International Journal of Heat and Mass Transfer 52 (2009) 543–547

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

On the scale effect and scale-up in the column apparatuses 1. Influence of the velocity distribution

K. Panayotova [a], M. Doichinova [b], Chr. Boyadjiev [b,*]

[a] Assen Zlatarov University, 1, Prof. Yakimov Bulv., Bourgas, Bulgaria
[b] Institute of Chemical Engineering, Bulgarian Academy of Sciences, Acad. St. Angelov street, Bl. 103, 1113 Sofia, Bulgaria

ARTICLE INFO

Article history:
Received 7 July 2008
Available online 6 September 2008

Keywords:
Column apparatuses
Mass transfer
Velocity distribution
Scale-up

ABSTRACT

A diffusion type of model is proposed for modeling of the scale effect in column apparatuses. 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. The effect of Fourier and Damkohler numbers on the process efficiency is analyzed. The present data show that mass transfer efficiency in column apparatuses decreases with the column diameter increase.

1. Introduction

The analysis of Rozen et al. [1] about the influence of the column size on the mass transfer efficiency shows that the process efficiency in column apparatuses decreases with the increase of column diameter. This scale-up effect is a result of the radial non-uniformity of the velocity distribution. The early paper from Boyadjiev [2] proposes a diffusion type of model for modeling this effect. For this purpose a convection-diffusion equation with volume reaction is used, where the convective transfer in the column apparatuses is a result of laminar or turbulent (large-scale pulsations) flows, while the diffusive transfer is molecular or turbulent (small-scale pulsations). The volume reaction is mass source (sink) as a result of chemical reactions or interphase mass transfer. This approach was used for modeling of airlift reactors [3,4] and an airlift photobioreactor by Boyadjiev and Merchuk [5].

2. Mathematical model

Let's 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:

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

where $u(r)$ and $c(r,z)$ are velocity and concentration distributions 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 $v = kc$ (mol m^{-3} s^{-1}) is obtained using the surface catalytic reaction rate v_s (mol m^{-2} s^{-1}) and the specific catalytic particles surface a (m^2 m^{-3}), i.e. $v = av_s$.

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

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

where ū is the average velocity at the cross-sections area of the column.

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

Different expressions for the velocity distribution in the column apparatuses permit the influence of the velocity distributions radial non-uniformities on the process efficiency to be analyzed:

$$u_n(r) = \bar{u}\left(\frac{n+1}{n} - \frac{2}{n}\frac{r^2}{r_0^2}\right), \quad n = 1, 2, \infty,$$
$$u_i(r) = \bar{u}\left(1 + a_i\frac{r^2}{r_0^2} + b_i\frac{r^4}{r_0^4}\right), \quad i = 1, 2, \quad (3)$$

where $n = 1$ (Poiseuille flow), $n = 2$, $n \to \infty$ (plug flow), $a_1 = 2$, $b_1 = -3$, $a_2 = -2$, $b_2 = 3$.

* Corresponding author.
E-mail address: chboyadj@bas.bg (Chr. Boyadjiev).

0017-9310/$ - see front matter © 2008 Elsevier Ltd. All rights reserved.
doi:10.1016/j.ijheatmasstransfer.2008.07.011

Nomenclature

u	Velocity (m s^{-1})	z	Axial coordinate (m)
$\bar{u}$	Average velocity (m s^{-1})	l	Column height (m)
c	Concentration (kg m^{-3})	q	Amount of reacted substance (kg m^{-2} s^{-1})
c_0	Initial concentration (kg m^{-3})	Fo	Fourier number
D	Diffusivity (m^{2}s^{-1})	Da	Damkohler number
k	Chemical reaction rate constant (s^{-1})	Q	Process efficiency
r	Radial coordinate (m)		
r_0	Column radius (m)		

The amount reacted substance will be used to determine the mass transfer efficiency of the column (q), i.e. the difference between the inlet and outlet average convective mass flux:

$$q = \bar{u}c_0 - \frac{2}{r_0^2}\int_0^{r_0} r\,u\,c(r,l)\mathrm{d}r, \quad \bar{u} = \frac{2}{r_0^2}\int_0^{r_0} r\,u(r)\mathrm{d}r, \tag{4}$$

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

3. 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. For this purpose dimensionless variables are used:

$$r = r_0R, \quad z = lZ, \quad u(r) = \bar{u}U(R), \quad c(r,z) = c_0C(R,Z). \tag{5}$$

Introducing Eq. (5) into Eqs. (1), (2), the dimensionless problem has the form:

$$U\frac{\partial C}{\partial Z} = Fo\left(\beta\frac{\partial^2 C}{\partial Z^2} + \frac{1}{R}\frac{\partial C}{\partial R} + \frac{\partial^2 C}{\partial R^2}\right) - DaC,$$
$$Z = 0, \quad C = 1; \quad 1 = U - \frac{1}{Pe}\frac{\partial C}{\partial Z},$$
$$R = 0, \quad \frac{\partial C}{\partial R} = 0; \quad R = 1, \quad \frac{\partial C}{\partial R} = 0, \tag{6}$$

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

$$Fo = \frac{Dl}{\bar{u}r_0^2}, \quad Da = \frac{kl}{\bar{u}}, \quad \beta = \left(\frac{r_0}{l}\right)^2. \tag{7}$$

The parameter β is small and the solution of (6) is possible to be obtained in the approximation $0 = \beta < 10^{-2}$:

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

The numerical solution of the problem (8) permits to obtain the relative mass transfer efficiency of the column (degree of the conversion):

$$Q = \frac{q}{\bar{u}c_0} = 1 - 2\int_0^1 RU(R)C_0(R,Z)\mathrm{d}R. \tag{9}$$

4. Velocity and concentration distributions

The dimensionless velocity distributions in (8) have the form:

$$U_0(R) = 1, \quad U_1(R) = 2 - 2R^2, \quad U_2(R) = 1 + 2R^2 - 3R^4,$$
$$U_3(R) = 1 - 2R^2 + 3R^4, \quad U_4(R) = \frac{3}{2} - R^2. \tag{10}$$

The differences between maximal and minimal velocity values $\Delta U_j = U_j^{\max} - U_j^{\min} (j = 1,\ldots,4)$ are the velocity distribution radial non-uniformity parameters ($\Delta U_1 = 2, \Delta U_2 = \Delta U_3 = \frac{4}{3}, \Delta U_4 = 1$).

On Fig. 1 are shown the velocity distributions U_j, $j = 0,\ldots,4$.

The solutions of the problem (8) for $Fo = 0.1$, $Da = 2$ for different velocity distributions are shown on Fig. 2.

5. Effect of the velocity distribution non-uniformity on the process efficiency

The numerical simulation based on the mathematical model (8), using different velocity profiles Eq. (10) gives the effect of the velocity radial non-uniformity on the process efficiency Q-Eq. (9) (see Fig. 3). The values of Q at $Z = 1$, $Da = 2$ are shown in Table 1.

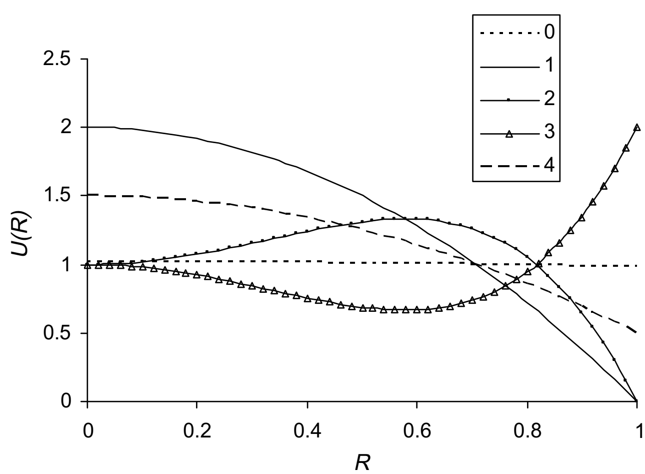

Fig. 1. Velocity distributions: 0-U_0; 1-U_1; 2-U_2; 3-U_3; 4-U_4.

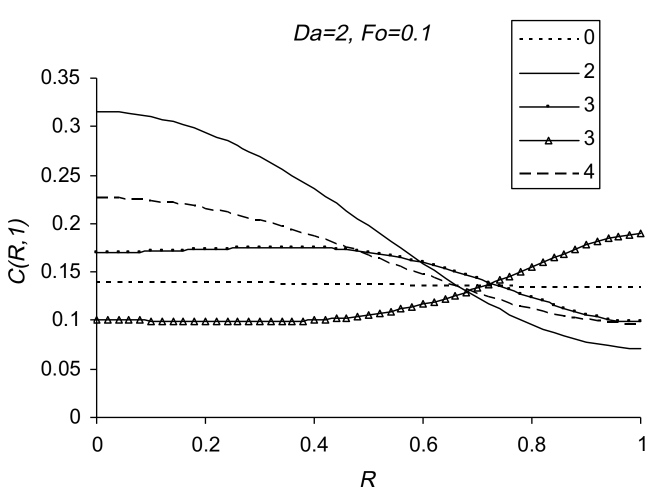

Fig. 2. Concentration distributions using the four velocity profiles: 0-U_0; 1-U_1; 2-U_2; 3-U_3; 4-U_4.

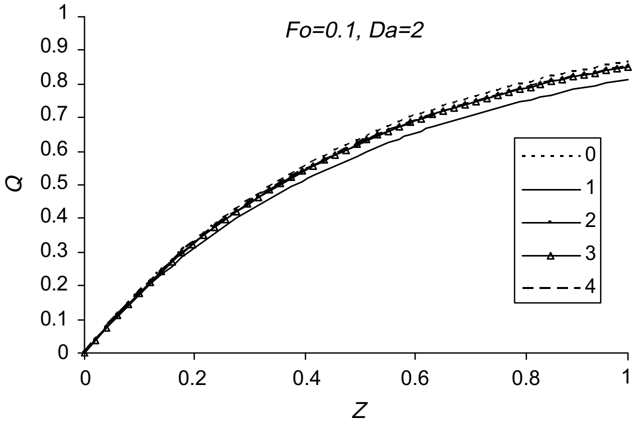

Fig. 3. Process efficiency for different velocity radial non-uniformity: 0-U_0; 1-U_1; 2-U_2; 3-U_3; 4-U_4.

Table 1
Process efficiency Q at $Z = 1$ and column height $H = Z$ at $Q = 0.8643$

Fo	U_0	U_1	U_2	U_3
0.1	$Q_0 = 0.8643$	$Q_1 = 0.8143$	$Q_2 = 0.8516$	$Q_3 = 0.8513$
Laboratory	$H_0 = 1$	$H_1 = 1.2$	$H_2 = 1.05$	$H_3 = 1.05$
0.01	$Q_0 = 0.8645$	$Q_1 = 0.7870$	$Q_2 = 0.8349$	$Q_3 = 0.8371$
Industrial	$H_0 = 1$	$H_1 = 1.34$	$H_2 = 1.12$	$H_3 = 1.12$

Table 2
Effect of the velocity radial non-uniformity on the process efficiency and column height

Fo	U_1	U_2	U_3
0.1	$\Delta Q_1 = 6\%$	$\Delta Q_2 = 1.4\%$	$\Delta Q_3 = 1.5\%$
Laboratory	$\Delta H_1 = 20\%$	$\Delta H_2 = 5\%$	$\Delta H_3 = 5\%$
0.01	$\Delta Q_1 = 9.8\%$	$\Delta Q_2 = 3.5\%$	$\Delta Q_3 = 3.3\%$
Industrial	$\Delta H_1 = 34\%$	$\Delta H_2 = 12\%$	$\Delta H_3 = 12\%$

Let's consider the effect of the velocity radial non-uniformity on the process efficiency decrease (in comparison with the plug flow):

$$\Delta Q_j = \frac{Q_0 - Q_j}{Q_j} \times 100\%, \quad j = 1, \ldots, 4. \tag{11}$$

The results obtained show (see Table 2) the influence of the increasing of the column radius and the velocity distribution radial non-uniformity parameter.

If consider the column heights H_j ($j = 1,\ldots,4$) for column efficiency $Q_0 = 0.8643$, $Fo = 0.1$ and $Da = 2$, i.e. the necessary column heights H_j ($j = 1,\ldots,4$) for to be realized the plug flow column efficiency. The results obtained show an increasing of the column heights (see Table 1) as a result of the velocity radial non-uniformity. The *relative column height increase* ΔH_j is possible to be obtained from:

$$\Delta H_j = \frac{H_j - H_0}{H_0} \times 100\%, \quad j = 1, \ldots, 4. \tag{12}$$

The numerical results (Table 2) show the necessity of an essential augmentation of the column height for to compensate the velocity distribution radial non-uniformity effect.

The comparison of the results in the last two tables show, that the effects of ΔU_2 and ΔU_3 are similar, i.e. the velocity distribution radial non-uniformity effects are caused from the *velocity non-uniformity* $\Delta U_j = U_j^{\max} - U_j^{\min} (j = 1, \ldots, 4)$, but not from the *velocity distribution* U_j, ($j = 1, \ldots, 4$).

6. Effect of Fourier and Damkohler numbers

The solution of problem (8) for $Z = 0.5$, $Da = 2$ for different values of Fourier number permits to obtain the Fourier number effect (Fig. 4).

Damkohler number effect is shown on the Fig. 5 ($Z = 0.5$, $Fo = 0.1$).

7. Scale effect

Let's consider a laboratory column ($Da = 2$, $Fo = 0.1$, $r_0 = 0.2$ m) and an industrial column ($Da = 2$, $Fo = 0.01$, $r_0 = 0.5$ m). On the Figs. 6,7 are shown the laboratory and industrial column efficiency. The scale effect on the efficiency $Q^{scale-up}$

$$\Delta Q_j^{\text{scale-up}} = \frac{Q_j^{\text{lab}} - Q_j^{\text{ind}}}{Q_j^{\text{ind}}} \times 100\%, \quad j = 1, 2, 3 \tag{13}$$

can be obtained using Table 1. The results are presented in Table 3 and Fig. 8.

The comparison between these two columns on the basis of Eq. (11) (ΔQ^{lab}, ΔQ^{ind}) and Eq. (12) (ΔH^{lab}, ΔH^{ind}) shows that the scale-up leads to a decrease of the column efficiency (for constant column height). If consider columns with a constant process efficiency, that leads to column height increase as result of the radius increase.

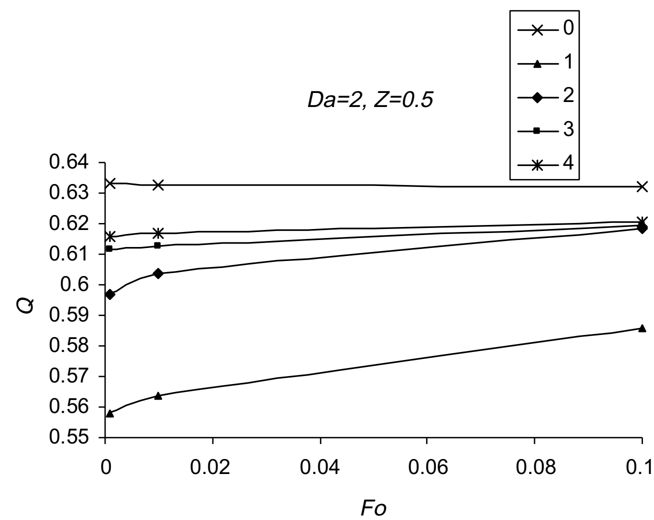

Fig. 4. Fourier number effect for different velocity profiles: 0-U_0; 1-U_1; 2-U_2; 3-U_3; 4-U_4.

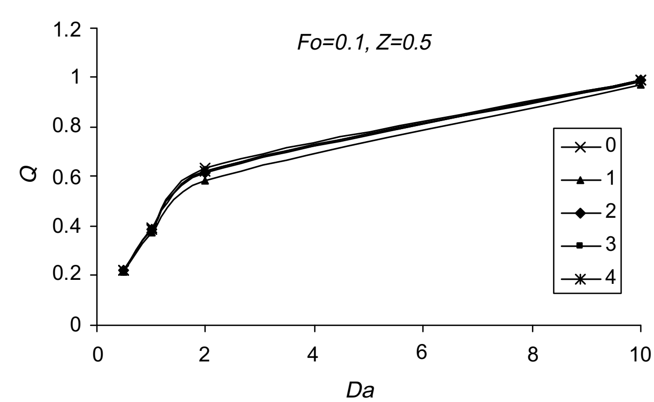

Fig. 5. Damkohler number effect for different velocity profiles: 0-U_0; 1-U_1; 2-U_2; 3-U_3; 4-U_4.

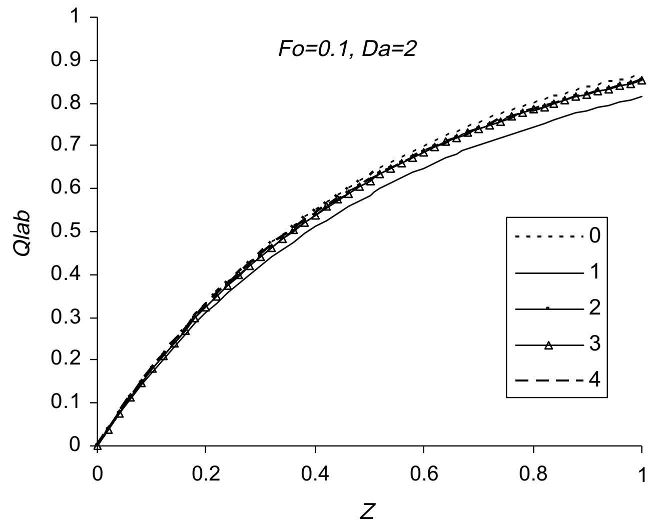

Fig. 6. Laboratory column efficiency for different velocity profiles: 0-U_0; 1-U_1; 2-U_2; 3-U_3; 4-U_4.

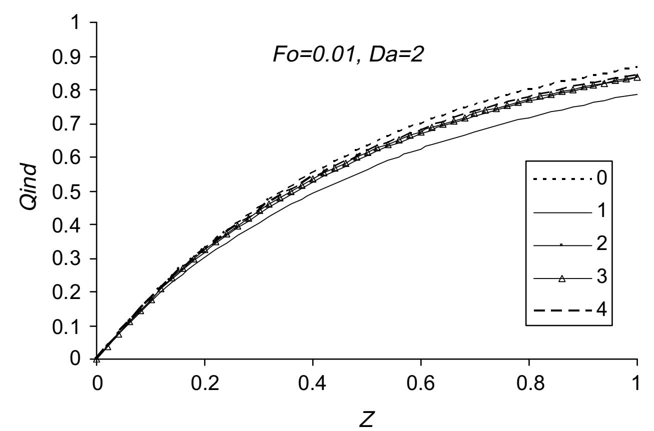

Fig. 7. Industrial column efficiency for different velocity profiles: 0-U_0; 1-U_1; 2-U_2; 3-U_3; 4-U_4.

Table 3
Comparison of the scale effect between different velocity profiles

	U_1	U_2	U_3
$\Delta Q^{\text{scale-up}}$	3.5%	1.9%	1.7%
$\Delta H^{\text{scale-up}}$	11.6%	6.6%	6.6%

The scale effect on the column height (at $Q = Q_0 = 0.8643$) is possible to be obtained using the values from Table 2:

$$\Delta H_j^{\text{scale-up}} = \frac{H_j^{\text{ind}} - H_j^{\text{lab}}}{H_j^{\text{lab}}} \times 100\%, \quad j = 1, 2, 3$$

and the results are shown in Table 3.

8. Results and discussion

In this study a convection-diffusion equation for the description of mass transfer processes in column apparatuses in the case of volume chemical reaction is used. Four different velocity distributions in the column are analyzed. Influence of the velocity distribution radial non-uniformity on the process efficiency is investigated.

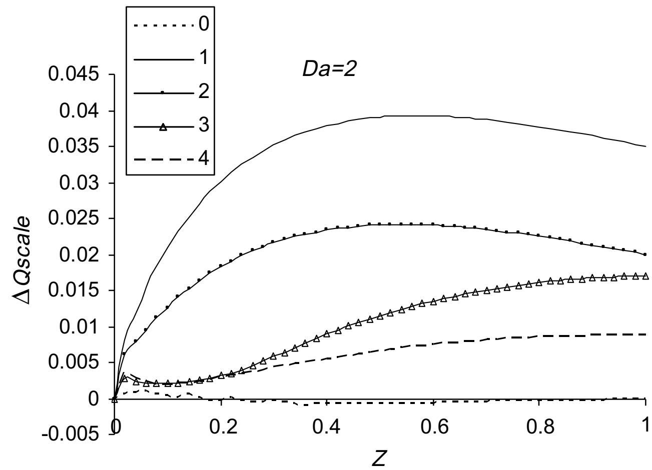

Fig. 8. Scale effect on the column efficiency for different velocity profiles: 0-U_0; 1-U_1; 2-U_2; 3-U_3; 4-U_4.

The presented data in Table 1 show that process efficiency of four of the velocity distributions is smaller than in case of plug flow (Q_0). It means that the process efficiency decrease as a result of radial non-uniformity of the velocity distribution. In Fig. 5 the influence of the Damkohler number on the process efficiency is noticed and the increase of the process efficiency when the volume chemical reaction rate increases can be seen.

Based on the numerical investigation it is shown (see Tables 1 and 2) that the process efficiency in the cases of different velocity distribution in a column with constant height decreases (6%) from $Q_0 = 0.8643$ to $Q_1 = 0.8145$ at $Z = 1$, $Fo = 0.1$ and it is due to the radial velocity non-uniformity. On the other hand the process efficiency at $Z = 1$,$Fo = 0.01$,$Q_1 = 0.7870$ (9.8%) decreases too, but as a result of the radius increase (from 0.2m to 0.5m). The influence of the radius on the process efficiency is demonstrated in Fig. 4, where the Fourier number effect is shown. As it is well seen the process efficiency decreases with the radius increase and the process efficiency in plug flow case is higher.

In addition the case of the process efficiency with constant value $Q_0 = 0.8643$ ($Fo = 0.1$ reached at $H_0 = 1$ ($Z = 1$)) at different column height is considered and the same value of the process efficiency for different velocity distribution is reached at $H_3 = 1.05$, $H_1 = 1.2$. It means that the column height depends on the radial non-uniformity of the velocity distribution (see Tables 1 and 2). The column height increases when radius of the column ($Fo = 0.01$) increases too.

9. Conclusion

This paper presents a theoretical analysis of the influence of velocity distribution on the process efficiency and scale-up in column apparatuses. The presented data show that process efficiency decreases as a result of the radial non-uniformity of the velocity distribution. This effect increases with the increase of column radius and will be named ‘scale effect’. The next work on the process efficiency will be connected with creation of a procedure for predicting of this effect. Therefore diffusion type of model will be used for the modeling of scale effect remainder.

Acknowledgement

This work was completed with the financial support of the National Science Fund, Ministry of Education and Science, Republic of Bulgaria, under Contract 1 TH-1506/2005.

References

[1] A.M. Rozen et al., Scale-up in Chemical Technology, A.M. Rozen, (Ed.), Chemistry, Moscow, 1980.
[2] Chr. Boyadjiev, Diffusion models and scale-up, Int. J. Heat Mass Tran. 49 (2006) 796–799.
[3] Chr. Boyadjiev, On the modeling of an air lift reactor, Int. J. Heat Mass Tran. 49 (2006) 2053–2057.
[4] Chr. Boyadjiev, Diffusion model of an airlift three-phase catalytic reactor and scale-up, Theor. Found. Chem. Eng. 40 (2006) 633–638.
[5] Chr. Boyadjiev, J. Merchuk, On the modeling of an airlift photobioreactor, J. Eng. Thermophys. 17 (2008) 134–141.