quad \left(\frac{\partial \bar{C}_{11}}{\partial Z}\right)_{Z=0} \equiv 0,
\end{aligned} \tag{0.4.8}$$

where

$$\begin{aligned}
K_0 &= \frac{k_0 l}{u_1^0}, \quad K_1 = k_1 t^0 b_0, \quad K_2 = k_2 t^0, \quad K_3 = k_0 t^0, \\
A(T, Z) &= \alpha(t_0 T, lZ) = \alpha(t, z) = 2 \int_0^1 R U(R) \frac{C_{11}(T, R, Z)}{\bar{C}_{11}(T, Z)} dR, \\
B(T, Z) &= \beta(t_0 T, lZ) = \beta(t, z) = 2 \int_0^1 R \frac{C_{13}(T, R, Z)}{\bar{C}_{13}(T, Z)} \frac{C_{23}(T, R, Z)}{\bar{C}_{23}(T, Z)} dR, \\
\bar{C}_{11}(T, Z) &= 2 \int_0^1 R C_{11}(T, R, Z) dR, \quad \bar{C}_{13}(T, Z) = 2 \int_0^1 R C_{13}(T, R, Z) dR, \\
\bar{C}_{23}(T, Z) &= 2 \int_0^1 R C_{23}(T, R, Z) dR.
\end{aligned} \tag{0.4.9}$$

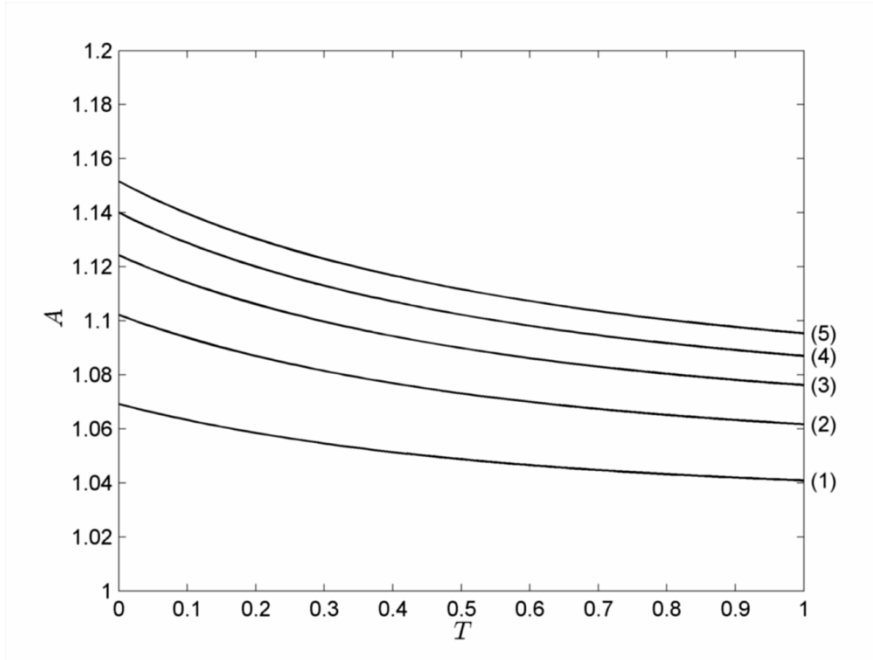
In (6.2.8)  $Z$  is a parameter in  $\bar{C}_{13}(T, Z)$ ,  $\bar{C}_{23}(T, Z)$  and  $T$  is a parameter in  $\bar{C}_{11}(T, Z)$ .

Practically, for lengthy (long-term) processes  $0 \leq \gamma \leq 10^{-2}$  and high columns ( $0 = \varepsilon \leq 10^{-2}$ ,  $0 = \text{Pe}^{-1} = \varepsilon \text{Fo} \leq 10^{-2}$  for  $\text{Fo} \leq 1$ ) the problem (6.2.8) has the form:

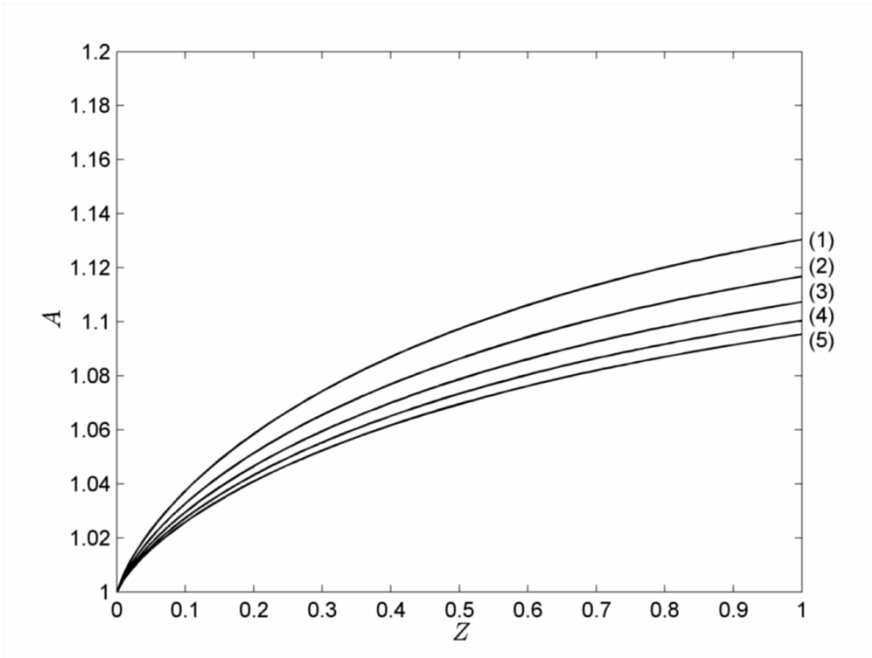
$$\begin{aligned}
A \frac{d\bar{C}_{11}}{dZ} + \frac{dA}{dZ} \bar{C}_{11} &= -K_0 (\bar{C}_{11} - \bar{C}_{13}); \\
\frac{d\bar{C}_{13}}{dT} &= K_3 (\bar{C}_{11} - \bar{C}_{13}) - BK_1 \bar{C}_{13} \bar{C}_{23} + K_2 \frac{c_{23}^0}{c_{11}^0} (1 - \bar{C}_{23}); \\
\frac{d\bar{C}_{23}}{dT} &= -BK_1 \frac{c_{11}^0}{c_{23}^0} \bar{C}_{13} \bar{C}_{23} + K_2 (1 - \bar{C}_{23}); \\
T = 0, \quad \bar{C}_{11} &\equiv 1, \quad \bar{C}_{13} \equiv 0, \quad \bar{C}_{23} \equiv 1; \quad Z = 0, \quad \bar{C}_{11} \equiv 1.
\end{aligned} \tag{0.4.10}$$

The solution of the model equations (3.2.11), using the multi-steps algorithm (see Chapter 9 and [7]), for the case  $0 = \varepsilon \leq 10^{-2}$ ,  $0 = \text{Pe}^{-1} = \varepsilon \text{Fo} \leq 10^{-2}$ ,  $\text{Fo} = 10^{-1}$ ,  $K_0 = K_1 = K_3 = c_{23}^0 = 1$ ,  $K_2 = 10^{-3}$ ,  $c_{11}^0 = 10^{-2}$ , permits to obtain the concentrations  $C_{11}(T, R, Z)$ ,  $C_{13}(T, R, Z)$ ,  $C_{23}(T, R, Z)$  and the functions  $\bar{C}_{11}(T, Z)$ ,  $\bar{C}_{13}(T, Z)$ ,  $\bar{C}_{23}(T, Z)$ ,  $A(T, Z)$ ,  $B(T, Z)$  in (6.2.9). The results for  $A(T, Z)$ ,  $B(T, Z)$  show that  $B(T, Z) \equiv 1$  and  $A(T, Z)$  is possible to be presented as a linear approximation:

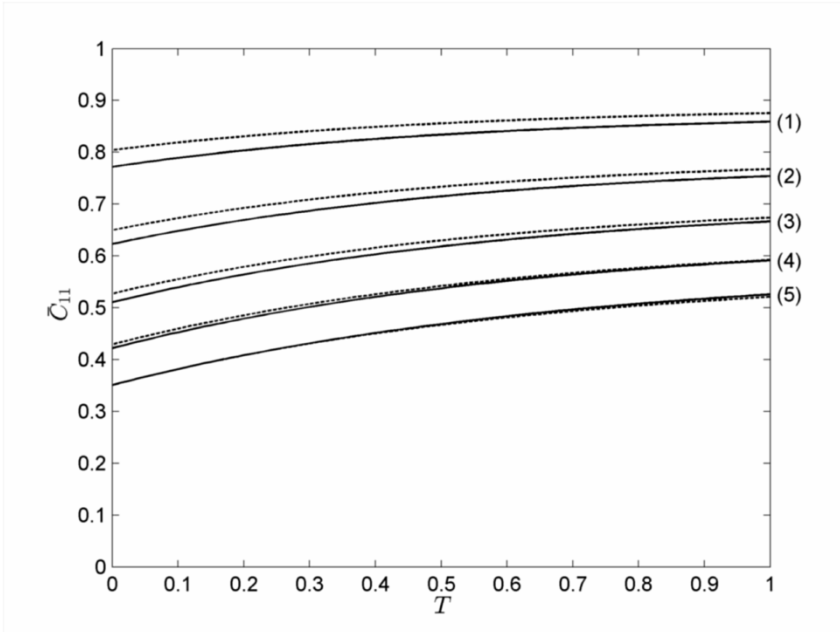
$$A = a_0 + a_2 Z + a_1 T. \tag{0.4.11}$$



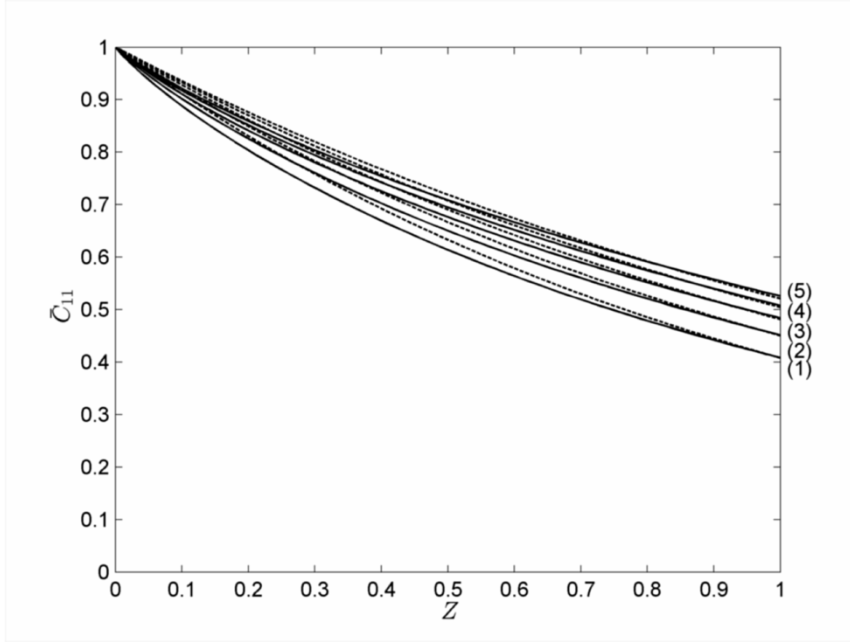
**Fig. 6.10** Function  $A(T, Z)$ : (1)  $Z = 0.2$ ; (2)  $Z = 0.4$ ; (3)  $Z = 0.6$ ; (4)  $Z = 0.8$ ; (5)  $Z = 1.0$



**Fig. 6.11** Function  $A(T, Z)$ : (1)  $T = 0.2$ ; (2)  $T = 0.4$ ; (3)  $T = 0.6$ ; (4)  $T = 0.8$ ; (5)  $T = 1.0$



**Fig. 6.12** Function  $\bar{c}_{11}(T, Z)$  in (6.2.9): (1)  $T = 0.2$ ; (2)  $T = 0.4$ ; (3)  $T = 0.6$ ; (4)  $T = 0.8$ ; (5)  $T = 1.0$ ; Dotted lines are solution of (6.2.10)



**Fig. 6.13** Function  $\bar{C}_{11}(T,Z)$  in (6.2.9): (1)  $Z = 0.2$ ; (2)  $Z = 0.4$ ; (3)  $Z = 0.6$ ; (4)  $Z = 0.8$ ; (5)  $Z = 1.0$ ; Dotted lines are solution of (6.2.10)

The obtained (“theoretical”) parameters values are  $a_0 = 1.0471$ ,  $a_z = 0.09025$ ,  $a_t = -0.03770$  (see Table 5.2). The functions  $\bar{C}_{11}(T,Z)$ ,  $A(T,Z)$  are presented in Figs. 6.10–6.13.

In the Figs. 6.12 and 5.13 are compared the function  $\bar{C}_{11}(T,Z)$  obtained in (6.2.9) (the lines) and the function  $\bar{C}_{11}(T,Z)$  obtained as a solution of the (6.2.10) (the dotted lines), where  $K_0 = K_1 = K_3 = c_{23}^0 = 1$ ,  $K_2 = 10^{-3}$ ,  $c_{11}^0 = 10^{-2}$  and  $A = 1.047 + 0.0902Z - 0.0377T$ ,  $B = 1$ .

The concentration  $C_{11}(0.6, R, Z)$  obtained as a solution of the problem (3.2.13) – (3.2.15) for the case  $Fo = 10^{-1}$ ,  $K_0 = K_1 = K_3 = c_{23}^0 = 1$ ,  $K_2 = 10^{-3}$ ,  $c_{11}^0 = 10^{-2}$  permits to be obtained the average concentration  $\bar{C}_{11}(0.6, Z)$  in (6.2.9) and “artificial experimental data” for different values of  $Z$ :

$$\begin{aligned} \bar{C}_{\text{exp}}^m(Z_n) &= (0.95 + 0.1S_m)\bar{C}_{11}(0.6, Z_n), \\ m &= 1, \dots, 10, \quad Z_n = 0.1n, \quad n = 1, 2, \dots, 10, \end{aligned} \quad (0.4.12)$$

where  $0 \leq S_m \leq 1$ ,  $m = 1, \dots, 10$  are obtained by means of a generator of random numbers. The obtained “artificial experimental” data (6.2.12) are used for the illustration of the parameter identification in the average concentrations models (6.2.10) by minimization of the least-squares functions  $Q_n$  and  $Q$ :

$$\begin{aligned} Q_n(Z_n, a_0, a_z, a_t) &= \sum_{m=1}^{10} [\bar{C}_{11}(0.6, Z_n, a_0, a_z, a_t) - \bar{C}_{\text{exp}}^m(Z_n)]^2, \\ Z_n &= 0.1n, \quad n = 1, 2, \dots, 10; \quad Q(a_0, a_z, a_t) = \sum_{n=1}^{10} Q_n(Z_n, a_0, a_z, a_t), \end{aligned} \quad (0.4.13)$$

where the values of  $\bar{C}_{11}(0.6, Z_n, a_0, a_z, a_t)$  are obtained as solutions of (6.2.10) for different  $Z_n = 0.1n$ ,  $n = 1, 2, \dots, 10$ .

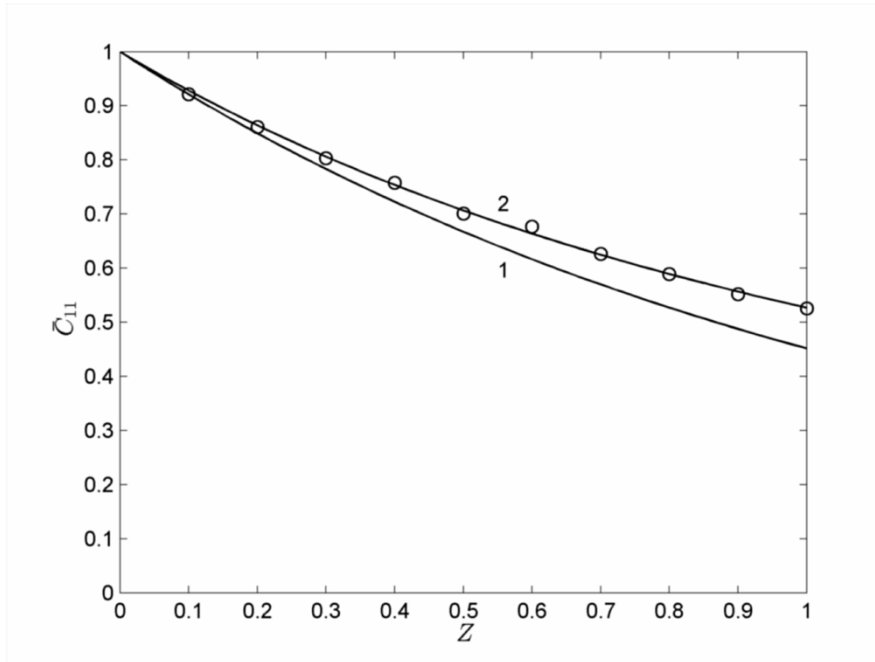


The obtained (“experimental”) values of  $a_0, a_z, a_t$  by minimization of  $Q, Q_1, Q_2, Q_3$  are presented in the Table 6.2.

“Theoretical values”	“Experimental values”				
	$Q$	$Q_1$	$Q_2$	$Q_3$	
$a_0$	1,0471	2,2291	0,7962	0,8721	0,9005
$a_z$	$9.9246 \times 10^{-2}$	0,6849	$7.3048 \times 10^{-4}$	$4.4452 \times 10^{-4}$	$3.1391 \times 10^{-4}$
$a_t$	$-3.7701 \times 10^{-2}$	-0,7892	$2.7259 \times 10^{-4}$	$1.8971 \times 10^{-4}$	$2.0352 \times 10^{-4}$

**Table 6.2**

On Fig. 6.14 are compared the average concentration  $\bar{c}_{11}(Z)$  (the lines) as a solution of (6.2.10) for the parameters values  $a_0, a_z, a_t$  obtained by the minimization of  $Q_1$  and  $Q$  in (5.2.13) with the “artificial experimental data” (6.2.12) (the points). The result presented shows that the parameters identification problems of the average concentration models is possible to be solved using experimental data obtained in a short column ( $Z = 0.1$ ) with a real diameter.



**Fig. 6.14** Function  $\bar{c}_{11}$ : 1 - minimization of  $Q_1$ ; 2 - minimization of  $Q$ ; (circles) - “artificial experimental data” (6.2.12)

## 2.2 Chemical adsorption

The convection-diffusion model of the non-stationary chemical adsorption [6, 7] has the form (3.2.18, 3.2.19):

$$\begin{aligned}
 \frac{\partial c_{11}}{\partial t} + u_1 \frac{\partial c_{11}}{\partial z} &= D_{11} \left( \frac{\partial^2 c_{11}}{\partial z^2} + \frac{1}{r} \frac{\partial c_{11}}{\partial r} + \frac{\partial^2 c_{11}}{\partial r^2} \right) - k_0 (c_{11} - c_{13}), \\
 \frac{dc_{13}}{dt} &= k_0 (c_{11} - c_{13}) - kc_{13}c_{23} = 0, \quad \frac{dc_{23}}{dt} = -kc_{13}c_{23}; \\
 t = 0, \quad c_{11} &\equiv c_{11}^0, \quad c_{13} \equiv 0, \quad c_{23} \equiv c_{23}^0;
 \end{aligned}
 \tag{0.4.14}$$

$$r = 0, \quad \frac{\partial c_{11}}{\partial r} \equiv 0; \quad r = r_0, \quad \frac{\partial c_{11}}{\partial r} \equiv 0;$$

$$z = 0, \quad c_{11} \equiv c_{11}^0, \quad u_1^0 c_{11}^0 \equiv u_1(r) c_{11}^0 - D_{11} \left( \frac{\partial c_{11}}{\partial z} \right)_{z=0}.$$

The use of the expressions (6.2.2)–(6.2.4) and averaging procedure (6.0.1)–(6.0.5) leads to the average concentration model of the chemical absorption:

$$\frac{\partial \bar{c}_{11}}{\partial t} + \alpha \bar{u}_1 \frac{\partial \bar{c}_{11}}{\partial z} + \frac{\partial \alpha}{\partial z} \bar{u}_1 \bar{c}_{11} = D_{11} \frac{\partial^2 \bar{c}_{11}}{\partial z^2} - k_0 (\bar{c}_{11} - \bar{c}_{13});$$

$$\frac{d \bar{c}_{13}}{dt} = k_0 (\bar{c}_{11} - \bar{c}_{13}) - \beta k \bar{c}_{13} \bar{c}_{23};$$

$$\frac{d \bar{c}_{23}}{dt} = -\beta k \bar{c}_{13} \bar{c}_{23};$$

$$t = 0, \quad \bar{c}_{11} \equiv c_{11}^0, \quad \bar{c}_{13} \equiv 0, \quad \bar{c}_{23} \equiv c_{23}^0; \quad z = 0, \quad \bar{c}_{11} \equiv c_{11}^0, \quad \left( \frac{\partial \bar{c}_{11}}{\partial z} \right)_{z=0} \equiv 0. \quad (0.4.15)$$

where  $\alpha = \alpha(t, z)$  and  $\beta = \beta(t, z)$  are presented in (6.2.6).

The using of the generalized variables (6.2.7) leads to:

$$\gamma \frac{\partial \bar{C}_{11}}{\partial T} + A \frac{\partial \bar{C}_{11}}{\partial Z} + \frac{\partial A}{\partial Z} \bar{C}_{11} = \text{Pe}^{-1} \frac{\partial^2 \bar{C}_{11}}{\partial Z^2} - K_0 (\bar{C}_{11} - \bar{C}_{13});$$

$$\frac{d \bar{C}_{13}}{dT} = K_3 (\bar{C}_{11} - \bar{C}_{13}) - BK c_{23}^0 \bar{C}_{13} \bar{C}_{23};$$

$$\frac{d \bar{C}_{23}}{dT} = -BK c_{11}^0 \bar{C}_{13} \bar{C}_{23};$$

$$T = 0, \quad \bar{C}_{11} \equiv 1, \quad \bar{C}_{13} \equiv 0, \quad \bar{C}_{23} \equiv 1; \quad Z = 0, \quad \bar{C}_{11} \equiv 1, \quad \left( \frac{\partial \bar{C}_{11}}{\partial Z} \right)_{Z=0} \equiv 0, \quad (0.4.16)$$

where

$$K = kt^0, \quad K_0 = \frac{k_0 l}{u_1^0}, \quad K_3 = k_0 t^0,$$

$$A(T, Z) = \alpha(t_0 T, lZ) = \alpha(t, z) = 2 \int_0^1 RU(R) \frac{C_{11}(T, R, Z)}{\bar{C}_{11}(T, Z)} dR,$$

$$B(T, Z) = \beta(t_0 T, lZ) = \beta(t, z) = 2 \int_0^1 R \frac{C_{13}(T, R, Z)}{\bar{C}_{13}(T, Z)} \frac{C_{23}(T, R, Z)}{\bar{C}_{23}(T, Z)} dR, \quad (0.4.17)$$

$$\bar{C}_{11}(T, Z) = 2 \int_0^1 RC_{11}(T, R, Z) dR, \quad \bar{C}_{13}(T, Z) = 2 \int_0^1 RC_{13}(T, R, Z) dR,$$

$$\bar{C}_{23}(T, Z) = 2 \int_0^1 RC_{23}(T, R, Z) dR.$$

In (6.2.8)  $Z$  is a parameter in  $\bar{C}_{13}(T, Z)$ ,  $\bar{C}_{23}(T, Z)$  and  $T$  is a parameter in  $\bar{C}_{11}(T, Z)$ .

Practically, for lengthy (long-term) processes  $0 \leq \gamma \leq 10^{-2}$  and high columns ( $0 = \varepsilon \leq 10^{-2}$ ,  $0 = \text{Pe}^{-1} = \varepsilon \text{Fo} \leq 10^{-2}$ ), the problem (6.2.8) has the form:

$$A \frac{d\bar{C}_{11}}{dZ} + \frac{dA}{dZ} \bar{C}_{11} = -K_0 (\bar{C}_{11} - \bar{C}_{13});$$

$$\frac{d\bar{C}_{13}}{dT} = K_3 (\bar{C}_{11} - \bar{C}_{13}) - BKc_{23}^0 \bar{C}_{13} \bar{C}_{23};$$

$$\frac{d\bar{C}_{23}}{dT} = -BKc_{11}^0 \bar{C}_{13} \bar{C}_{23};$$

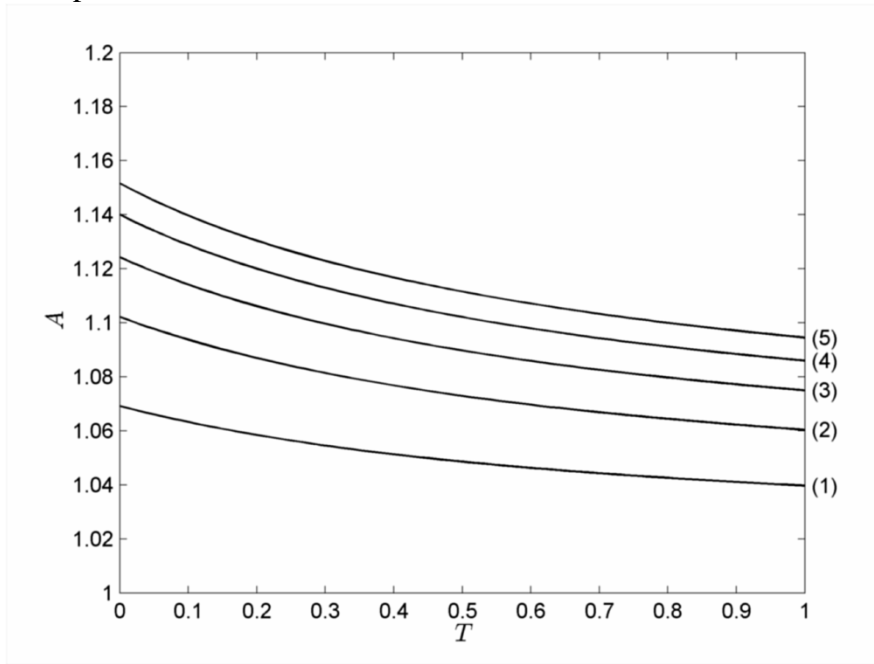
$$T = 0, \quad \bar{C}_{13} = 0, \quad \bar{C}_{23} = 1; \quad Z = 0, \quad \bar{C}_{11} = 1. \quad (0.4.18)$$

The solution of the model equations (3.2.23) for the case  $0 = \varepsilon \leq 10^{-2}$ ,  $0 = \text{Pe}^{-1} = \varepsilon \text{Fo} \leq 10^{-2}$ ,  $\text{Fo} = 10^{-1}$ ,  $K = K_0 = K_3 = c_{23}^0 = 1$ ;  $c_{11}^0 = 10^{-2}$ , permits to obtain the average concentrations  $\bar{C}_{11}(T, Z)$ ,  $\bar{C}_{13}(T, Z)$ ,  $\bar{C}_{23}(T, Z)$  and the functions  $A(T, Z)$ ,  $B(T, Z)$  in (6.2.9). The results for  $A(T, Z)$ ,  $B(T, Z)$  show that  $B(T, Z) \equiv 1$  and  $A(T, Z)$  is possible to be presented as a linear approximation:

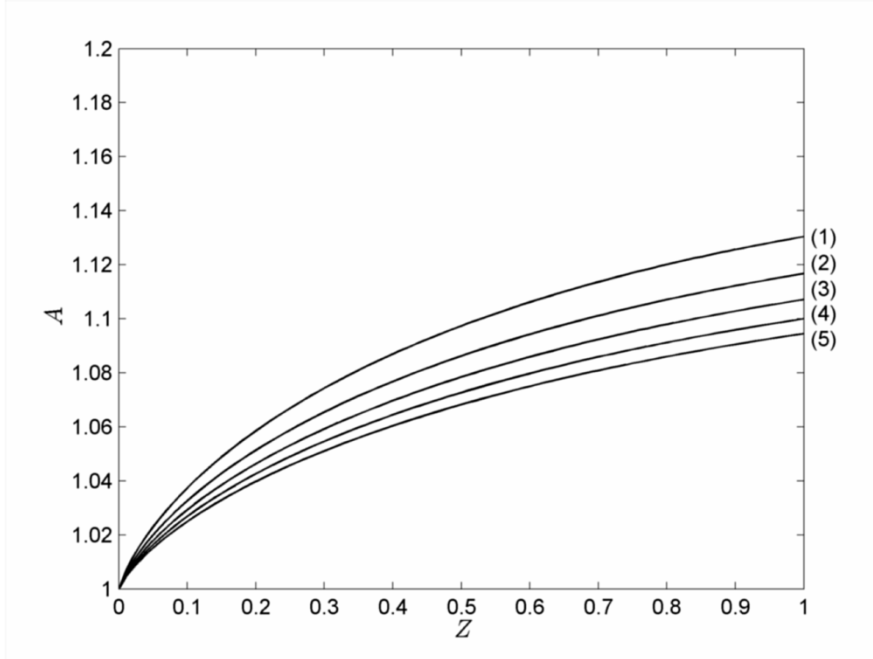
$$A = a_0 + a_z Z + a_t T. \quad (0.4.19)$$

The obtained (“theoretical”) parameter values are  $a_0 = 1.0471$ ,  $a_z = 9.9247 \cdot 10^{-2}$ ,  $a_t = -3.7696 \cdot 10^{-2}$ . The function  $A(T, Z)$  is presented in Figs. 6.15 and 6.16.

The parameters identification of the chemical adsorption models is similar to the physical adsorption case.



**Fig. 6.15** Function  $A(T, Z)$ : (1)  $Z = 0.2$ ; (2)  $Z = 0.4$ ; (3)  $Z = 0.6$ ; (4)  $Z = 0.8$ ; (5)  $Z = 1.0$



**Fig. 6.16** Function  $A(T,Z)$ : (1)  $T = 0.2$ ; (2)  $T = 0.4$ ; (3)  $T = 0.6$ ; (4)  $T = 0.8$ ; (5)  $T = 1.0$

In the cases of physical absorption [1–4] in a high counter-current gas-liquid column the mass transfer process model has to be presented in a two-coordinate system (see (3.1.8)):

$$U_j(R) \frac{\partial C_j}{\partial Z_j} = \text{Fo}_j \left( \frac{1}{R} \frac{\partial C_j}{\partial R} + \frac{\partial^2 C_j}{\partial R^2} \right) + (-1)^j K_j (C_1 - C_2);$$

$$R = 0, \quad \frac{\partial C_j}{\partial R} \equiv 0; \quad R = 1, \quad \frac{\partial C_j}{\partial R} \equiv 0; \quad j = 1, 2;$$

$$Z_1 = 0, \quad C_1 \equiv 1; \quad Z_2 = 0, \quad C_2 \equiv 0. \quad (0.4.20)$$

### 1. Convection-diffusion type model

Let us consider the convection-diffusion type model (8.0.1), where the velocity distributions in the phases are of Poiseuille type [5] and the difference between the phase velocities is in the average velocities, only:

$$U_1 = U_2 = 2 - 2R^2. \quad (0.5.1)$$

From (8.0.1) and (8.1.1) it is possible to obtain the next form of the problem for computer modelling of the absorption processes in counter-current column apparatuses:

$$(2 - 2R^2) \frac{\partial C_1}{\partial Z_1} = \text{Fo}_1 \left( \frac{1}{R} \frac{\partial C_1}{\partial R} + \frac{\partial^2 C_1}{\partial R^2} \right) - K_1 (C_1 - C_2);$$

$$R = 0, \quad \frac{\partial C_1}{\partial R} \equiv 0; \quad R = 1, \quad \frac{\partial C_1}{\partial R} \equiv 0; \quad Z_1 = 0, \quad C_1 \equiv 1. \quad (0.5.2)$$

$$(2 - 2R^2) \frac{\partial C_2}{\partial Z_2} = \text{Fo}_2 \left( \frac{1}{R} \frac{\partial C_2}{\partial R} + \frac{\partial^2 C_2}{\partial R^2} \right) + K_2 (C_1 - C_2);$$

$$R = 0, \quad \frac{\partial C_2}{\partial R} \equiv 0; \quad R = 1, \quad \frac{\partial C_2}{\partial R} \equiv 0; \quad Z_2 = 0, \quad C_2 \equiv 0. \quad (0.5.3)$$

#### 1.1. Calculation problem

The numerical solution of the equations set (8.1.2), (8.1.3) is possible if an iterative procedure is used [6], where the concentration distributions in the column will be obtained in two matrix forms on every iteration step  $s$ :

$$\begin{aligned} C_1^s(R, Z_1) &= \|a_{\rho\zeta_1}^s\|, \quad \rho = 1, 2, \dots, \rho^0, \quad \zeta_1 = 1, 2, \dots, \zeta^0, \\ 0 \leq R \leq 1, \quad 0 \leq Z_1 \leq 1, \quad R &= \frac{\rho-1}{\rho^0-1}, \quad Z_1 = \frac{\zeta_1-1}{\zeta^0-1}, \quad \rho^0 = \zeta^0. \end{aligned} \quad (0.5.4)$$

$$\begin{aligned} C_2^s(R, Z_2) &= \|b_{\rho\zeta_2}^s\|, \quad \rho = 1, 2, \dots, \rho^0, \quad \zeta_2 = 1, 2, \dots, \zeta^0, \\ 0 \leq R \leq 1, \quad 0 \leq Z_2 \leq 1, \quad R &= \frac{\rho-1}{\rho^0-1}, \quad Z_2 = \frac{\zeta_2-1}{\zeta^0-1}. \end{aligned} \quad (0.5.5)$$

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

$$\begin{aligned} C_2^0(R, Z_2) &= \|b_{\rho\zeta_2}^0\| \equiv 0, \quad \rho = 1, 2, \dots, \rho^0, \quad \zeta_2 = 1, 2, \dots, \zeta^0; \\ C_1^0(R, Z_1) &= \|a_{\rho\zeta_1}^0\|, \quad \rho = 1, 2, \dots, \rho^0, \quad \zeta_1 = 1, 2, \dots, \zeta^0, \end{aligned} \quad (0.5.6)$$

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

$$\begin{aligned} (2-2R^2) \frac{\partial C_1^0}{\partial Z_1} &= \text{Fo}_1 \left( \frac{1}{R} \frac{\partial C_1^0}{\partial R} + \frac{\partial^2 C_1^0}{\partial R^2} \right) - K_1 C_1^0; \\ R=0, \quad \frac{\partial C_1^0}{\partial R} &\equiv 0; \quad R=1, \quad \frac{\partial C_1^0}{\partial R} \equiv 0; \quad Z_1=0, \quad C_1^0 \equiv 1. \end{aligned} \quad (0.5.7)$$

The solution of (8.1.7) permits to obtain a new function:

$$\begin{aligned} C_1^0(R, Z_1) &= C_1^0(R, 1-Z_2) = \hat{C}_1^0(R, Z_2) = \|\hat{a}_{\rho\zeta_2}^0\|, \\ \rho &= 1, 2, \dots, \rho^0, \quad \zeta_2 = 1, 2, \dots, \zeta^0. \end{aligned} \quad (0.5.8)$$

The iterative step  $s$  is the solution of the problem:

$$\begin{aligned} (2-2R^2) \frac{\partial C_2^s}{\partial Z_2} &= \text{Fo}_2 \left( \frac{1}{R} \frac{\partial C_2^s}{\partial R} + \frac{\partial^2 C_2^s}{\partial R^2} \right) + K_2 (\hat{C}_1^{(s-1)} - C_2^s); \\ R=0, \quad \frac{\partial C_2^s}{\partial R} &\equiv 0; \quad R=1, \quad \frac{\partial C_2^s}{\partial R} \equiv 0; \quad Z_2=0, \quad C_2^s \equiv 0, \end{aligned} \quad (0.5.9)$$

where  $\hat{C}_1^{(s-1)}(R, Z_2) = \|\hat{a}_{\rho\zeta_2}^{(s-1)}\|$ ,  $\rho = 1, 2, \dots, \rho^0$ ,  $\zeta_2 = 1, 2, \dots, \zeta^0$ .

The solution of (8.1.9) permits to obtain a new function:

$$\begin{aligned} C_2^s(R, Z_2) &= C_2^s(R, 1-Z_1) = \hat{C}_2^s(R, Z_1) = \|\hat{b}_{\rho\zeta_1}^s\|, \\ \rho &= 1, 2, \dots, \rho^0, \quad \zeta_1 = 1, 2, \dots, \zeta^0, \end{aligned} \quad (0.5.10)$$

which will be used for solving (8.1.2) at the  $s^{\text{th}}$  iterative step:

$$\begin{aligned} (2-2R^2) \frac{\partial C_1^s}{\partial Z_1} &= \text{Fo}_1 \left( \frac{1}{R} \frac{\partial C_1^s}{\partial R} + \frac{\partial^2 C_1^s}{\partial R^2} \right) - K_1 (C_1^s - \hat{C}_2^s); \\ R=0, \quad \frac{\partial C_1^s}{\partial R} &\equiv 0; \quad R=1, \quad \frac{\partial C_1^s}{\partial R} \equiv 0; \quad Z_1=0, \quad C_1^s \equiv 1. \end{aligned} \quad (0.5.11)$$

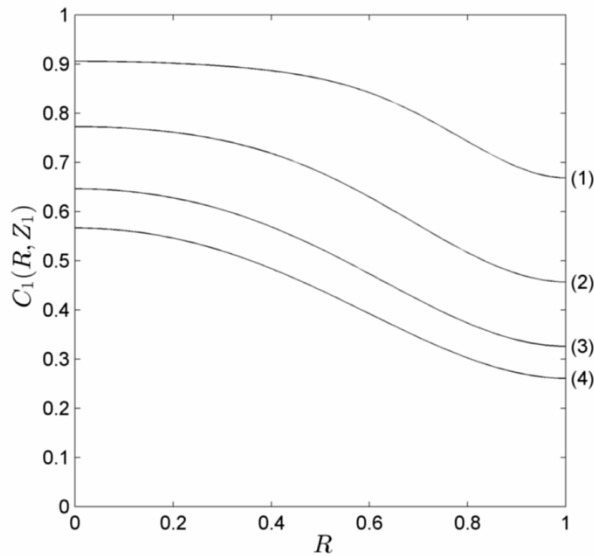
The solution of the problem (8.1.2), (8.1.3) is possible to be obtained using MATLAB program. It solves the equations (8.1.9), (8.1.11) through iterative procedure, using the built-in MATLAB function *pdepe*, which solves the initial-boundary value problems for parabolic partial differential equations. The obtained matrices  $\hat{C}_1^{s-1}$  (from (8.1.11)) and  $\hat{C}_2^s$  (from (8.1.9)) are introduced in (8.1.9) and (8.1.11) respectively using the built-in MATLAB function *interp2*.

The stop criterion of the iterative procedure is the condition:

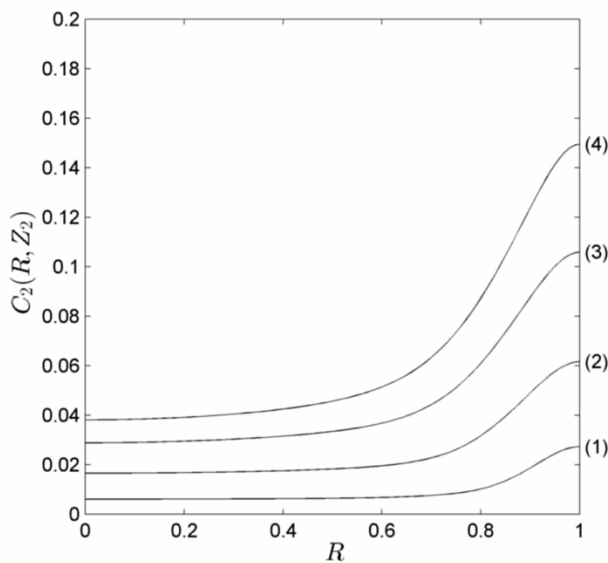
$$\left| \frac{a_{\rho\zeta_1}^s - a_{\rho\zeta_1}^{(s-1)}}{a_{\rho\zeta_1}^s} \right| \leq 10^{-3}, \quad \rho = 1, 2, \dots, \rho^0, \quad \zeta_1 = 1, 2, \dots, \zeta^0. \quad (0.5.12)$$

### 1.2. Concentration distributions

A solution of the problem (8.1.2), (8.1.3) is obtained for the case  $Fo_1 = 0.1$ ,  $Fo_2 = 0.01$ ,  $K_1 = 1$ ,  $K_2 = 0.1$  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 on Fig. 8.1 and Fig.8.2. These results permit to obtain  $\bar{C}_j(Z_j), A_j(Z_j), j = 1, 2$  in (6.1.7) (Figs. 6.1–6.4) and “theoretical” parameters values (6.1.9) presented in Table 6.1



**Fig. 8.1** 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. 8.2** 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)-  $C_2(R, 1)$ .

### 1.3. Absorption process efficiency

The solution of the problem (8.1.2), (8.1.3) permit to obtain the absorption efficiency  $g$  and the gas absorption degree  $G$  in the column using the inlet and outlet average convective mass flux at the cross-sectional area surface in the column:

$$g = u_1^0 c_1^0 - \frac{2}{r_0^2} \int_0^{r_0} r u_1(r) c_1(r, l) dr, \quad G = \frac{g}{u_1^0 c_1^0}. \quad (0.5.13)$$

The absorption degree in generalized variables (3.1.4) has the form:

$$G = 1 - 2 \int_0^1 R U_1(R) C_1(R, 1) dR. \quad (0.5.14)$$

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

$$G_0 = 1 - 2 \int_0^1 R C_1(R, 1) dR \quad (0.5.15)$$

and the reduction in the process efficiency due to the radial non-uniformity of the velocity is shown in Table 8.1.

**Table 8.1** Absorption degree

#### 2. Average-concentration model

In the cases of unknown velocity distribution in high counter-current columns the average-concentration model (6.1.10) is possible to be used for the physical absorption modeling:

$$\begin{aligned} (a_{01} + a_{11} Z_1) \frac{d\bar{C}_1}{dZ_1} + a_{11} \bar{C}_1 &= -K_{01} (\bar{C}_1 - \bar{C}_2); \quad Z_1 = 0, \quad \bar{C}_1(0) = 1. \\ (a_{02} + a_{12} Z_2) \frac{d\bar{C}_2}{dZ_2} + a_{12} \bar{C}_2 &= K_{02} (\bar{C}_1 - \bar{C}_2); \quad Z_2 = 0, \quad \bar{C}_2(0) = 0, \end{aligned} \quad (0.6.1)$$

where  $a_{0j}, a_{1j}, j = 1, 2$  are the "theoretical" parameters values presented in Table 6.1.

#### 2.1. Calculation problem

The numerical solution of the equation set (8.2.1) is possible if MATLAB and an iterative procedure are used [6], where the average concentration distributions in the column will be obtained in two vectors forms on every iteration step  $s$ :

$$\bar{C}_1^s(Z_1) = \|m_{\zeta_1}^s\|, \quad \zeta_1 = 1, 2, \dots, \zeta^0, \quad 0 \leq Z_1 \leq 1, \quad Z_1 = \frac{\zeta_1 - 1}{\zeta^0 - 1}. \quad (0.6.2)$$

$$\bar{C}_2^s(Z_2) = \|n_{\zeta_2}^s\|, \quad \zeta_2 = 1, 2, \dots, \zeta^0, \quad 0 \leq Z_2 \leq 1, \quad Z_2 = \frac{\zeta_2 - 1}{\zeta^0 - 1}. \quad (0.6.3)$$

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

$$\bar{C}_2^0(Z_2) = \|n_{\zeta_2}^0\| \equiv 0, \quad \zeta_2 = 1, 2, \dots, \zeta^0; \quad \bar{C}_1^0(Z_1) = \|m_{\zeta_1}^0\|, \quad \zeta_1 = 1, 2, \dots, \zeta^0, \quad (0.6.4)$$

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

$$(a_{01} + a_{11}Z_1) \frac{d\bar{C}_1^0}{dZ_1} + a_{11}\bar{C}_1^0 = -K_1\bar{C}_1^0; \quad Z_1 = 0, \quad \bar{C}_1^0(0) \equiv 1. \quad (0.6.5)$$

As a result is possible to obtain

$$\hat{C}_1^0(Z_2) = \bar{C}_1^0(Z_1 = 1 - Z_2). \quad (0.6.6)$$

The iterative procedure  $s$  is the sequentially solving the equations:

$$(a_{02} + a_{12}Z_2) \frac{d\bar{C}_2^s}{dZ_2} + a_{12}\bar{C}_2^s = K_2(\hat{C}_1^{(s-1)} - \bar{C}_2^s); \quad Z_2 = 0, \quad \bar{C}_2^s(0) \equiv 0; \quad (0.6.7)$$

$$(a_{01} + a_{11}Z_1) \frac{d\bar{C}_1^s}{dZ_1} + a_{11}\bar{C}_1^s = -K_1(\bar{C}_1^s - \hat{C}_2^s); \quad Z_1 = 0, \quad \bar{C}_1^s(0) \equiv 1, \quad (0.6.8)$$

where

$$\hat{C}_1^{(s-1)}(Z_2) = \bar{C}_1^{(s-1)}(Z_1 = 1 - Z_2), \quad \hat{C}_2^s(Z_1) = \bar{C}_2^s(Z_2 = 1 - Z_1). \quad (0.6.9)$$

The stop criterion of the iterative procedure is the condition:

$$\left| \frac{m_{\zeta_1}^s - m_{\zeta_1}^{(s-1)}}{m_{\zeta_1}^s} \right| \leq 10^{-3}, \quad \zeta_1 = 1, 2, \dots, \zeta^0. \quad (0.6.10)$$

The solving of the problem (8.2.7), (8.2.8) was obtained by MATLAB program, using iterative algorithm. First it solves the equation (8.2.7) using  $\hat{C}_1^{(s-1)}(Z_2) = \bar{C}_1^{(s-1)}(Z_1 = 1 - Z_2)$  and the built-in MATLAB function *ode45*, which solves non-stiff differential equations by medium order method. The obtained matrix  $\hat{C}_2^s(Z_1) = \bar{C}_2^s(Z_2 = 1 - Z_1)$  is introduced in (8.2.8) using the built-in MATLAB interpolation function *interp1*. The presented approach is used for the parameter identification in Chap. 6.