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Some problems in the column apparatuses modeling

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The solutions of some theoretical problems of the column apparatuses modeling in the cases of one-, two- and three-phase processes are presented in the approximation of the mechanics of continua. The effect of the radial non-uniformity of the velocity distribution, the effect of the tangential flow and simultaneous mass and heat transfer processes in one-phase column are analyzed. The possibility for obtaining the interphase distribution of the mass transfer resistances in two-phase columns is shown. An iterative numerical algorithm for non-stationary processes modeling in three-phase columns is also presented.

Key words: modeling, column apparatus, one phase, two phases, three phases, mass transfer, heat transfer.

INTRODUCTION

The fundamental modeling problems in column apparatuses are a result of the complicated hydrodynamic behavior of the flows in the columns. The presence of different phases (gas, liquid and solid) leads to the necessity for formulation of two or three phases hydrodynamic problem. At the other side the equations of the interphase surface, where boundary conditions must be formulated, are practically unknown. As a result the solution of the interphase mass transfer problem is not possible because the velocity function in the convection-diffusion equation is unknown.

The interphase mass transfer problem in column apparatuses may be modeled using a new approach based on the approximations of the mechanics of continua [1-4], where the mathematical point is equivalent to a small (elementary) physical volume, sufficiently small with respect to the apparatus volume, but at the same time sufficiently large with respect to the intermolecular volumes of the medium. As a result the mathematical description of the processes presents the mass balance in this elementary volume in the form of a convection-diffusion type of model, using the convection-diffusion equations. These types of models [1-4] allow a qualitative analysis of the process in order to obtain the main, small and slight physical effects (mathematical operators in the models), and to reject the slight effects (operators).

The use of the convection-diffusion type of models for modeling (quantifying) of the processes in column apparatuses is not possible because the velocity function in the convection-diffusion equations is unknown. The problem can be avoided if the average values of the velocities and concentrations over the cross-sectional area of the column are used, i.e. the medium elementary volume (in the physical approximations of the mechanics of continua [1-4]) will be equivalent to a small cylinder with radius r_0 and a height, which is sufficiently small with respect to the column height and at the same time sufficiently large with respect to the intermolecular distances in the medium.

The main part of the problems in one-phase columns is the decrease of the processes efficiency as a result of the effect of radial non-uniformity of the velocity distribution. This problem can be avoided by using a tangential inlet of the flow in the column, which is very useful in the cases of simultaneous mass and heat transfer processes.

Theoretical analysis of the interphase distribution of the mass transfer resistances in two-phase columns allows obtaining the optimal gas-liquid dispersion, i.e. a system of gas-liquid drops (liquid-gas bubbles) in the case when the main part of the interphase mass transfer resistance is in the gas (liquid) phase.

ONE-PHASE MODEL

Let's consider a liquid motion in a column reactor with radius r_0 (m) and height l (m), where a homogeneous chemical reaction between two liquid components is realized. If the difference between the component concentrations is very large, then the chemical reaction will be of first order.

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Convection–diffusion type of model

If the velocity u [m.s^{-1}] and concentration c [kg.m^{-3}] distributions in the column are defined as:

$$u = u(r), \quad c = c(r,z), \tag{1}$$

the convection–diffusion type of model [4] can be expressed as:

$$u\frac{\partial c}{\partial z} = D\left(\frac{\partial^2 c}{\partial z^2} + \frac{1}{r}\frac{\partial c}{\partial r} + \frac{\partial^2 c}{\partial r^2}\right) - kc;$$

$$z = 0, \quad c(r,0) \equiv c_0, \quad \bar{u}\, c_0 \equiv u c_0 - D\frac{\partial c}{\partial z};$$

$$r = 0, \quad \frac{\partial c}{\partial r} \equiv 0; \quad r = r_0, \quad \frac{\partial c}{\partial r} \equiv 0, \tag{2}$$

where D [m^2.s^{-1}] is diffusivity, k [s^{-1}] – chemical reaction rate constant, $\bar{u}$, c_0 - input values of the average velocity and concentration.

The qualitative analysis of the model (2) will be made using generalized variables:

$$r = r_0 R, \quad z = lZ, \quad u(r) = u(r_0 R) = \bar{u}U(R),$$

$$c(r,z) = c(r_0 R, lZ) = c_0 C(R,Z), \quad \varepsilon = \left(\frac{r_0}{l}\right)^2, \tag{3}$$

Where r_0, l, $\bar{u}$, c_0 are the characteristic (inherent) scales (maximal or average values) of the variables. Introducing the generalized variables (3) in (2), the convection–diffusion type of model can be written as:

$$U(R)\frac{\partial C}{\partial Z} = \text{Fo}\left(\varepsilon\frac{\partial^2 C}{\partial Z^2} + \frac{1}{R}\frac{\partial C}{\partial R} + \frac{\partial^2 C}{\partial R^2}\right) - \text{Da}C;$$

$$Z = 0, \quad C \equiv 1, \quad 1 \equiv U - \text{Pe}^{-1}\frac{\partial C}{\partial Z};$$

$$R = 0, \quad \frac{\partial C}{\partial R} \equiv 0; \quad R = 1, \quad \frac{\partial C}{\partial R} \equiv 0, \tag{4}$$

where $\varepsilon = \text{Fo}^{-1}\text{Pe}^{-1}$, $\text{Fo} = \frac{Dl}{\bar{u}r_0^2}$, $\text{Pe} = \frac{\bar{u}l}{D}$, $\text{Da} = \frac{kl}{\bar{u}}$ are the Fourier, Damkohler and Peclet numbers, respectively.

In the cases of big values of the average velocity ($0 = \text{Fo} \le 10^{-2}$), from the convection–diffusion type of model (4) may obtain a convection type of model:

$$U(R)\frac{\partial C}{\partial Z} = -\text{Da}C; \quad Z = 0, \quad \text{C} \equiv 1. \tag{5}$$

The effect of the chemical reaction rate is negligible if $0 = \text{Da} \le 10^{-2}$ and as a result $C \equiv 1$.

When a fast chemical reaction takes place ($\text{Da} \ge 10^{-2}$), the terms in the model must be divided by Da and the approximation $0 = \text{Da} \le 10^{-2}$ has to be applied. The result is:

$$0 = \frac{\text{Fo}}{\text{Da}}\left(\frac{1}{R}\frac{dC}{dR} + \frac{d^2 C}{dR^2}\right) - C;$$

$$R = 0, \quad \frac{dC}{dR} = 0; \quad R = 1, \quad \frac{dC}{dR} = 0, \tag{6}$$

i.e. the model (6) is diffusion type.

Average concentration model

The average velocity and concentration at the column cross-sectional area can be presented as

$$\bar{u} = \frac{2}{r_0^2}\int_0^{r_0} r u(r)\,dr, \quad \bar{c}(z) = \frac{2}{r_0^2}\int_0^{r_0} r c(r,z)\,dr. \tag{7}$$

The convection–diffusion type of model (2) assumes the velocities and concentration distributions to be presented [3, 4] by the average functions (7):

$$u(r) = \bar{u}\,\tilde{u}(r), \quad c(r,z) = \bar{c}(z)\;\tilde{c}(r,z), \tag{8}$$

where $\tilde{u}(r)$ and $\tilde{c}(r,z)$ represent the radial non-uniformity of both the velocity and the concentration distributions, satisfying the conditions:

$$\frac{2}{r_0^2}\int_0^{r_0} r\tilde{u}(r)\,dr = 1, \qquad \frac{2}{r_0^2}\int_0^{r_0} r\;\tilde{c}(r,z)\,dr = 1. \tag{9}$$

An average concentration model may be obtained [1-4] if the expressions (8) were placed into the model equations (2) and then multiplied by r and integrated with respect to r over the interval [0, r_0]. The result is:

$$\alpha\bar{u}\frac{\partial\bar{c}}{\partial z} + \frac{d\alpha}{dz}\bar{u}\bar{c} = D\frac{\partial^2\bar{c}}{\partial z^2} - k\bar{c};$$

$$z = 0, \quad \bar{c}(0) = c_0, \quad \frac{\partial\bar{c}}{\partial z} = 0, \tag{10}$$

where

$$\alpha = \alpha(z) = \frac{2}{r_0^2}\int_0^{r_0} r\tilde{u}\tilde{c}\,dr. \tag{11}$$

The use of the generalized variables:

$$Z = \frac{z}{l}, \quad \bar{C} = \frac{\bar{c}}{c_0}, \quad \alpha(z) = \alpha(lZ) = A(Z), \tag{12}$$

leads to:

$$A\frac{d\bar{C}}{dZ} + \frac{dA}{dZ}\bar{C} = \text{Pe}^{-1}\frac{d^2\bar{C}}{dZ^2} - \text{Da}\,\bar{C};$$

$$Z = 0, \quad \bar{C} = 1, \quad \frac{d\bar{C}}{dZ} = 0. \tag{13}$$

In the cases

$0=\mathrm{Fo}\leq 10^{-2}$, $0=\mathrm{Pe}^{-1}=\varepsilon\mathrm{Fo}\leq 10^{-2}$, $\varepsilon<1$

(see (5)) the model (13) has the convective form:

$$A\frac{d\bar{C}}{dZ}+\frac{dA}{dZ}\bar{C}=-\mathrm{Da}\,\bar{C};\quad Z=0,\quad \bar{C}=1. \qquad (14)$$

The function $A(Z)$ in (13, 14) represents the effect of the velocity radial non-uniformity on the mass transfer efficiency in the column apparatus:

$$A(Z)=\alpha(z)=\frac{2}{r_0^2}\int_0^{r_0} r\tilde{u}\tilde{c}\,dr, \qquad (15)$$

where

$$\tilde{u}(r)=\frac{u(r)}{\bar{u}}=U(R),$$

$$\tilde{c}(r,z)=\frac{c(r,z)}{\bar{c}(z)}=\frac{C(R,Z)}{\bar{C}(Z)},$$

$$\bar{C}(Z)=\frac{\bar{c}(z)}{c_0}=2\int_0^1 RC(R,Z)\,dR \qquad (16)$$

and as a result one can obtain the following equation:

$$A(Z)=2\int_0^1 RU(R)\frac{C(R,Z)}{\bar{C}(Z)}dR\,. \qquad (17)$$

Effect of the radial non-uniformity of the velocity distribution

The case of parabolic velocity distribution (Poiseuille flow) will be used as an example:

$$u(r)=\bar{u}\left(2-2\frac{r^2}{r_o^2}\right). \qquad (18)$$

From (3, 18) follows:

$$U(R)=2-2R^2\,. \qquad (19)$$

The model (4) may raise several particular cases that permit to obtain $C(R,Z)$, $\bar{C}(Z)$ and to present results for $A(Z)\geq 1$, using different approximations:

$$\mathrm{Fo}=1,\quad \mathrm{Da}=1,2,\quad A(Z)=a_0,$$

$$a_0=\frac{1}{N}\sum_{n=1}^{N}A(Z_n);$$

$$\mathrm{Fo}=0,0.1,\quad \mathrm{Da}=1,2,\quad A(Z)=1+aZ,$$

$$a=\frac{1}{N}\sum_{n=1}^{N}\frac{A(Z_n)-1}{Z_n};\quad 0<Z_n<1. \qquad (20)$$

The obtained values of α, α_0 in (20) are shown in Table 1.

The equations (13, 14) allow to obtain expressions for the concentration axial gradient:

$$\frac{d\bar{C}}{dZ}=-A^{-1}\frac{dA}{dZ}\bar{C}+A^{-1}\,\mathrm{Pe}^{-1}\frac{d^2\bar{C}}{dZ^2}-A^{-1}\,\mathrm{Da}\,\bar{C};$$

$$\frac{d\bar{C}}{dZ}=-A^{-1}\frac{dA}{dZ}\bar{C}-A^{-1}\,\mathrm{Da}\,\bar{C}. \qquad (21)$$

From (8) follows that $\tilde{u}=1$ if the velocity radial non-uniformity is absent ($u=\bar{u}$), i.e. $A=\alpha=1$ (see (9, 11, 15)). The presence of a radial non-uniformity of the axial velocity in the columns leads to $A>1$, i.e. a decrease of the concentration axial gradient and process efficiency [4]. In Table 1 are shown the process efficiencies (conversion degree) in the cases of presence (G) and absence (G_0) of a radial non-uniformity of the axial velocity in the column:

$$G=1-2\int_0^1 RU(R)C(R,1)\,dR,\quad G_0=1-\bar{C}(1)\,. \qquad (22)$$

Table 1. Parameter values and values of process efficiencies (conversion degree)

	a	a_0	G	G_0
Da=1, Fo=0	0.5511		0.5568	0.6734
Da=1, Fo=0.1	0.2463		0.5938	0.6452
Da=1, Fo=1		1.02	0.6211	0.6281
Da=2, Fo=0	1.3623		0.7806	0.8516
Da=2, Fo=0.l	0.4547		0.8115	0.8502
Da=2, Fo=1		1.04	0.8481	0.8538

The values in Table 1 demonstrate that the radial non-uniformity of the axial velocity component leads to a substantial decrease of the conversion degree.

Effect of the tangential flow

Let’s consider a cylindrical column with axial input of gas (liquid) flow (Fig.1a). The axial and radial velocity components $u_z=u_z(r,z)$, $u_r=u_r(r,z)$ satisfy the continuity equation:

$$\frac{\partial u_z}{\partial z}+\frac{\partial u_r}{\partial r}+\frac{u_r}{r}=0\,;$$

$$z=0,\quad u_z(r,0)=u_z^0(r),\quad r=r_0,\quad u_r(r_0,z)\equiv 0, \qquad (23)$$

where $u_z^0(r)$ is the input distribution of the axial velocity component as a result of the geometric conditions at the axial input of the column. The velocity components $u_z(r,z)$, $u_r(r,z)$ can be obtained as a solution of the Navier-Stokes equations in boundary layer approximation, i.e. to solve the problem of the gas (liquid) jet in immobile gas (liquid). As a result the radial non-uniformity of the axial velocity component exists for the columns with limited height. In these conditions the conversion degree increase is related to the decrease of the radial non-uniformity of the axial velocity component (special geometric conditions at the axial input of the column).

A possibility for a partial reduction of the radial non-uniformity of the axial velocity component is to use a column with tangential enter [5] of the gas (liquid) flow (Fig.1b) in the column input.

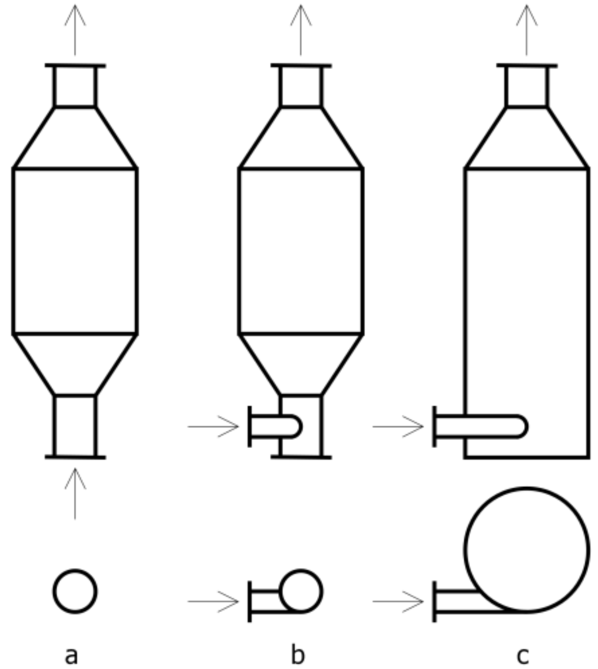

Fig. 1. Cylindrical column with: **a -** axial gas (liquid) flow; **b** - tangential gas (liquid) flow in column inlet; **c-** tangential gas (liquid) flow in the column working area.

A maximal reduction of the radial non-uniformity of the axial velocity component is to use a column with tangential enter [6] of the gas (liquid) flow (Fig.1c) in the column working area.
In the cases of tangential input of the flow in the column, the velocity components $u_z=u_z(r,z,\varphi)$ $u_r=u_r(r,z,\varphi)$, $u_\varphi=u_\varphi(r,z,\varphi)$ satisfy the continuity equation:

$$\frac{\partial u_z}{\partial z}+\frac{1}{r}\frac{\partial u_\varphi}{\partial \varphi}+\frac{\partial u_r}{\partial r}+\frac{u_r}{r}=0;$$
$$z=0,\quad 0\le r<r_0,\quad 0\le\varphi\le 2\pi,$$
$$u_z\left(0,r,\varphi\right)\equiv\bar{u}=\frac{Q}{\pi r_0^2};$$
$$r=r_0,\quad 0<z\le l,\quad 0\le\varphi\le 2\pi,\quad u_r\left(z,r_0,\varphi\right)\equiv 0;$$
$$\varphi=0,\quad u_\varphi\left(0,r_0,0\right)\equiv u_\varphi^0=\frac{Q}{\pi r_{00}^2}, \tag{24}$$

where Q ($m^3.s^{-1}$) is gas (liquid) flow rate in the column and r_{00} is the column inlet radius.

The applying of generalized variables:

$$z=lZ,\quad r=r_0R,\quad \varphi=2\pi\Phi,$$
$$u_z=\bar{u}U_z,\quad u_r=\bar{u}\frac{r_0}{l}U_r,\quad u_\varphi=u_\varphi^0U_\varphi \tag{25}$$

leads to

$$\frac{1}{R}\frac{\partial U_\varphi}{\partial \varphi}+2\pi\frac{\bar{u}r_0}{u_\varphi^0 l}\left(\frac{\partial U_z}{\partial Z}+\frac{\partial U_r}{\partial R}+\frac{U_r}{R}\right)=0;$$
$$Z=0,\quad 0\le R<1,\quad 0\le\Phi\le 1,\quad U_z\left(0,R,\Phi\right)\equiv 1;$$
$$R=1,\quad 0<Z\le 1,\quad 0\le\Phi\le 1,\quad U_r\left(Z,1,\Phi\right)\equiv 0;$$
$$\Phi=0,\quad U_\varphi\left(0,1,0\right)\equiv 1. \tag{26}$$

Practically $\bar{u} \ll u_\varphi^0$ and the following approximation can be used:

$$0=2\pi\frac{\bar{u}r_0}{u_\varphi^0 l}\le 10^{-2}, \tag{27}$$

i.e. $$\frac{\partial U_\varphi}{\partial \varphi}=0 \tag{28}$$

and from (26) follows:

$$\frac{\partial U_z}{\partial Z}+\frac{\partial U_r}{\partial R}+\frac{U_r}{R}=0;$$
$$Z=0,\quad 0\le R<1,\quad U_z\left(0,R\right)\equiv 1;$$
$$R=1,\quad 0<Z\le 1,\quad U_r\left(Z,1\right)\equiv 0. \tag{29}$$

From model (29) follows that practically $U_z(R,Z)\equiv 1$, $U_r(Z,R)\equiv 0$ (except for the thin boundary layer at the wall).

The presented theoretical analysis shows that using tangential input of the flow in the column area leads to a significant decrease of the velocity radial non-uniformity and as a result to an increase of the conversion degree in the columns.

Simultaneous mass and heat transfer processes

The heat and mass transfer kinetics theory shows [3], that the process rate depends on the characteristic velocity in the boundary layer. The big difference between these velocities leads to a substantial increase of the heat transfer rate through the column wall in the cases of axial and tangential input of the flows ($\bar{u} \ll u_\varphi^0$).

Let's consider simultaneous mass and heat transfer processes in a column chemical reactor, where the velocity, concentration and temperature t (deg) distributions in the column are denoted as:

$$u=u\left(r\right),\quad c=c\left(r,z\right),\quad t\left(r,z\right). \tag{30}$$

The mass and heat transfer model in the physical approximations of the mechanics of continua [1-4] can be expressed as:

$$u\frac{\partial c}{\partial z}=D\left(\frac{\partial^2 c}{\partial z^2}+\frac{1}{r}\frac{\partial c}{\partial r}+\frac{\partial^2 c}{\partial r^2}\right)-kc;$$

$$z=0,\quad c(r,0)\equiv c_0,\quad \bar{u}\,c_0\equiv uc_0-D\frac{\partial c}{\partial z},$$

$$r=0,\quad \frac{\partial c}{\partial r}\equiv 0;\qquad r=r_0,\quad \frac{\partial c}{\partial r}\equiv 0. \tag{31}$$

$$u\frac{\partial t}{\partial z}=\frac{\lambda}{\rho c_p}\left(\frac{\partial^2 t}{\partial z^2}+\frac{1}{r}\frac{\partial t}{\partial r}+\frac{\partial^2 t}{\partial r^2}\right)+\frac{q}{\rho c_p}kc;$$

$$z=0,\quad t(r,0)\equiv t_0,\quad \bar{u}\,t_0\equiv u\,t_0-\frac{\lambda}{\rho c_p}\frac{\partial t}{\partial z};$$

$$r=r_0,\quad t\equiv t_s;\quad -\lambda\frac{\partial t}{\partial r}\equiv k_0, \tag{32}$$

where ρ (kg.m^{-3}) is density, c_p [J.kg^{-1}.deg^{-1}] – specific heat at constant pressure, λ [J.m^{-1}.s^{-1}.deg^{-1}] – thermal conductivity, q [J.kg^{-1}] – heat effect of the chemical reaction, k_0 [J.m^{-2}.s^{-1}] – local heat transfer flux. In the model (31, 32) $D,k,\lambda,\rho,c_p,q,k_0$ are temperature functions, where $t_0\le t\le t_s$ or $t_s\le t\le t_0$ in the case of endothermic (q<0) or exothermic (q>0) chemical reaction. Practically the difference $|t_0-t_s|$ is not so big and in (31, 32) may use constant values of $D,k,\lambda,\rho,c_p,q,k_0$ at $t^*=(t_0+t_s)/2$.

From the condition t_s=const follows that the volume heat generation in the column is equal to the interface heat transfer through the column wall:

$$2\pi\int\limits_0^{r_0} rqkc\,dr=-2\pi r_0\lambda\left(\frac{\partial t}{\partial r}\right)_{r=r_0},$$

$$-\lambda\left(\frac{\partial t}{\partial r}\right)_{r=r_0}=\frac{r_0qk}{2}\bar{c}(z)=k_0(z). \tag{33}$$

A qualitative analysis of the model (31, 32) will be made using generalized variables:

$$r=r_0R,\quad z=lZ,\quad u(r)=u(r_0R)=\bar{u}U(R),$$
$$c(r,z)=c(r_0R,lZ)=c_0C(R,Z),$$
$$t(r,z)=t(r_0R,lZ)=t^*T(R,Z), \tag{34}$$

where $r_0,l,\bar{u},c_0,t^*$ are the characteristic (inherent) scales (maximal or average values) of the variables. The introduction of generalized variables (34) in (31, 32) leads to:

$$U(R)\frac{\partial C}{\partial Z}=\frac{Dl}{\bar{u}r_0^2}\left(\frac{r_0^2}{l^2}\frac{\partial^2 C}{\partial Z^2}+\frac{1}{R}\frac{\partial C}{\partial R}+\frac{\partial^2 C}{\partial R^2}\right)-\frac{kl}{\bar{u}}C;$$

$$Z=0,\quad C(R,0)\equiv 1,\quad 1\equiv U(R)-\frac{D}{\bar{u}l}\frac{\partial C}{\partial Z};$$

$$R=0,\quad \frac{\partial C}{\partial R}\equiv 0;\qquad R=1,\quad \frac{\partial C}{\partial R}\equiv 0. \tag{35}$$

$$U(R)\frac{\partial T}{\partial Z}=\frac{\lambda l}{\bar{u}\rho c_p r_0^2}\left(\frac{r_0^2}{l^2}\frac{\partial^2 T}{\partial Z^2}+\frac{1}{R}\frac{\partial T}{\partial R}+\frac{\partial^2 T}{\partial R^2}\right)+\frac{qlkc_0}{\bar{u}\rho c_p t^*}C;$$

$$Z=0,\quad T(R,0)\equiv T_0,\quad 1\equiv U(R)-\frac{\lambda}{T_0\bar{u}\rho c_p l}\frac{\partial T}{\partial Z},\quad T_0=\frac{t_0}{t^*}.$$

$$R=1,\quad T\equiv T_s;\quad \frac{\partial T}{\partial R}\equiv-\frac{r_0^2qkc_0}{2\lambda t^*}\bar{C}(Z),\quad T_s=\frac{t_s}{t^*}. \tag{36}$$

In the cases of very high columns it may use the approximation $0=\frac{r_0^2}{l^2}\le 10^{-2}$ and the models (35, 36) are of parabolic type. If the average velocity $\bar{u}$ is very high, it may use the approximations $0=\frac{Dl}{\bar{u}r_0^2}\le 10^{-2}$ and $0=\frac{\lambda l}{\bar{u}\rho c_p r_0^2}\le 10^{-2}$, i.e. the models (32, 33) are of convective type:

$$U(R)\frac{\partial C}{\partial Z}=-\frac{kl}{\bar{u}}C;\quad Z=0,\quad C(R,0)\equiv 1. \tag{37}$$

$$U(R)\frac{\partial T}{\partial Z}=\frac{qlkc_0}{\bar{u}\rho c_p t^*}C;\quad Z=0,\quad T(R,0)\equiv T_0. \tag{38}$$

Average temperature model

The average temperature at the column cross-sectional area can be presented as

$$\bar{t}(z)=\frac{2}{r_0^2}\int\limits_0^{r_0} rt(r,z)\,dr. \tag{39}$$

The velocities and temperature distributions can be presented by the average functions (7, 39):

$$u(r)=\bar{u}\,\tilde{u}(r),\quad t(r,z)=\bar{t}(z)\tilde{t}(r,z), \tag{40}$$

where $\tilde{u}(r,z)$ and $\tilde{t}\,(r,z)$ represent the radial non-uniformity of both the velocity and the temperature distributions, satisfying the conditions:

$$\frac{2}{r_0^2}\int\limits_0^{r_0} r\tilde{u}(r)\,dr=1,\qquad \frac{2}{r_0^2}\int\limits_0^{r_0} r\,\tilde{t}(r,z)\,dr=1. \tag{41}$$

An average temperature model may be obtained if the expressions (40) are put into the model equations (32) and then multiplied by r and integrated with respect to r over the interval $[0,r_0]$. The result is:

$$\alpha_t\bar{u}\frac{d\bar{t}}{dz}+\frac{d\alpha_t}{dz}\bar{u}\,\bar{t}=\frac{\lambda}{\rho c_p}\frac{d^2\bar{t}}{dz^2};$$

$$z=0,\quad \bar{t}(0)=t_0,\quad \frac{d\bar{t}}{dz}=0, \tag{42}$$

where

$$\alpha_t = \alpha_t\left(z\right) = \frac{2}{r_0^2}\int\limits_0^{r_0} r\tilde{u}\tilde{t}\,dr. \qquad (43)$$

The use of generalized variables:

$$Z = \frac{z}{l}, \quad \overline{T} = \frac{\overline{t}}{t_0}, \quad \alpha_t\left(z\right) = \alpha_t\left(lZ\right) = A_t\left(Z\right), \qquad (44)$$

leads to:

$$A_t\frac{d\overline{T}}{dZ} + \frac{dA_t}{dZ}\overline{T} = \frac{\lambda t_0}{\rho c_p \overline{u} l^2}\frac{d^2T}{dZ^2};$$

$$Z = 0, \quad \overline{T} = 1, \quad \frac{d\overline{T}}{dZ} = 0. \qquad (45)$$

Similar to (17) the function $A_t(Z)$ may be obtained after solution of the problems (35) and (36):

$$A_t\left(Z\right) = 2\int\limits_0^1 RU\left(R\right)\frac{T\left(R,Z\right)}{\overline{T}\left(Z\right)}dR,$$

$$\overline{T}\left(Z\right) = \frac{\overline{t}\left(z\right)}{t^*} = 2\int\limits_0^1 RT\left(R,Z\right)dR. \qquad (46)$$

TWO-PHASE MODEL

The convection-diffusion models are used [6-11] for qualitative analysis of the processes in two-phase columns. A new possibility is the determination of the interphase distribution of the mass transfer resistances in gas-liquid systems.

Interphase distribution of the mass transfer resistances

Let's consider a physical absorption in a co-current gas–liquid bubble column with a radius r_0 and working zone height l, where the interphase mass transfer rate across the gas-liquid boundary is $k(c_1-\chi c_2)$ and χ is the Henry's constant. If ε_1 and ε_2 are the gas and liquid parts of the medium elementary volume ($\varepsilon_1+\varepsilon_2=1$) in the column (gas and liquid holdup coefficients), the convection-diffusion equations have the forms:

$$\varepsilon_1 u_1\frac{\partial c_1}{\partial z} = \varepsilon_1 D_1\left(\frac{\partial^2 c_1}{\partial z^2} + \frac{1}{r}\frac{\partial c_1}{\partial r} + \frac{\partial^2 c_1}{\partial r^2}\right) - k\left(c_1 - \chi c_2\right),$$

$$\varepsilon_2 u_2\frac{\partial c_2}{\partial z} = \varepsilon_2 D_2\left(\frac{\partial^2 c_2}{\partial z^2} + \frac{1}{r}\frac{\partial c_2}{\partial r} + \frac{\partial^2 c_2}{\partial r^2}\right) + k\left(c_1 - \chi c_2\right), \qquad (47)$$

where $u_1(r)$, $u_2(r)$ are velocity distributions in the gas and liquid phases, $c_i(z,r)$ and $D_i(i=1,2)$ are the concentration distributions and the diffusivities of the absorbed substance in the gas and liquid. The boundary conditions of the model equations have the form:

$$z = 0, \quad c_1\left(0,r\right) \equiv c_1^0, \quad \overline{u}_1 c_1^0 \equiv u_1\left(r\right)c_1^0 - D_1\left(\frac{\partial\, c_1}{\partial\, z}\right)_{z=0};$$

$$z = 0, \quad c_2\left(0,r\right) \equiv c_2^0, \quad \overline{u}_2 c_2^0 \equiv u_2\left(r\right)c_2^0 - D_2\left(\frac{\partial\, c_2}{\partial\, z}\right)_{z=0};$$

$$r = 0, \quad \frac{\partial c_1}{\partial r} = \frac{\partial c_2}{\partial r} \equiv 0; \quad r = r_0, \quad \frac{\partial c_1}{\partial r} = \frac{\partial c_2}{\partial r} \equiv 0, \qquad (48)$$

where $\bar{u}_i$, c_i^0, $i=1,2$ are the average velocities and the input concentrations in the gas and liquid phases. Practically $c_2^0=0$.

A qualitative analysis of the model may be made, using dimensionless (generalized) variables:

$$R = \frac{r}{r_0}, \quad Z = \frac{z}{l}, \quad U_1 = \frac{u_1}{\overline{u}_1}, \quad U_2 = \frac{u_2}{\overline{u}_2}, \quad C_1 = \frac{c_1}{c_1^0}, \quad C_2 = \frac{c_2\chi}{c_1^0}. \qquad (49)$$

The model (47, 48) in generalized variables (49) has the form:

$$U_1\left(R\right)\frac{\partial C_1}{\partial Z} = \mathrm{Fo}_1\left(\varepsilon\frac{\partial^2 C_1}{\partial Z^2} + \frac{1}{R}\frac{\partial C_1}{\partial R} + \frac{\partial^2 C_1}{\partial R^2}\right) - K\left(C_1 - C_2\right);$$

$$U_2\left(R\right)\frac{\partial C_2}{\partial Z} = \mathrm{Fo}_2\left(\varepsilon\frac{\partial^2 C_2}{\partial Z^2} + \frac{1}{R}\frac{\partial C_2}{\partial R} + \frac{\partial^2 C_2}{\partial R^2}\right) + K\frac{\varepsilon_1\overline{u}_1\chi}{\varepsilon_2\overline{u}_2}\left(C_1 - C_2\right);$$

$$Z = 0, \quad C_1\left(0,R\right) \equiv 1, \quad 1 = U_1\left(R\right) - \mathrm{Pe}_1^{-1}\left(\frac{\partial C_1}{\partial Z}\right)_{Z=0};$$

$$Z = 0, \quad C_2\left(0,R\right) \equiv 0, \quad \left(\frac{\partial C_2}{\partial Z}\right)_{Z=0} \equiv 0;$$

$$R = 0, \quad \frac{\partial C_i}{\partial R} \equiv 0; \quad R = 1, \quad \frac{\partial C_i}{\partial R} \equiv 0; \quad i = 1,2, \qquad (50)$$

where

$$K = \frac{k_0 l}{\varepsilon_1\overline{u}_1}, \quad \mathrm{Fo}_i = \frac{D_i l}{\overline{u}_i r_0^2}, \quad \mathrm{Pe}_1 = \frac{\overline{u}_1 l}{D_1}, \quad i = 1,2. \qquad (51)$$

If denote:

$$\rho_0 = \frac{\varepsilon_1\overline{u}_1\chi}{\varepsilon_2\overline{u}_2}, \quad \rho_1 = K, \quad \rho_2 = \rho_0\rho_1,$$

$$\rho_1 + \rho_2 = 1, \quad \rho_1 = \frac{1}{1+\rho_0}, \quad \rho_2 = \frac{\rho_0}{1+\rho_0}, \qquad (52)$$

the parameters ρ_1 and ρ_2 can be considered as mass transfer resistances in the gas and liquid phases and from (50) it may obtain directly models of the physical absorption in the cases of highly ($\chi\to 0$, $\rho_0\to 0$, $\rho_2\to 0$, $C_2\equiv 0$) and slightly ($\chi\to\infty$, $\rho_0\to\infty$, $\rho_1\to 0$, $C_1\equiv 1$) soluble gases. The use of model (50) for prediction of the distribution of mass transfer resistances allows an optimal organization of the absorption process, i.e. absorption in gas-liquid drops systems, when the resistance is in the gas phase ($\rho_2 \le 10^{-2}, \rho_0 \le 10^{-2}$), or absorption in liquid-gas bubble systems, when the resistance is in the liquid phase ($\rho_1 \le 10^{-2}, \rho_0 \ge 10^2$).

THREE-PHASE MODEL

The convection-diffusion models in three -phase systems [12, 13] are very often characterized by a fixed solid phase, where there is no diffusion transfer. As a result, the process in the solid phase is usually non-stationary. One of the main problems in these cases is the solution of the set of model equations.

Non-stationary processes modeling

Let's consider a non-stationary absorption-adsorption process in column apparatuses in a cylindrical coordinate system (τ,z,r), where τ (s) is the time. A co-current liquid-gas bubbles flow moves through a fixed solid adsorbent particles bed. A component of the gas phase absorbs physically in the liquid phase and after that adsorbs physically in the adsorbent particles. A chemical reaction takes place in the adsorbent particles between adsorbed component and the active centers (AC) in the adsorbent.

The concentrations of the absorbed component in the gas (i=1) and liquid (i=2) phases are $c_i(\tau,z,r)$, while $c_3(\tau,z,r)$ and $c_0(\tau,z,r)$ are the concentrations of the absorbed component and AC in the solid phase, respectively. The interphase mass transfer rates of the physical absorption and adsorption are $k(c_1-\chi c_2)$ and $k_\alpha(c_2-c_3)$.

The chemical reaction rate in the solid phase is $k_0c_3c_0$. As a result the convection-diffusion model of this absorption-adsorption process has the form:

$$\varepsilon_1\frac{\partial c_1}{\partial\tau}+\varepsilon_1 u_1\frac{\partial c_1}{\partial z}=$$

$$=\varepsilon_1 D_1\left(\frac{\partial^2 c_1}{\partial z^2}+\frac{1}{r}\frac{\partial c_1}{\partial r}+\frac{\partial^2 c_1}{\partial r^2}\right)-k\left(c_1-\chi c_2\right),$$

$$\varepsilon_2\frac{\partial c_2}{\partial\tau}+\varepsilon_2 u_2\frac{\partial c_2}{\partial z}=\varepsilon_2 D_2\left(\frac{\partial^2 c_2}{\partial z^2}+\frac{1}{r}\frac{\partial c_2}{\partial r}+\frac{\partial^2 c_2}{\partial r^2}\right)+$$

$$+k\left(c_1-\chi c_2\right)-k_a\left(c_2-c_3\right),$$

$$\varepsilon_0\frac{\partial c_3}{\partial\tau}=k_a\left(c_2-c_3\right)-k_0c_3c_0,$$

$$\varepsilon_0\frac{\partial c_0}{\partial\tau}=-k_0c_3c_0,\ \varepsilon_0+\varepsilon_1+\varepsilon_2=1,$$

with initial and boundaries conditions

$$\tau\equiv 0,\quad c_1\equiv c_1^0,\quad c_2\equiv 0,\quad c_3\equiv 0,\quad c_0\equiv c_0^0;$$

$$z=0,\quad c_1\equiv c_1^0,\quad \bar{u}_1c_1^0\equiv u_1\left(r\right)c_1^0-D_1\left(\frac{\partial c_1}{\partial z}\right)_{z=0};$$

$$z=0,\quad c_2\equiv 0,\quad \left(\frac{\partial c_2}{\partial z}\right)_{z=0}\equiv 0;$$

$$r=0,\quad \frac{\partial c_1}{\partial r}=\frac{\partial c_2}{\partial r}\equiv 0;\quad r=r_0,\quad \frac{\partial c_1}{\partial r}=\frac{\partial c_2}{\partial r}\equiv 0. \tag{54}$$

In the presented model (53, 54) ε_i, D_i are phase part and diffusivity in the solid (i=0), gas (i=1) and liquid (i=2) phases (D_0=0), k,k_α,k_0- absorption and adsorption interphase mass transfer coefficients and a chemical reaction rate constant, respectively.

The use of dimensionless (generalized) variables permit a qualitative analysis of the model (53, 54) to be made, where as characteristic scales average velocities, initial concentrations, characteristic time τ_0 (s) and column parameters (r_0,h) are used:

$$T=\frac{\tau}{\tau_0},R=\frac{r}{r_0},Z=\frac{z}{l},U_i\left(R\right)=\frac{u_i\left(r\right)}{\bar{u}_i},$$

$$C_i\left(T,Z,R\right)=\frac{c_i\left(\tau,z,r\right)}{c_i^0},\quad c_2^0=\frac{c_1^0}{\chi},$$

$$C_3\left(T,Z,R\right)=\frac{c_3\left(\tau,z,r\right)}{c_3^0},\ C_0\left(T,Z,R\right)=\frac{c_0\left(\tau,z,r\right)}{c_0^0},$$

$$i=1,2. \tag{55}$$

The convection-diffusion model in dimensionless variables can be written in the following way:

$$\frac{l}{\bar{u}_1\tau_0}\frac{\partial C_1}{\partial T}+U_1\frac{\partial C_1}{\partial Z}=$$

$$=\frac{D_1 l}{\bar{u}_1 r_0^2}\left(\frac{r_0^2}{l^2}\frac{\partial^2 C_1}{\partial Z^2}+\frac{1}{R}\frac{\partial C_1}{\partial R}+\frac{\partial^2 C_1}{\partial R^2}\right)-\frac{kl}{\varepsilon_1\bar{u}_1}\left(C_1-C_2\right),$$

$$\frac{l}{\bar{u}_2\tau_0}\frac{\partial C_2}{\partial\tau}+U_2\frac{\partial C_2}{\partial Z}=$$

$$=\frac{D_2 l}{\bar{u}_2 r_0^2}\left(\frac{r_0^2}{l^2}\frac{\partial^2 C_2}{\partial Z^2}+\frac{1}{R}\frac{\partial C_2}{\partial R}+\frac{\partial^2 C_2}{\partial R^2}\right)+$$

$$+\frac{kl\chi}{\varepsilon_2\bar{u}_2}\left(C_1-C_2\right)-\frac{k_a l}{\varepsilon_2\bar{u}_2}\left(C_2-\frac{\chi c_3^0}{c_1^0}C_3\right),$$

$$\frac{\partial C_3}{\partial T}=\frac{k_a\tau_0}{\varepsilon_0}\left(\frac{c_1^0}{\chi c_3^0}C_2-C_3\right)-\frac{k_0\tau_0c_0^0}{\varepsilon_0}C_3C_0,$$

$$\frac{\partial C_0}{\partial T}=-\frac{k_0\tau_0c_3^0}{\varepsilon_0}C_3C_0. \tag{56}$$

$$T=0,\quad C_1\equiv 1,\quad C_2\equiv 0,\quad C_3\equiv 0,\quad C_0\equiv 1;$$
$$Z=0,\quad C_1\equiv 1,\quad 1\equiv U_1(R)-\frac{D_1}{\bar{u}_1 l}\left(\frac{\partial C_1}{\partial Z}\right)_{Z=0};$$
$$Z=0,\quad C_2\equiv 0,\quad \left(\frac{\partial C_2}{\partial Z}\right)_{Z=0}\equiv 0;$$
$$R=0,\quad \frac{\partial C_1}{\partial R}=\frac{\partial C_2}{\partial R}\equiv 0;\quad R=1,\quad \frac{\partial C_1}{\partial R}=\frac{\partial C_2}{\partial R}\equiv 0. \tag{57}$$

The presented model (56, 57) is the basis for a qualitative analysis of the mass transfer processes in three- phase column apparatuses, i.e. the role of the different physical effects in the complicated absorption-adsorption process.

One of the main problems in three-phase systems is the long-time process. In this case approximations must be used:

$$0=\frac{l}{\bar{u}_1\tau_0}\le 10^{-2},\quad 0=\frac{l}{\bar{u}_2\tau_0}\le 10^{-2} \tag{58}$$

and the model (56, 57) has the form:

$$U_1\frac{\partial C_1}{\partial Z}=\frac{D_1 l}{\bar{u}_1 r_0^2}\left(\frac{r_0^2}{l^2}\frac{\partial^2 C_1}{\partial Z^2}+\frac{1}{R}\frac{\partial C_1}{\partial R}+\frac{\partial^2 C_1}{\partial R^2}\right)-\frac{kl}{\varepsilon_1\bar{u}_1}(C_1-C_2);$$
$$Z=0,\quad C_1\equiv 1,\quad 1\equiv U_1(R)-\frac{D_1}{\bar{u}_1 l}\left(\frac{\partial C_1}{\partial Z}\right)_{Z=0};$$
$$R=0,\quad \frac{\partial C_1}{\partial R}\equiv 0;\quad R=1,\quad \frac{\partial C_1}{\partial R}\equiv 0. \tag{59}$$

$$U_2\frac{\partial C_2}{\partial Z}=\frac{D_2 l}{\bar{u}_2 r_0^2}\left(\frac{r_0^2}{l^2}\frac{\partial^2 C_2}{\partial Z^2}+\frac{1}{R}\frac{\partial C_2}{\partial R}+\frac{\partial^2 C_2}{\partial R^2}\right)+$$
$$+\frac{kl\chi}{\varepsilon_2\bar{u}_2}(C_1-C_2)-\frac{k_a l}{\varepsilon_2\bar{u}_2}\left(C_2-\frac{\chi c_3^0}{c_1^0}C_3\right);$$
$$Z=0,\ C_2\equiv 0,\left(\frac{\partial C_2}{\partial Z}\right)_{Z=0}\equiv 0;$$
$$R=0,\ \frac{\partial C_2}{\partial R}\equiv 0;\ R=1,\ \frac{\partial C_2}{\partial R}\equiv 0. \tag{60}$$

$$\frac{dC_3}{dT}=\frac{k_a\tau_0}{\varepsilon_0}\left(\frac{c_1^0}{\chi c_3^0}C_2-C_3\right)-\frac{k_0\tau_0 c_0^0}{\varepsilon_0}C_3C_0;$$
$$T=0,\quad C_3\equiv 0. \tag{61}$$

$$\frac{dC_0}{dT}=-\frac{k_0\tau_0 c_3^0}{\varepsilon_0}C_3C_0;\quad T=0,\quad C_0\equiv 1. \tag{62}$$

Considering problems (59, 60) *T* is parameter, while in (61, 62) the parameters are *Z* and *R*.

The presented convection-diffusion model (59-62) may be used for qualitative analysis only, but it is the base for the creation of average concentration model.

Average concentration model

Using the dimensionless form of average concentrations the concentrations in (59-62) can be written as:

$$C_i(T,Z,R)=\bar{C}_i(T,Z)\tilde{C}_i(R),$$
$$\bar{C}_i(T,Z)=2\int_0^1 RC_i(T,Z,R)\,dR,$$
$$2\int_0^1 R\tilde{C}_i(R)\,dR=1,\ i=0,1,2,3. \tag{63}$$

The average concentration model can be obtained if the expressions (63) are put into the model equations (59-62) and then multiplied by *R* and integrated with respect to *R* over the interval [0, 1]. The result is:

$$A_1\frac{d\bar{C}_1}{dZ}+\frac{dA_1}{dZ}\bar{C}_1=\mathrm{Pe}_1^{-1}\frac{d^2\bar{C}_1}{dZ^2}-K_1\left(\bar{C}_1-\bar{C}_2\right);$$
$$Z=0,\quad \bar{C}_1\equiv 1,\quad \frac{d\bar{C}_1}{dZ}\equiv 0. \tag{64}$$

$$A_2\frac{d\bar{C}_2}{dZ}+\frac{dA_2}{dZ}\bar{C}_2=$$
$$=\mathrm{Pe}_2^{-1}\frac{d^2\bar{C}_2}{dZ^2}+K_2\left(\bar{C}_1-\bar{C}_2\right)-K_a\left(\bar{C}_2-K_3\bar{C}_3\right);$$
$$Z=0,\ \bar{C}_2\equiv 0,\ \frac{d\bar{C}_2}{dZ}\equiv 0. \tag{65}$$

$$\frac{d\bar{C}_3}{dT}=K_0\frac{k_a}{k_0}\left(K_3^{-1}\bar{C}_2-\bar{C}_3\right)-K_0c_0^0B\bar{C}_3\bar{C}_0;$$
$$T=0,\quad \bar{C}_3\equiv 0. \tag{66}$$

$$\frac{d\bar{C}_0}{dT}=-K_0c_3^0BC_3C_0;\ T=0,\quad \bar{C}_0\equiv 1. \tag{67}$$

In the problems (64-67) the expressions are used:

$$A_i(Z)=2\int_0^1 RU(R)\frac{C_i(T,Z,R)}{\bar{C}(T,Z)}dR,\quad \mathrm{Pe}_i=\frac{\bar{u}_i l}{D_i},\quad i=1,2,$$
$$B(Z)=2\int_0^1 R\frac{C_3(T,Z,R)}{\bar{C}_3(T,Z)}\frac{C_0(T,Z,R)}{\bar{C}_0(T,Z)}dR,\quad K_a=\frac{k_a l}{\varepsilon_2\bar{u}_2},$$
$$K_0=\frac{k_0\tau_0}{\varepsilon_0},\quad K_1=\frac{kl}{\varepsilon_1\bar{u}_1},\quad K_2=\frac{kl\chi}{\varepsilon_2\bar{u}_2},\quad K_3=\frac{\chi c_3^0}{c_1^0}. \tag{68}$$

In the problems (64, 65) *T* is parameter, while in (66, 67) the parameter is *Z* and for solution of the set of equations (64-67) will be used a numerical iterative algorithm.

Iterative algorithm

The solution of (64-67) may be obtained as four matrix forms:

$$\bar{C}_1(T,Z)=\left\|\bar{C}_{1\theta\zeta}\right\|,\quad \bar{C}_2(T,Z)=\left\|\bar{C}_{2\theta\zeta}\right\|,$$
$$\bar{C}_3(T,Z)=\left\|\bar{C}_{3\theta\zeta}\right\|,\quad \bar{C}_0(T,Z)=\left\|\bar{C}_{0\theta\zeta}\right\|;$$
$$T=0.01\theta,\ \theta=1,2,...,100;\quad Z=0.01\zeta,\ \zeta=1,2,...,100\ . \tag{69}$$

A multi-step approach for different values of $T=0.01\theta,$ ($\theta=1,2,...,100$) will be used, where the upper index (*θ*) will be the step number too. As a zero step (*θ*=0) will be used:

$$\bar{C}_1^0(T,Z)=\left\|C_{(1)0\zeta}\right\|,\quad \bar{C}_2^0(T,Z)=\left\|\bar{C}_{(2)0\zeta}\right\|,$$
$$\bar{C}_3^0=\left\|\bar{C}_{(3)0\zeta}\right\|\equiv 0,\quad \bar{C}_0^0(T,Z)=\left\|\bar{C}_{(0)0\zeta}\right\|\equiv 1$$
$$Z=0.01\zeta,\quad \zeta=1,2,...,100\ , \tag{70}$$

where $\bar{C}_1^0(T,Z)=\left\|C_{(1)0\zeta}\right\|,\ \bar{C}_2^0(T,Z)=\left\|\bar{C}_{(2)0\zeta}\right\|$ are solutions of (64, 65) for $\bar{C}_3^0=\left\|\bar{C}_{(3)0\zeta}\right\|\equiv 0$:

$$A_1\frac{d\bar{C}_1^0}{dZ}+\frac{dA_1}{dZ}\bar{C}_1^0=\mathrm{Pe}_1^{-1}\frac{d^2\bar{C}_1^0}{dZ^2}-K_1\left(\bar{C}_1^0-\bar{C}_2^0\right);$$
$$Z=0,\quad \bar{C}_1^0\equiv 1,\quad \frac{d\bar{C}_1^0}{dZ}\equiv 0.$$
$$A_2\frac{d\bar{C}_2^0}{dZ}+\frac{dA_2}{dZ}\bar{C}_2^0=\mathrm{Pe}_2^{-1}\frac{d^2\bar{C}_2^0}{dZ^2}+K_2\left(\bar{C}_1^0-\bar{C}_2^0\right)-K_a\bar{C}_2^0;$$
$$Z=0,\ \bar{C}_2^0\equiv 0,\ \frac{d\bar{C}_2^0}{dZ}\equiv 0. \tag{71}$$

The first step is the solutions of (66, 67) $\bar{C}_3^1(T,Z)=\left\|\bar{C}_{(3)\theta\zeta}^1\right\|,\ \bar{C}_0^1(T,Z)=\left\|\bar{C}_{(0)\theta\zeta}^1\right\|$ for $\bar{C}_2=\bar{C}_2^0(T,Z)=\left\|C_{(2)0\zeta}\right\|,\ Z=0.01\zeta,\ \zeta=1,2,...,100$:

$$\frac{d\bar{C}_3^1}{d\mathrm{T}}=K_0\frac{k_a}{k_0}\left(K_3^{-1}\bar{C}_2^0-\bar{C}_3^1\right)-K_0c_0^0B\bar{C}_3^1\bar{C}_0^1;$$
$$\mathrm{T}=0,\ \bar{C}_3^1\equiv 0.$$
$$\frac{d\bar{C}_0^1}{d\mathrm{T}}=-K_0c_3^0BC_3^1C_0^1;\ \ \mathrm{T}=0,\quad \bar{C}_0^1\equiv 1. \tag{72}$$

As a result the solutions for *T*=0.01 – $\hat{C}_0^1$(Z) and the polynomial approximation $\hat{C}_3^1$(Z) may be obtained:

$$\hat{C}_3^1(Z)=\bar{C}_3^1(0.01,Z)=\left\|\bar{C}_{(3)1\zeta}^1\right\|=\sum_{j=1}^{5}\ \bar{\theta}_j^{(1)}Z^{j-1},$$
$$\hat{C}_0^1(Z)=\bar{C}_0^1(0.01,Z)=\left\|\bar{C}_{(0)1\zeta}^1\right\|,$$
$$Z=0.01\zeta,\ \zeta=1,2,...,100. \tag{73}$$

The solution of (64, 65) at the first step leads to:

$$A_1\frac{d\bar{C}_1^1}{dZ}+\frac{dA_1}{dZ}\bar{C}_1^1=\mathrm{Pe}_1^{-1}\frac{d^2\bar{C}_1^1}{dZ^2}-K_1\left(\bar{C}_1^1-\bar{C}_2^1\right);$$
$$Z=0,\quad \bar{C}_1^1\equiv 1,\quad \frac{d\bar{C}_1^1}{dZ}\equiv 0.$$
$$A_2\frac{d\bar{C}_2^1}{dZ}+\frac{dA_2}{dZ}\bar{C}_2^1=$$
$$=\mathrm{Pe}_2^{-1}\frac{d^2\bar{C}_2^1}{dZ^2}+K_2\left(\bar{C}_1^1-\bar{C}_2^1\right)-K_a\left(\bar{C}_2^1-\sum_{j=1}^{5}\bar{\theta}_j^{(1)}Z^{j-1}\right);$$
$$Z=0,\quad \bar{C}_2^1\equiv 0,\quad \frac{d\bar{C}_2^1}{dZ}\equiv 0. \tag{74}$$

The step (*θ*) is the solutions of (66, 67) $\bar{C}_3^\theta(T,Z)=\left\|\bar{C}_{(3)\theta\zeta}^\theta\right\|,\ \bar{C}_0^\theta(T,Z)=\left\|\bar{C}_{(0)\theta\zeta}^\theta\right\|$ for $\bar{C}_2=\bar{C}_2^{\theta-1}(T,Z)=\left\|C_{(2)(\theta-1)\zeta}\right\|,$ $Z=0.01\zeta,\quad \zeta=1,2,...,100$:

$$\frac{d\bar{C}_3^\theta}{d\mathrm{T}}=K_0\frac{k_a}{k_0}\left(K_3^{-1}\bar{C}_2^{\theta-1}-\bar{C}_3^\theta\right)-K_0c_0^0B\bar{C}_3^\theta\bar{C}_0^\theta;$$
$$T=0,\quad \bar{C}_3^\theta=\hat{C}_3^{\theta-1}(Z).$$
$$\frac{d\bar{C}_0^\theta}{d\mathrm{T}}=-K_0c_3^0BC_3^\theta C_0^\theta;\qquad T=0,\quad \bar{C}_0^\theta=\hat{C}_0^{\theta-1}(Z). \tag{75}$$

As a result the solutions for *T*=0.01 - $\hat{C}_0^\theta$(Z) and the polynomial approximations $\hat{C}_3^\theta$(Z) may be obtained:

$$\hat{C}_3^\theta(Z)=\bar{C}_3^\theta(0.01,Z)=\left\|\bar{C}_{(3)\theta\zeta}^\theta\right\|=\sum_{j=1}^{5}\ \bar{\theta}_j^{(\theta)}Z^{j-1},$$
$$\hat{C}_0^\theta(Z)=\bar{C}_0^\theta(0.01,Z)=\left\|\bar{C}_{(0)\theta\zeta}^\theta\right\|,$$
$$Z=0.01\zeta,\ \zeta=1,2,...,100\ . \tag{76}$$

At the step *θ* the solution of (64, 65) leads to:

$$A_1\frac{d\bar{C}_1^\theta}{dZ}+\frac{dA_1}{dZ}\bar{C}_1^\theta=\mathrm{Pe}_1^{-1}\frac{d^2\bar{C}_1^\theta}{dZ^2}-K_1\left(\bar{C}_1^\theta-\bar{C}_2^\theta\right);$$
$$Z=0,\quad \bar{C}_1^\theta\equiv 1,\quad \frac{d\bar{C}_1^\theta}{dZ}\equiv 0.$$

$$A_2 \frac{d\bar{C}_2^{\theta}}{dZ} + \frac{dA_2}{dZ}\bar{C}_2^{\theta} =$$
$$= \mathrm{Pe}_2^{-1}\frac{d^2\bar{C}_2^{\theta}}{dZ^2} + K_2\left(\bar{C}_1^{\theta} - \bar{C}_2^{\theta}\right) - K_a\left(\bar{C}_2^{\theta} - \sum_{j=1}^{5}\bar{\theta}_j^{(\theta)} Z^{j-1}\right);$$
$$Z = 0, \quad \bar{C}_2^{\theta} \equiv 0, \quad \frac{d\bar{C}_2^{\theta}}{dZ} \equiv 0. \qquad (77)$$

The stop criterion is θ=100.

The obtained results can be presented as:

$$\left\|\breve{C}_{(1)\theta\zeta}\right\| = \left\|\bar{C}_{(1)\theta\zeta}^{(\theta)}\right\|, \ \left\|\breve{C}_{(2)\theta\zeta}\right\| = \left\|\bar{C}_{(2)\theta\zeta}^{(\theta)}\right\|,$$
$$\left\|\breve{C}_{(3)\theta\zeta}\right\| = \left\|\bar{C}_{(3)\theta\zeta}^{(\theta)}\right\|, \ \left\|\breve{C}_{(0)\theta\zeta}\right\| = \left\|\bar{C}_{(0)\theta\zeta}^{(\theta)}\right\|;$$
$$\theta = 1,...,100; \quad \zeta = 1,...,100.$$

CONCLUSIONS

The solutions of some theoretical problems of the column apparatuses modeling in the cases of one-, two- and three-phase processes are presented in the approximation of the mechanics of continua.
In the cases of one-phase processes the effect of the radial non-uniformity of the velocity distribution, the effect of the tangential flow and the simultaneous mass and heat transfer processes are shown.

A possibility to obtain the interphase distribution of the mass transfer resistances in two-phase columns is shown.

The modeling of three-phase processes in column apparatuses is analysed. An iterative numerical algorithm for non-stationary processes modeling is presented.

The presented approach is used for solution of the SO_2 problem in power engineering [14, 15].

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ПРОБЛЕМИ ПРИ МОДЕЛИРАНЕ НА КОЛОННИ АПАРАТИ

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(Резюме)

В приближенията на механиката на непрекъснатите среди са представени теоретични решения при моделирането на колонни апарати в случаите на една, две и три фази. Анализирани са ефектите от разпределението на радиалната неравномерност на скоростта, наличието на тангенциален поток, както и топло и масопреносните процеси в колона с една фаза. Показана е възможността за получаване на съпротивленията при междуфазно масопренасяне в колона с две фази. Представен е числен алгоритъм за моделиране на нестационарни процеси в колона с три фази.