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On the scale effect and scale-up in the column apparatuses. 2. Scale effect modeling

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ABSTRACT

The mass transfer with chemical reaction model is investigated. A diffusion type of model is proposed for modeling of the scale effect in column apparatuses, where the velocity and concentration distributions are replaced with theirs average values at the cross-section areas of the column. The obtained results show that scale effect is related with one parameter which is possible to be calculated using experimental data for average concentration at some different points at the column height.

1. Introduction

The theoretical analysis of the mass transfer with volume chemical reaction in the column apparatuses shows [1] that process efficiency decrease as a result of the radial non-uniformity of the velocity distribution. This effect increase with the column radius increase and will be named "scale effect".

In the laboratory column model with small diameters the velocity distribution is almost "plug flow" type practically.

The radial non-uniformity of the velocity distribution as a result of the constructive faults of the column inlet leads to the scale effect in an industrial column.

An improvement in the inlet construction permit to decrease the scale effect but the remainder of scale effect must be predicted in the industrial column model.

The modeling of the scale effect will be made using average concentration models [2].

2. Average concentration model

Let us consider a gas motion in a column with radius r_0 through catalyze particles layer. One of the gas components reacts on the catalytic interface. If the volume concentration of the active sites at the catalytic interface is very big, a volume chemical reaction of first order is possible.

The volume chemical reaction and the non-uniformity of radial velocity distribution lead to convective and diffusion mass transfer, i.e. a convection–diffusion equation with volume reaction can be used for the mathematical description of the process:

$$u\frac{\partial c}{\partial z} = D\left(\frac{\partial^2 c}{\partial z^2} + \frac{1}{r}\frac{\partial c}{\partial r} + \frac{\partial^2 c}{\partial r^2}\right) - kc^n; \quad z = 0, \quad c = c_0,$$

$$\bar{u}c_0 = uc_0 - D\frac{\partial c}{\partial z}; \quad r = 0, \quad \frac{\partial c}{\partial r} = 0; \quad r = r_0, \frac{\partial c}{\partial r} = 0, \tag{1}$$

where deferent velocity distributions presented in [1] are used.

The average velocity and concentration for the cross-section's area of the column [2] are:

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

The velocity $u(r)$ and concentration $c(r,z)$ distributions may be presented by help of the average functions (2):

$$u(r) = \bar{u}\tilde{u}(r), \quad c(r,z) = \bar{c}(z)\tilde{c}(r,z), \tag{3}$$

where for the function of radial non-uniformities $\tilde{u}(r)$, $\tilde{c}(r,z)$ was obtained:

$$\frac{2}{r_0^2}\int_0^{r_0} r\tilde{u}(r)dr = 1, \qquad \frac{2}{r_0^2}\int_0^{r_0} r\tilde{c}(r,z)dr = 1. \tag{4}$$

The average concentration model may be obtained [2] if put Eq. (3) in Eq. (1), multiply with r and integrate over r in the interval $[0, r_0]$:

$$\alpha(r_0,z)\bar{u}\frac{d\bar{c}}{dz} + \frac{d\alpha}{dz}\bar{u}\bar{c} = D\frac{d^2\bar{c}}{dz^2} - k\bar{c}; \quad z = 0, \quad \bar{c} = c_0, \quad \frac{dc}{dz} = 0, \tag{5}$$

where scale effect function $\alpha(r_0,z)$ is result of the velocity and concentration radial non-uniformities:

$$\alpha(r_0,z) = \frac{2}{r_0^2}\int_0^{r_0} r\tilde{u}(r)\tilde{c}(r,z)dr, \quad \alpha(r_0,0) = 1. \tag{6}$$

The function α is possible to be obtained using the solution of the problem (1) in dimensionless variables [1]:

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Nomenclature

u	velocity (m s^{-1})	r_0	column radius (m)
$\bar{u}$	average velocity (m s^{-1})	z	axial coordinate (m)
c	concentration (kg m^{-3})	l	column height (m)
c_0	initial concentration (kg m^{-3})	q	amount of reacted substance (kg m^{-2} s^{-1})
D	diffusivity (m^2 s^{-1})	Fo	Fourier number
k	chemical reaction rate constant (s^{-1})	Da	Damkohler number
r	radial coordinate (m)		

$$r = r_0 R, \quad z = lZ, \quad u(r) = \bar{u}U(R), \quad c(r,z) = c_0 C(R,Z),$$
$$\bar{c}(z) = \bar{c}(lZ) = c_0 \bar{C}(Z), \tag{7}$$

i.e.

$$U\frac{\partial C}{\partial Z} = F_0\left(\beta\frac{\partial^2 C}{\partial Z^2} + \frac{1}{R}\frac{\partial C}{\partial R} + \frac{\partial^2 C}{\partial R^2}\right) - DaC,$$
$$Z = 0, C = 1; \frac{\partial C}{\partial Z} = Pe(U-1); \quad R = 0, \quad \frac{\partial C}{\partial R} = 0; \quad R = 1, \quad \frac{\partial C}{\partial R} = 0, \tag{8}$$

where Fo and Da are similar to the Fourier and Damkohler numbers:

$$Fo = \frac{Dl}{\bar{u}r_0^2}, \quad Da = \frac{kl}{\bar{u}}, \quad \beta = \left(\frac{r_0}{l}\right)^2. \tag{9}$$

Will be investigated [1] different dimensionless velocity distributions in Eq. (8):

$$U_0(R) = 1, \quad U_1(R) = 2 - 2R^2, \quad U_2(R) = 1 + 2R^2 - 3R^4,$$
$$U_3(R) = 1 - 2R^2 + 3R^4, \quad U_4(R) = \frac{3}{2} - R^2.$$

As a result from Eqs. (3) and (7) were obtained:

$$\tilde{u}(r) = U(R), \quad \tilde{c}(r,z) = \frac{C(R,Z)}{\bar{C}(Z)}. \tag{10}$$

If put Eq. (10) in Eq. (6) α is as follow in dimensionless variables:

$$A(Z) = \alpha(r_0, lz) = \frac{2}{\bar{C}(Z)}\int_0^1 RU(R)C(R,Z)dR, \tag{11}$$

where the dimensionless concentration $C(R,Z)$ is solution of Eq. (8) and the average dimensionless concentration $\bar{C}(Z)$ is obtained from:

$$\bar{C}(Z) = 2\int_0^1 RC(R,Z)dR. \tag{12}$$

The values of the average concentration $\bar{C}$ and the scale effect function $A(Z)$ were obtained in the case of $Fo = 0.1$, $Da = 2$ ($r_0 = 0.2$ m) and $Fo = 0.01$, $Da = 2$ ($r_0 = 0.5$ m) (see Fig. 1a and b).

From Fig. 1a and b is seen that the maximal scale effect exist in the cases of a Poiseuille flow ($U = U_1$) while for plug flow ($U = U_0$) the scale effect absent ($\tilde{u} = \tilde{c} = 1$, i.e. $A \equiv 1$). Because of this will be consider the modeling of the Poiseuille flow scale effect only.

The scale effect function is possible to be presented using the linear and quadratic approximation (see Table 1):

$$A(Z) = 1 + aZ,$$
$$A(Z) = 1 + a_1 Z + a_2 Z^2. \tag{13}$$

In Fig. 2a and b are shown the comparison between the function $A(Z)$ and its polynomial (linear and quadratic) approximations.

3. Scale effect modeling

The connection between scale effect and radial velocity non-uniformity shows that the creation of the model which gives radial non-uniformity will allow the modeling of a scale effect, i.e. influence of radius r_0 on α.

The influence of the column radius r_0 on the function $A(z) = \alpha(r_0, lz)$ is a result of the parameter F_0 influence on the solution $C(R,Z)$ (see Eqs. (8), (9), (11)).

Consider the dimensionless form of Eq. (5) using Eq. (7):

$$A(Z)\frac{\partial \bar{C}}{\partial Z} = \frac{1}{Pe}\frac{\partial^2 \bar{C}}{\partial Z^2} - \left(Da + \frac{\partial A}{\partial Z}\right)\bar{C}, \quad Z = 0, \quad \bar{C} = 1; \quad \frac{d\bar{C}}{dZ} = 0, \tag{14}$$

where $Pe = \bar{u}l/D$, i.e. $Pe^{-1} = \beta Fo$.

The models of Eqs. (5) and (13) show that average concentration model is equivalent to the longitudinal diffusion model with volume reaction where the chemical reaction rate is corrected with the effect of the velocity and concentration distributions radial non-uniformity.

The determination of $A(z)$ in polynomial form Eq. (13) permits to obtain the average concentration $\bar{C}(Z,a), \bar{C}(Z,a_1,a_2)$ ($C(Z,a)$, $C(Z,a_1,a_2)$ in Fig. 3a and b) in the column, using Eq. (14). It is compared in Fig. 3a and b with the values for $\bar{C}(Z)$ ($C(Z)$ in Fig. 3a and b) obtained from Eq. (12).

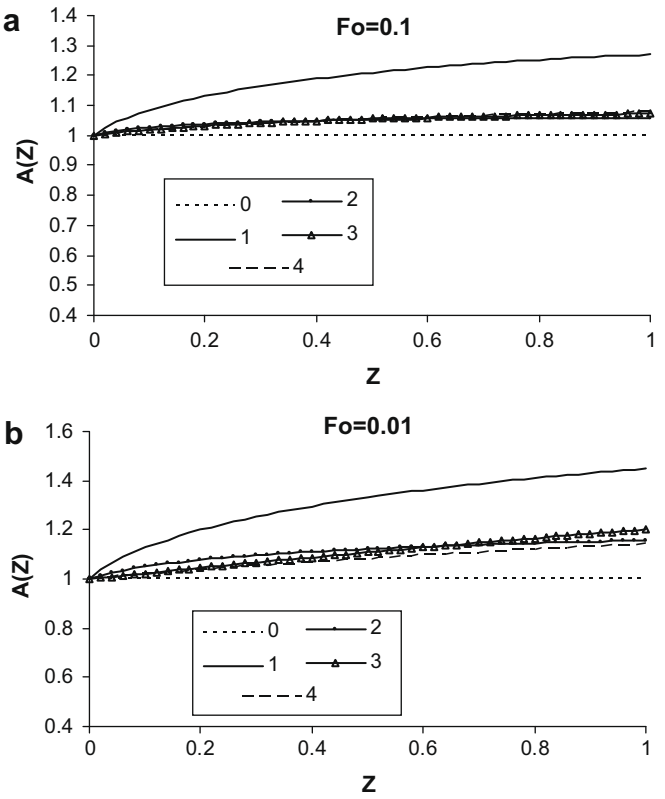

Fig. 1. (a) Scale effect function: 0 – U_0; 1 – U_1; 2 – U_2; 3 – U_3; 4 – U_4. (b) Scale effect function: 0 – U_0; 1 – U_1; 2 – U_2; 3 – U_3; 4 – U_4.

Table 1
Approximation parameters values.

U	U_1
Fo	
0.1	$a = 0.4347$ $a_1 = -0.3732$ $a_2 = 0.6221$
0.01	$a = 0.6778$ $a_1 = -0.5362$ $a_2 = 0.9538$

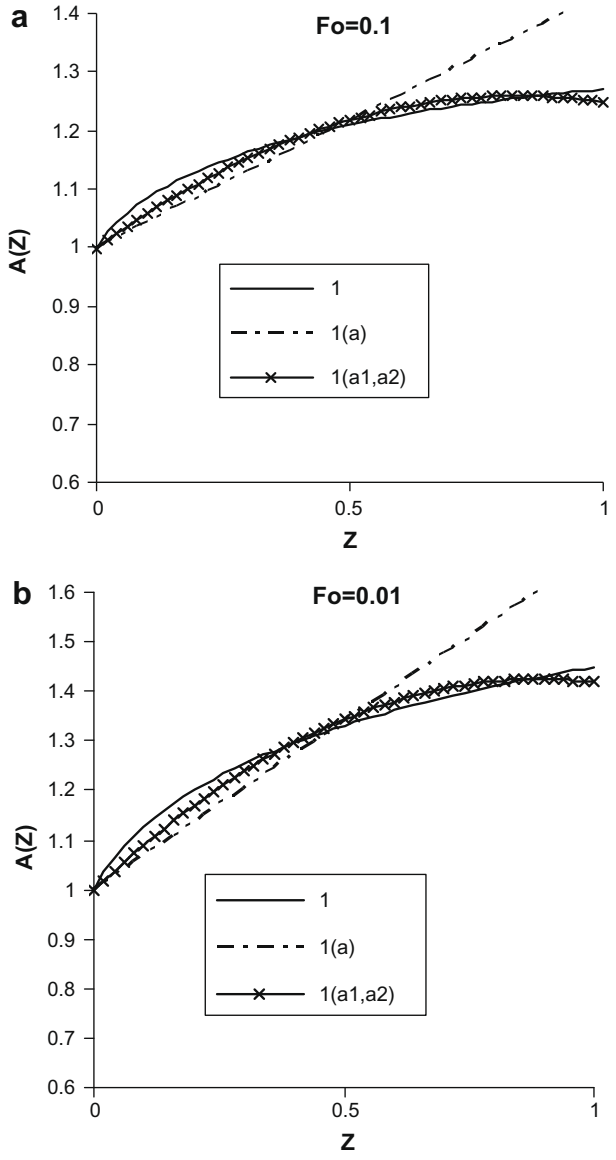

Fig. 2. (a) The comparison between the function $A(Z)$ and its polynomial (linear and quadratic) approximations $1 - U_1$. (b) The comparison between the function $A(Z)$ and its polynomial (linear and quadratic) approximations $1 - U_1$.

4. Parameters identification

The results from Fig. 3 demonstrate the possibility to present the scale effect by one parameter (a).

Let us consider a case of linear approximation for $A(Z)$. As result the Eq. (14) have the form:

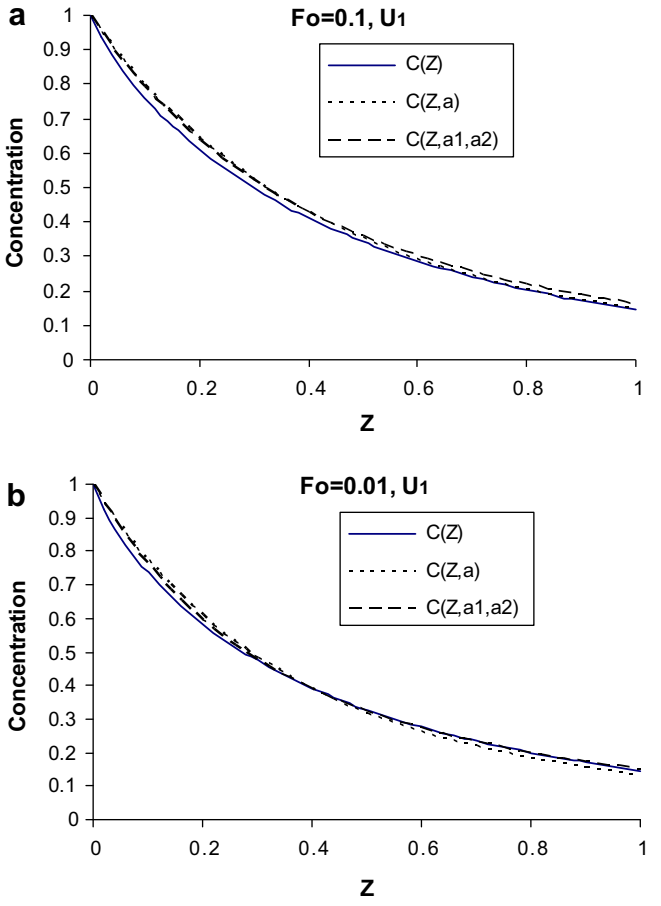

Fig. 3. (a) Comparison between concentration distribution functions calculated for different approximations of the scale effect function $A(Z)$. (b) Comparison between concentration distribution functions calculated for different approximations of the scale effect function $A(Z)$.

$$(1+aZ)\frac{\partial \bar{C}}{\partial Z} = \frac{1}{Pe}\frac{\partial^2 \bar{C}}{\partial Z^2} - (Da+a)\bar{C}; \quad Z=0, \quad \bar{C}=1; \quad \frac{d\bar{C}}{dZ}=0. \tag{15}$$

The identification of the scale effect parameter a using experimental data for the average concentration is possible.

The parameter identification of the model Eq. (15) will be made by minimization of the least square function Φ:

$$\Phi(\alpha) = \sum_{i=1}^{N}\sum_{j=1}^{M}\left[\bar{C}(Z_i) - \bar{C}_{ij}^{\exp}(Z_i)\right]^2. \tag{16}$$

In Eq. (16) $\bar{C}(Z_i)$, $i = 1,\ldots,N$ are calculated values of the average dimensionless concentration using Eq. (14). The concentrations $\bar{C}^{\exp}(Z_i)$, $i = 1,\ldots,N$ are "experimental data" which are obtained using Eq. (12) (where $C(R,Z)$ is exact solution obtained from the model Eq. (8)) and random numbers δ_j ($j = 1\ldots,M$), obtained by generator for random numbers:

$$\bar{C}_{ij}^{\exp}(Z_i) = \bar{C}(Z_i)[0.95+\delta_j], \quad 0 \leqslant \delta_j \leqslant 1, \quad i = 1,\ldots,N, j = 1,\ldots,M \quad (N=10). \tag{17}$$

Table 2
Parameter values a.

Z	0.2	0.4	0.6	0.8	1
Fo					
0.1	$a = -0.573$	$a = 1.3311$	$a = 6.333$	$a = 14.656$	$a = 25.1758$
0.01	$a = -0.537$	$a = 1.4753$	$a = 5.988$	$a = 13.317$	$a = 22.2965$

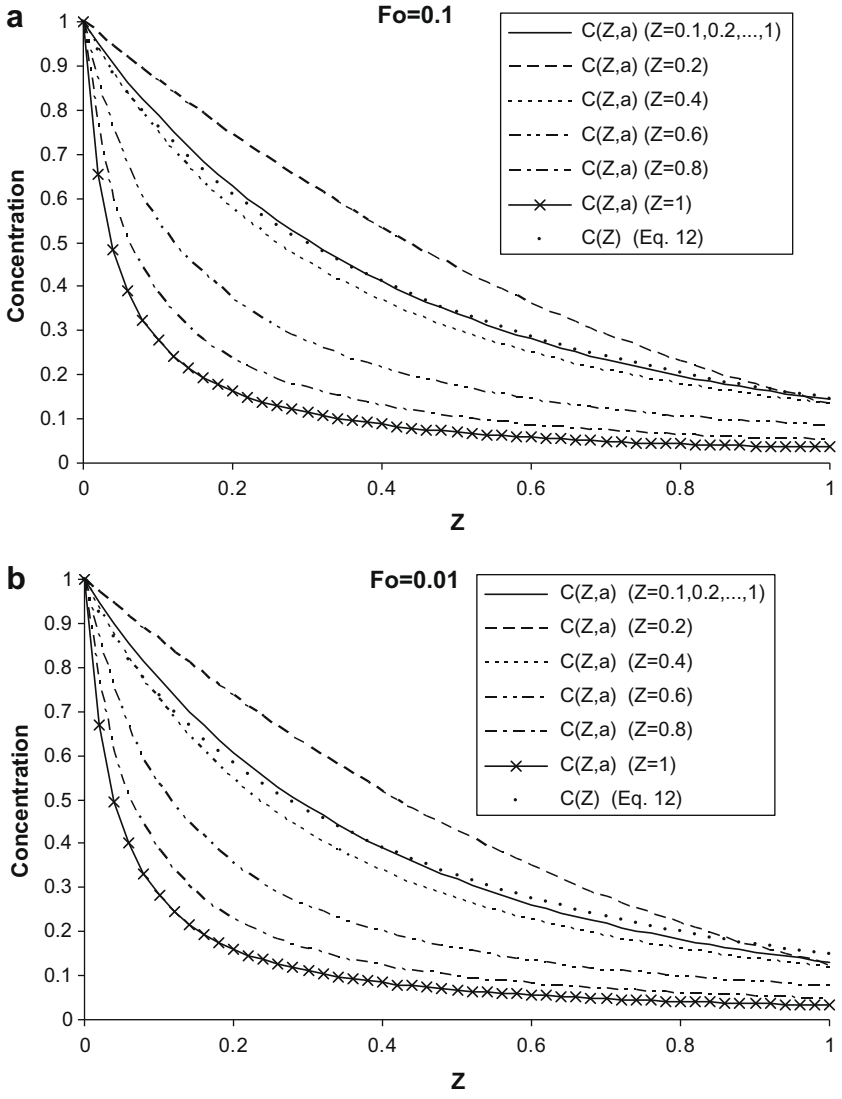

Fig. 4. (a) Comparison between concentration distribution functions calculated for different values of parameter *a*. (b) Comparison between concentration distribution functions calculated for different values of parameter *a*.

Obviously the maximal relative error of "experimental data" is ±5%.

The next calculations are made for the case:

$$Fo = 10^{-1}(Fo = 10^{-2}), \quad Da = 2, \quad Zj = 0.1j, \quad i = j = 1, \ldots, 10 \quad (18)$$

and the values of the parameter a which minimize the least square function Φ (Eq. (16)) are $a = 0.6357$ ($Fo = 0.1$), $a = 0.6773$ ($Fo = 0.01$).

The next cases are parameter identification using ten "experimental data" values in one point only ($Z = 0.2$, 0.4, 0.6, 0.8, 1) (see Table 2).

In Fig. 4a and b are shown concentration distribution functions calculated from Eq. (15), where the parameter a is obtained using ten "experimental data" separate points ($Z = 0.2; Z = 0.4; \ldots; Z = 1$).

5. Conclusions

The obtained results show that scale effect is possible to be presented with one parameter which must be calculated using experimental data for average concentration at some different points at the column height. It gives opportunity to use some different values for average concentration at one point at the middle column height because of this the idea of hydrodynamic modeling [3] to use experimental data of columns with real diameter and small column height will not be realized successfully.

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