ИЗСЛЕДВАНЕ ВЛИЯНИЕТО НА СКОРОСТНИТЕ ПРОФИЛИ ВЪРХУ ЕФЕКТИВНОСТТА НА ПРОЦЕСА И МАЩАБНИЯ ЕФЕКТ ЗА КОЛОННИ АПАРАТА

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INFLUENCE OF THE VELOCITY DISTRIBUTION ON THE PROCESS EFFICIENCY AND SCALE-UP IN COLUMN APPARATUSES

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ABSTRACT

A theoretical analysis of the influence of velocity distribution on the process efficiency and scale-up in column apparatuses is presented. The mass transfer with chemical reaction model is investigated. The influence of the radial non uniformity of the velocity distribution on the mass transfer efficiency, column height and scale-up is obtained.

Key words: column apparatuses, mass transfer, velocity distribution

INTRODUCTION

A chemical engineer is generally concerned with the industrial implantation of processes in which the chemical or microbiological conversion of material takes place in conjunction with the transfer of mass, heat, and momentum. These processes are scale-dependent, i.e., they behave differently on a small scale (in laboratories or pilot plant) than they do on a large scale (in production). Also included are heterogeneous chemical reactions and most unit operations. Understandably, chemical engineers have always wanted to find ways of simulating these processes in models in order to gain knowledge which will then assist in designing new industrial plants. Occasionally, they are faced with the same problem for another reason: an industrial facility already exists but does not function properly, if at all, and suitable measurements have to be carried out in order to discover the cause of these difficulties as well to provide a solution [1]. Many experimental data show [2] that mass transfer efficiency in column apparatuses decreases with the column diameter increase. The theory of scale-up [1-3] explains this scale effect as a result of the velocity distribution radial non-uniformity for the cross-section's area of the column. A theoretical analysis of this effect is possible on the base of convection-diffusion equation with volume reaction [4, 5]. The convective transfer in the column apparatuses is result of a laminar or turbulent (large-scale pulsations) flows. The diffusive transfer is molecular or turbulent (small – scale pulsations). The volume reaction is mass source as a result of chemical reactions or interphase mass transfer.

MATHEMATICAL MODEL

Let's consider gas motion in the column with radius r_0 through catalyze particles layer. One of the gas components reacts on 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 radial velocity distribution non-uniformity lead to convective and diffusion mass transfer i.e. a convection-diffusion equation with volume reaction can be used for mathematical description of the process:

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

where $u(r)$ and $c(r, z)$ are velocity and concentration distribution in the column.

The radial gas velocity component is equal to zero if the catalytic particle distribution in the column is uniform. The volume reaction rate is obtained using the surface catalytic reaction rate and specific catalytic particles surface.

The boundary conditions are the inlet concentration (c_0) and mass balance of the active gas component:

$$z = 0, \quad c = c_0, \quad \bar{u}c_0 = uc_0 - D\frac{\partial c}{\partial z},$$
$$r = 0, \quad \frac{\partial c}{\partial r} = 0; \quad r = r_0, \quad \frac{\partial c}{\partial r} = 0, \qquad (2)$$

where $\bar{u}$ is the average velocity at the cross-section area of the column.

In Eq.(2) is supposed that a symmetric radial velocity distribution will leads to symmetric concentration distribution too.

The velocity distribution in the column will be used by expression:

$$u(r) = 2 + a_i\frac{r^2}{r_0^2} + b_i\frac{r^4}{r_0^4}, \qquad (3)$$

which permits to obtain velocity distributions with different radial non-uniformities for $i=1, 2$:

$$a_1 = 0.8, \qquad b_1 = -1 ;$$
$$a_2 = -0.8, \qquad b_2 = 1. \qquad (4)$$

In (3) for average velocity is used

$$\bar{u} = \frac{2}{r_0^2}\int_0^{r_0} ru(r)dr = 2 + \frac{a_i}{2} + \frac{b_i}{3}, \quad i = 1,2. \qquad (5)$$

As a mass transfer efficiency of the column will be used the amount of the reacted substance (q), i.e. the difference between inlet and outlet convective mass flow:

$$q = \bar{u}c_0 - \frac{2}{r_0^2}\int_0^{r_0} r\,u\,c(r,l)dr, \qquad (6)$$

where l is the column height (catalytic layer thickness).

DIMENSIONLESS PROBLEM SOLUTION

The solution of the problem Eqs.(1, 2) permits to obtain the mass transfer efficiency q in the column under the influence of the velocity distribution radial non-uniformity ε. For this purpose must be used dimensionless variables:

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

If put Eq. (7) in Eqs. (1, 2) the dimensionless problem has the form:

$$U\frac{\partial C}{\partial Z} = Fo\left(\beta\frac{\partial^2 C}{\partial Z^2} + \frac{1}{R}\frac{\partial C}{\partial R} + \frac{\partial^2 C}{\partial R^2}\right) - DaC,$$

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

$$R = 0, \quad \frac{\partial C}{\partial R} = 0; \quad R = 1, \quad \frac{\partial C}{\partial R} = 0, \tag{8}$$

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

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

The parameter β is small ($\beta << 1$) and the solution of (8) is possible to obtain using a perturbation method [5]:

$$C(R,Z) = C_0(R,Z) + \beta C_1(R,Z) + \beta^2 C_2(R,Z) + ..., \tag{10}$$

where C_0 , C_1 and C_2 are solutions of the problems:

$$U\frac{\partial C_0}{\partial Z} = Fo\left(\frac{1}{R}\frac{\partial C_0}{\partial R} + \frac{\partial^2 C_0}{\partial R^2}\right) - DaC_0,$$

$$Z = 0, \quad C_0 = 1; \; R = 0, \quad \frac{\partial C_0}{\partial R} = 0; \quad R = 1, \quad \frac{\partial C_0}{\partial R} = 0; \tag{11}$$

$$U\frac{\partial C_i}{\partial Z} = Fo\left(\frac{\partial^2 C_{i-1}}{\partial Z^2} + \frac{1}{R}\frac{\partial C_i}{\partial R} + \frac{\partial^2 C_i}{\partial R^2}\right) - DaC_i,$$

$$Z = 0, \quad C_i = 1; \; R = 0, \quad \frac{\partial C_i}{\partial R} = 0; \quad R = 1, \quad \frac{\partial C_i}{\partial R} = 0, \quad i = 1,2. \tag{12}$$

The solution of the problem (8) (or equations set (11, 12)) permits to obtain the relative mass transfer efficiency of the column (degree of the conversion):

$$Q = \frac{q}{\bar{u}c_0} = 1 - 2\int_0^1 R\,U(R)C(R,Z)dR. \tag{13}$$

VELOCITY AND CONCENTRATION DISTRIBUTIONS

The dimensionless velocity distribution in (8) has the form:

$$U(R) = c_i + d_i R^2 + e_i R^4. \tag{14}$$

On the Fig. 1 are shown velocity distributions for different values of c_i ,d_i and e_i (c_1=0.9677, d_1=0.3871, e_1=*-0.4839* and c_2=1.0345, d_2=-0.4138 e_2=0.5173) .

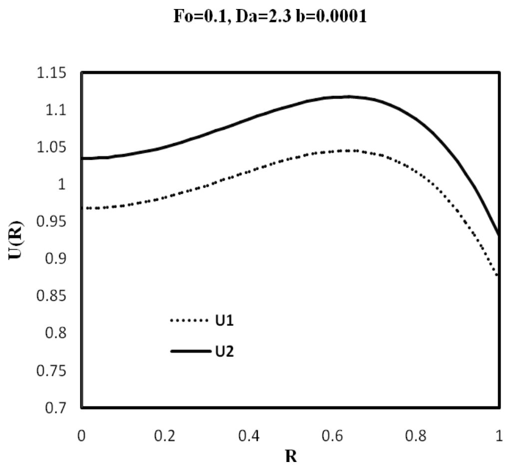

Fig. 1 Velocity distributions

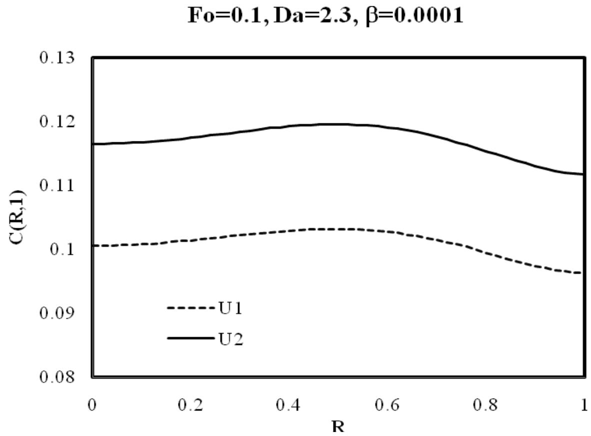

Fig. 2. Concentration distributions

After the solutions of Esq. (11, 12) for *Fo=0.1, Da=2.3, β=0.0001* the concentration distributions are shown on the Fig.2.

EFFECT OF THE VELOCITY NON UNIFORMITY

Let consider the concrete process:

$$\beta = 0.01, \qquad Fo = 0.1, \qquad Da = 2.3 . \tag{15}$$

If put Eq. (15) in Eqs. (11, 12) the solution of the problem permits to obtain the effect of the velocity radial non uniformity (ε) on the process efficiency (Q) (see Fig. 3).

Let denote Q_1 and Q_2 process efficiency for U_1 and U_2, *(Z=0.8)* respectively. From Fig.3 can see the effect ΔQ of the velocity non uniformity on the process efficiency:

$$\Delta Q = \frac{Q_1 - Q_2}{Q_2} = 0.0400 . \tag{16}$$

If denote on the Fig.3 $Z=H_1$ and $Z=H_2$ the column height for U_1 and U_2, *(Q=0.8)*, the effect (ΔH) of the velocity non uniformity (ε) on the column height is:

$$\Delta H = \frac{H_2 - H_1}{H_1} = 0.1111 . \tag{17}$$

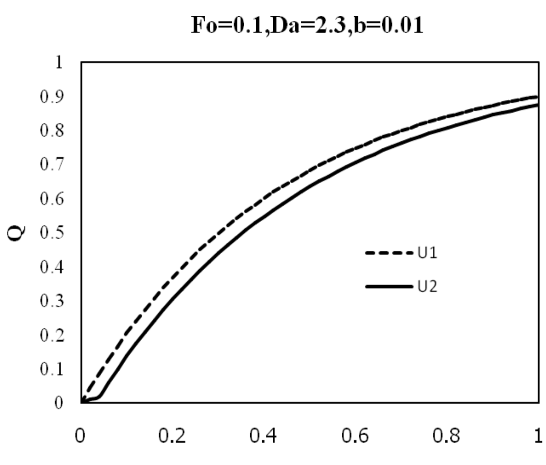

Fig. 3. Process efficiency for different velocity radial non uniformity

SCALE EFFECT

Let consider "model" column (*Da=2.3, Fo=0.1,* β*=0.0001* and r_0*=0.1m*) and "industrial" column (*Da=2.3, Fo=0.001*, β*=0.01* and r_0*=1m*) where the ratio of its diameters is 0.1. On the Figs. 4, 5 are shown "model" and "industrial" column efficiency. The scale effect on the efficiency

$$\Delta Q_{scal} = \frac{Q_{\mathrm{mod}} - Q_{ind}}{Q_{ind}}.100\% \qquad (18)$$

is shown on the Fig.6.

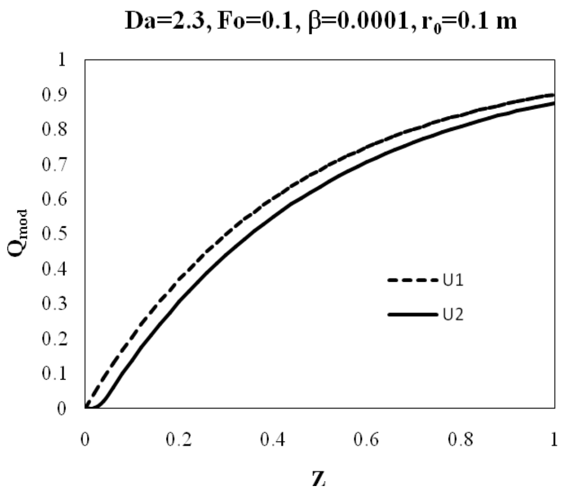

Fig. 4 "Model" column efficiency

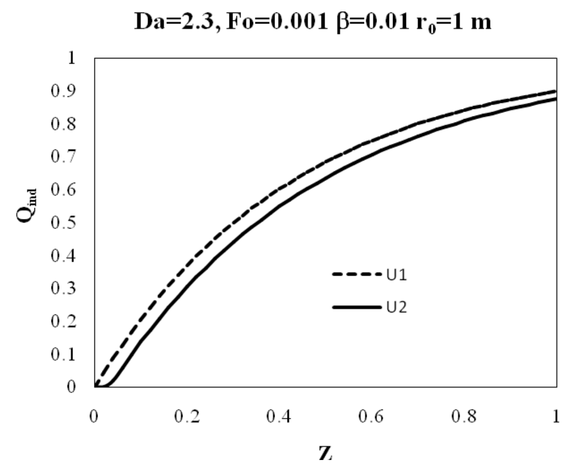

Fig. 5"Industrial" column efficiency

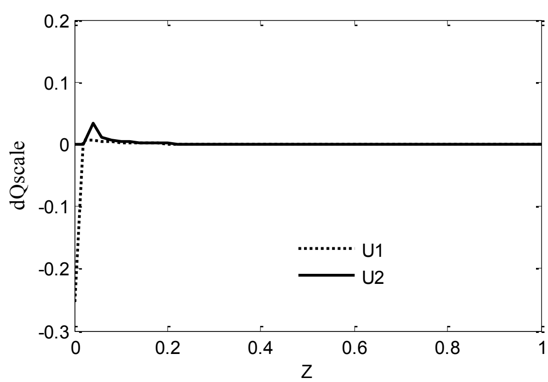

Fig.6. Scale effect on the column efficiency

The comparison between these two columns on the bases of (16) (ΔQ_{mod}, ΔQ_{ind}) and (17) (ΔH_{mod}, ΔH_{ind}) shows

ΔQ_{mod}=2.98%, ΔQ_{ind}=4.01%,

ΔH_{mod} =11.43% ΔH_{ind}=11.11%

i.e. the scale – up leads to decrease of the column efficiency (for constant column height) and increase the column height (for constant column efficiency).

CONCLUSIONS

The results obtained show that in the cases of plug flow the column radius do not influence the process efficiency (the curves in Figs. 4, 5 are identical).

The scale effect is result of the radial non uniformity of the velocity distribution.

The process efficiency decreases in the 'model' column (2.98%) from $Q_{mod}=0.8167\ (U_2)$ to $Q_{mod}=0.8410\ (U_1)$ for $Z=0.8$ as a result of the velocity radial non uniformity and to $Q_{ind}=0.8167(U_2)$ in the 'industrial' column (4.01%) as a result of the radius increase (from $0.1m$ to $1m$).

At the same conditions the column height increases (11.43%) from $H_{mod}=0.7\ (U_1)$ to $H_{mod}=0.78\ (U_2)$ for $Q_{mod}=0.8$ for the 'model' column and to $H_{ind}=0.8(U_2)$ for the 'industrial' column (11.11%).

In many cases the radial velocity distribution in 'model' column is almost uniform and all scale effect is 'concentrated' in the 'industrial' column. That is why the scale-up problem solution [1, 2] has two steps:

- a decrease of the scale effect as a result of the radial velocity non uniformity decrease using different devices at the column inlet;
- calculation (modeling) of the scale effect remainder.

The solution of the second problem must use diffusion type of model.

NOMENCLATURE

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

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