Bulgarian Chemical Communications, Volume 52, Special Issue F (pp. 20-24) 2020 DOI: 10.34049/bcc.52.F.0003

Convective type models of chemical processes in column apparatuses

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Received: August 1, 2020; Accepted: August 10, 2020

A new approach for the chemical processes modeling in column apparatuses is presented in industrial column apparatuses. An exact approach for solutions of the equations in the convective type models is used. The use of experimental data for the average concentration at the column end, for a concrete process and column, permits to obtain the model parameters related with the radial non-uniformity of the velocity. These parameter values permit to use the average-concentration model for modeling of chemical processes with different reaction rates.

INTRODUCTION

The modeling and simulation of the chemical processes in column apparatuses is possible, using the new approach [1-3] on the basis of the physical approximations of the mechanics of continua, where the mathematical point (in the phase volume or on the surface between the phases) is equivalent to a small (elementary) physical volume, which is sufficiently small with respect to the apparatus volume, but at the same time sufficiently large with respect to the intermolecular volumes in the medium. On this base convection-diffusion and average-concentration type models are presented.

The convection-diffusion type models permit the qualitative analysis of the processes. These models are the base of the average-concentration models which allow a quantitative analysis of the chemical processes in column apparatuses [4].

In the case of the chemical reactions in industrial column apparatuses the effects of the radial component of velocity and the axial diffusion transfer are not negligible and must be taken into account in the convection-diffusion and average-concentration type models [6]. The use of the perturbations method [4, 5] permits to obtain approximation solutions of the model equations. In this paper an exact approach for solutions of the equations in the convective type models of industrial chemical processes in column apparatuses will be presented.

Convection-Diffusion Model

A theoretical analysis of the effect of the radial velocity components and the axial diffusion transfer in industrial column chemical reactors will be presented in the case, when the radial velocity component is not equal to zero for pseudo-first order chemical reactions. In the stationary case, the convection-diffusion model [3, 4] has the form:

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

$$r=0,\quad \frac{\partial c}{\partial r}\equiv 0;\quad r=r_0,\quad \frac{\partial c}{\partial r}\equiv 0;\quad z=0,\quad c\equiv c^0,\quad u^0c^0\equiv uc^0-D\frac{\partial c}{\partial z}.$$

$$\frac{\partial u}{\partial z}+\frac{\partial v}{\partial r}+\frac{v}{r}=0;\quad r=r_0,\quad v\left(r_0,z\right)\equiv 0,\quad z=0,\quad u=u\left(r,0\right). \tag{2}$$

In (1, 2) $c\left(r,z\right), D,$ are the concentrations [kg-mol.m^{-3}] and the diffusivities [m^2.s^{-1}] of the reagents in the fluid, $u\left(r,z\right)$ and $v\left(r,z\right)$ - the axial and radial velocity components [m.s^{-1}], $\left(r,z\right)$ - the radial and axial coordinates [m], k - chemical reaction rate constant, u^0, c^0 - input (z=0) velocity and concentrations.

The theoretical analysis of the model (1, 2) will be made using the generalized variables [1]:

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$$r = r_0 R, \quad z = lZ, \quad \varepsilon = \frac{r_0}{l}, \quad c(r,z) = c(r_0 R, lZ) = c^0 C(R,Z),$$
$$u(r,z) = u(r_0 R, lZ) = u^0 U(R,Z), \quad v(r,z) = v(r_0 R, lZ) = u^0 \varepsilon V(R,Z). \tag{3}$$

As a result, from (1-3) it may be obtained:

$$U\frac{\partial C}{\partial Z} + V\frac{\partial C}{\partial R} = \mathrm{Fo}\left(\varepsilon^2 \frac{\partial^2 C}{\partial Z^2} + \frac{1}{R}\frac{\partial C}{\partial R} + \frac{\partial^2 C}{\partial R^2}\right) - \mathrm{Da}\, C;$$
$$R = 0, \quad \frac{\partial C}{\partial R} \equiv 0; \quad R = 1, \quad \frac{\partial C}{\partial R} \equiv 0; \quad Z = 0, \quad C \equiv 1, \quad 1 \equiv U - \varepsilon^2\, \mathrm{Fo}\frac{\partial C}{\partial Z}. \tag{4}$$

$$\frac{\partial U}{\partial Z} + \frac{\partial V}{\partial R} + \frac{V}{R} = 0; \quad R = 1, \quad V(1,Z) \equiv 0; \quad Z = 0, \quad U = U(R,0). \tag{5}$$

In (5) are used the parameters:

$$\mathrm{Fo} = \frac{D_i l}{u^0 r_0^2}, \quad \mathrm{Da} = \frac{kl}{u^0}, \tag{6}$$

where Fo and Da are the Fourier and Damkohler numbers, respectively. In industrial conditions the parameters $\mathrm{Fo} < 10^{-2}$ are small and the model (4) has a convective form:

$$U\frac{\partial C}{\partial Z} + V\frac{\partial C}{\partial R} = -\mathrm{Da}\, C;$$
$$Z = 0, \quad C \equiv 1; \quad R = 1, \quad \frac{\partial C}{\partial R} \equiv 0. \tag{7}$$

Axial and Radial Velocity Components

The theoretical analysis of the change in the radial non-uniformity of the axial velocity component (effect of the radial velocity component) in a column can be made by an appropriate hydrodynamic model, where the average velocity at the cross section of the column is a constant (inlet average axial velocity component), while the radial non-uniformity of the axial velocity component decreases along the column height and as a result a radial velocity component is initiated. In generalized variables (3) the model can be used:

$$U = (2 - 0.4Z) - 2(1 - 0.4Z)R^2, \quad V = 0.2\left(R - R^3\right), \tag{8}$$

where the velocity components satisfy equation (5). The velocity components (8) are presented on Figs. 1, 2.

Eq. (7) is solved using the Method of Lines [6], by discretizing it in respect to $R_i = i/n$, $i = 0,...,n$, with 3 points central finite difference scheme, thus transforming it from partial differential equation to a system of ordinary differential equations in respect to *Z*:

The problem (9) is stiff, that's why it is solved using MATLAB variable-step, variable-order solver ode15s, using second order backward differentiation formulas (BDF, also known as Gear's method).

$$U(R_0,Z)\frac{dC_0}{dZ} = -\mathrm{Da}\, C_0;$$
$$U(R_i,Z)\frac{dC_i}{dZ} = -V(R_i)\frac{C_{i+1} - C_{i-1}}{R_{i+1} - R_{i-1}} - \mathrm{Da}\, C_i; \tag{9}$$
$$U(R_n,Z)\frac{dC_n}{dZ} = -\mathrm{Da}\, C_n;$$
$$Z = 0, \quad C_0 \equiv 1, \quad C_i \equiv 1, \quad C_n \equiv 1; \quad i = 1,...,n-1.$$

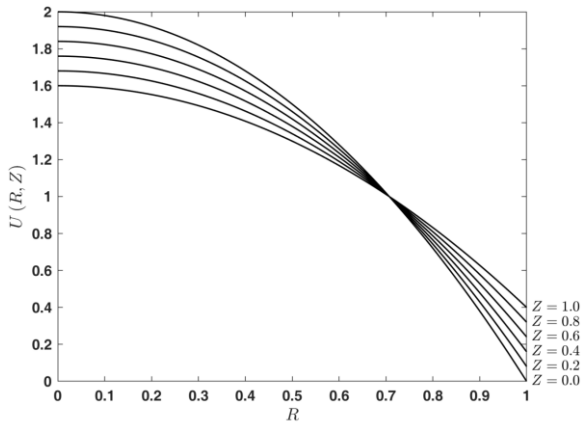

Fig. 1. Axial velocity component $U(R,Z)$ for different $Z = 0,\ 0.2,\ 0.4,\ 0.6,\ 0.8,\ 1.0$.

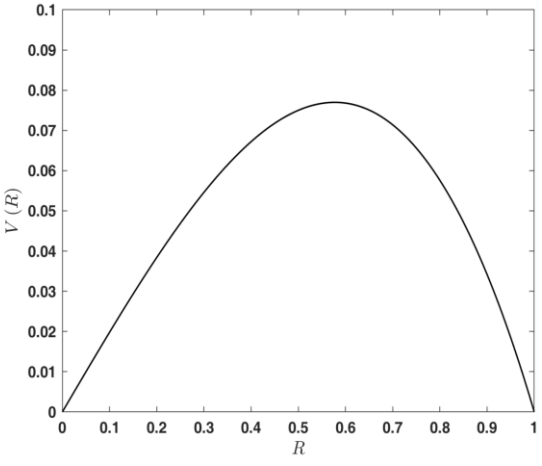

Fig. 2. Radial velocity component $V(R)$.

The solutions of (7) in the case $\mathrm{Da}=1$ are presented on Fig. 3.

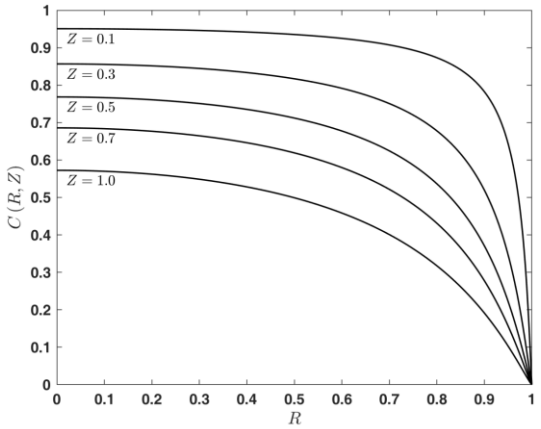

Fig. 3. Concentration distributions $C(R,Z)$ for different Z = 0.1, 0.3, 0.5, 0.7, 1.0.

Average-Concentration Model

The functions $u(r,z), v(r,z), c(r,z)$ in (1) can be presented with the help of the average values of the velocity and concentration at the column cross-sectional area [1-3]:

$$\bar{u}=\frac{2}{r_0^2}\int_0^{r_0} ru(r)\,dr,\quad \bar{c}(z)=\frac{2}{r_0^2}\int_0^{r_0} rc(r,z)\,dr, \tag{10}$$

i.e.

$$u(r,z)=\bar{u}U(R,Z),\quad v(r,z)=\varepsilon\bar{u}V(R),\quad c(r,z)=\bar{c}(z)\,\tilde{c}(r,z). \tag{11}$$

As a result, the following is obtained [3]:

$$\alpha(z)\bar{u}\frac{d\bar{c}}{dz}+\left[\beta(z)+\varepsilon\gamma(z)\right]\bar{u}\bar{c}_i=D\frac{d^2\bar{c}}{dz^2}-k\bar{c}; \tag{12}$$

$$z=0,\quad \bar{c}\equiv c^0,\quad \frac{d\bar{c}}{dz}\equiv 0,$$

where

$$\alpha(z)=\frac{2}{r_0^2}\int_0^{r_0} rU\tilde{c}\,dr,\quad \beta(z)=\frac{2}{r_0^2}\int_0^{r_0} rU\frac{\partial\tilde{c}}{\partial z}\,dr,\quad \gamma(z)=\frac{2}{r_0^2}\int_0^{r_0} rV\frac{\partial\tilde{c}}{\partial r}\,dr,$$

$$\tilde{c}(r,z)=\tilde{C}(R,Z),\quad U=U(R,Z),\quad V=V(R). \tag{13}$$

The theoretical analysis of the model (12) will be made using the following generalized variables and functions:

$$z=lZ,\quad r=r_0R,\quad \bar{c}(z)=c^0\bar{C}(Z),\quad \bar{C}(Z)=2\int_0^1 RC(R,Z)\,dR,$$

$$\tilde{c}(r,z)=\frac{c(r,z)}{\bar{c}(z)}=\frac{C(R,Z)}{\bar{C}(Z)}=\tilde{C}(R,Z),\quad \alpha(z)=A(Z)=2\int_0^1 RU(R,Z)\tilde{C}(R,Z)\,dR, \tag{14}$$

$$\beta(z)=\beta(lZ)=B(Z)=2\int_0^1 RU(R,Z)\frac{\partial\tilde{C}}{\partial Z}\,dR,\quad \gamma(z)=\gamma(lZ)=G(Z)=2\int_0^1 RV(R)\frac{\partial\tilde{C}}{\partial R}\,dR$$

and as a result:

$$A(Z)\frac{d\bar{C}}{dZ}+\left[B(Z)+G(Z)\right]\bar{C}=\varepsilon^2\,\mathrm{Fo}\frac{d^2\bar{C}}{dZ^2}-\mathrm{Da}\,\bar{C}; \tag{15}$$

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

In industrial conditions $\mathrm{Fo}<10^{-2}$ and the model (15) has the convective form:

$$A(Z)\frac{d\bar{C}}{dZ}+\left[B(Z)+G(Z)\right]\bar{C}=-\mathrm{Da}\,\bar{C}; \tag{16}$$

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

The solution of (7) and (14) permits to obtain the average concentrations ("theoretical" values) $\bar{C}(Z_n)$ and functions *A(Z$_n$), B(Z$_n$) G(Z$_n$), Z$_n$ = 0.1(n+1), n = 0,1,...,9*, which are presented (points) on Figs. 4, 5.

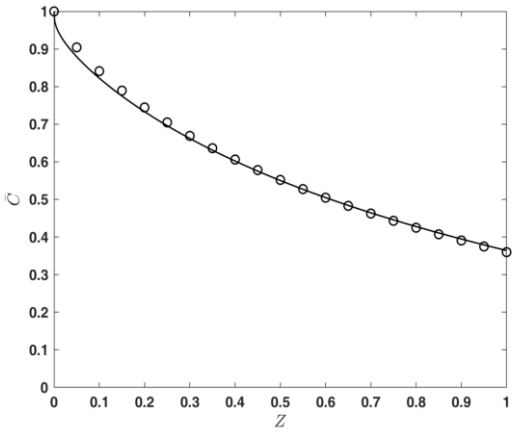

Fig. 4. Average concentrations $\bar{C}(Z)$: "theoretical" values $\bar{C}(Z_n), Z_n=0.1(n+1),\quad n=0,1,...,9$ (points); solution of (18) (lines)

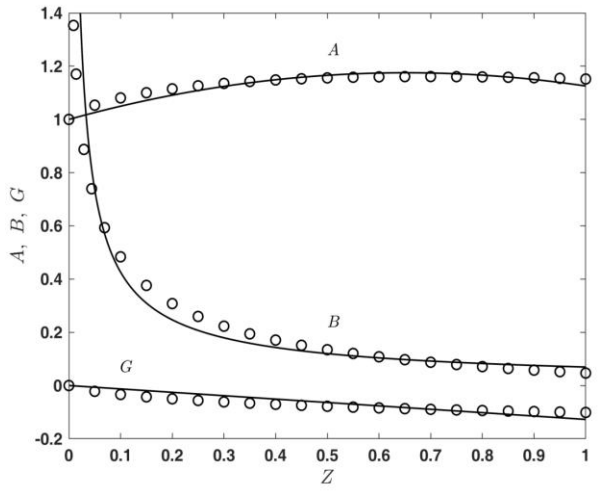

Fig. 5. Functions $A(Z_n)$, $B(Z_n)$ $G(Z_n)$, $Z_n = 0.1(n+1)$, $n = 0,1,\ldots,9$ (points) and their quadratic and linear approximations (17) (lines).

From Fig. 5 is seen, that the functions $A(Z), B(Z), G(Z)$ can be presented as the following approximations:

$$A(Z) = 1 + a_1 Z + a_2 Z^2, \quad B(Z) = b_1 Z^{b_2}, \quad G(Z) = gZ. \tag{17}$$

As a result, the model (16) has the form:

$$\left(1 + a_1 Z + a_2 Z^2\right)\frac{d\bar{C}}{dZ} + \left(b_1 Z^{b_2} + gZ\right)\bar{C} = -\mathrm{Da}\,\bar{C}; \tag{18}$$

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

where the parameters $P(a_1, a_2, b_1, b_2, g)$ must be obtained using experimental data.

Parameters Identification

The value of the function $\bar{C}(1)$ obtained from (7) and (14) permits to obtain the artificial experimental data $\bar{C}^m_{\exp}(1)$ for the column end ($Z = 1$):

$$\bar{C}^m_{\exp}(1) = \left(0.95 + 0.1B_m\right)\bar{C}(1), \quad m = 1,\ldots,10, \tag{19}$$

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

The obtained artificial experimental data (19) can be used for the illustration of the parameters P identification in the average concentrations model (18) by the minimization of the least-squares function:

$$Q(P) = \sum_{m=1}^{10}\left[\bar{C}(1,P) - \bar{C}^m_{\exp}(1)\right]^2, \tag{20}$$

where the values of $\bar{C}(1,P)$ are obtained after the solution of (17) for $Z = 1$.

The obtained ("experimental") parameter values (Table 1) are used for the solution of (18) and the results (lines) are compared with the average "theoretical" concentration values $\bar{C}(Z_n)$, $Z_n = 0.1(n+1)$, $n = 0,1,\ldots,9$ (points) on Fig. 4.

Table 1. Parameters $P(a_1, a_2, b_1, b_2, g)$.

Parameters	"Theoretical" values	"Experimental" values
a_1	0.5373	0.5850
a_2	−0.4118	−0.4226
b_1	0.0695	0.0697
b_2	−0.7878	−0.6726
g	−0.1274	−0.1361

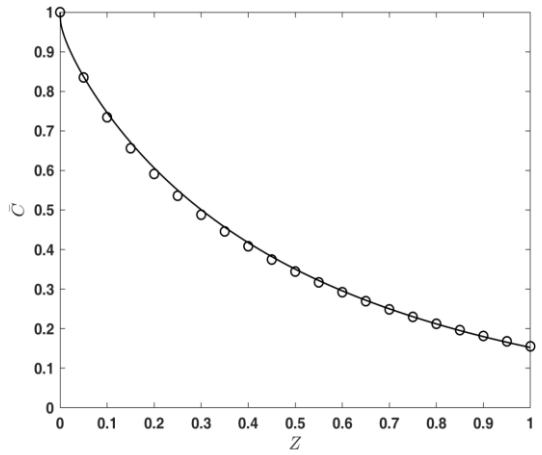

Fig. 6. Average concentrations $\bar{C}(Z)$ for $\mathrm{Da} = 2$: "theoretical" values $\bar{C}(Z_n)$, $Z_n = 0.1(n+1)$, $n = 0,1,\ldots,9$ (points); solution of (18) (lines).

Effect of the Chemical Reaction Rate

The effect of the chemical reaction rate will be obtained in the case when $\mathrm{Da} = 2$ in the models (7) and (18). The solution of (7) and (14) permits to obtain the theoretical values of the average concentration (points), which are compared (Fig. 6) with the solution of the average-concentration model equation (18), where the obtained experimental parameters values (Table 1) are used.

CONCLUSIONS

A new approach for the chemical processes modeling in column apparatuses, is presented in industrial column apparatuses. An exact approach for solutions of the equations in the convective type models is used. The use of experimental data, for the average concentration at the column end, for a concrete process and column, permits to obtain the model parameters related to the radial non-uniformity of the velocity. These parameter values permit to use the average-concentration model for modeling of chemical processes with different reaction rates.

NOTATIONS

$c(r,z)$ − concentration [kg-mol.m^{-3}]

D − diffusivity [m^2.s^{-1}]

$u(r,z)$ − axial velocity component [m.s^{-1}]

$v(r,z)$ − radial velocity component [m.s^{-1}]

(r,z) − radial and axial coordinates [m]

k − chemical reaction rate constant [s^{-1}]

Fo − Fourier number

Da − Damkohler number

Acknowledgements: *this work is supported by the project of fundamental scientific research 19-58-18004, conducted by RFBR and the National Science Fund of Bulgaria under contract no KP 06 RUSIA-3 from 27 Sep. 2019, "Modeling, simulation and experimental investigations of the interphase mass transfer and separation in distillation, absorption, adsorption and catalytic processes in industrial column apparatuses".*

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