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The Simulation of Multicomponent Sorption Processes with Axial Diffusion

Awad R. Mansour[a]
[a] CHEMICAL ENGINEERING DEPARTMENT JORDAN UNIVERSITY OF SCIENCE & TECHNOLOGY, IRBID, JORDAN

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The Simulation of Multicomponent Sorption Processes with Axial Diffusion

AWAD R. MANSOUR

CHEMICAL ENGINEERING DEPARTMENT
JORDAN UNIVERSITY OF SCIENCE & TECHNOLOGY
IRBID, JORDAN

Abstract

A generalized complex model has been developed to numerically simulate multicomponent adsorption kinetics of binary and ternary systems. The model takes into account fluid resistance, internal and external diffusion resistances with axial diffusion, and a highly nonlinear equilibrium isotherm. Excellent agreement with previously published experimental data with and without axial diffusion has been obtained. The general computer program developed in this study can be accurately used for any number of components in any complex multicomponent sorption studies.

INTRODUCTION

Multicomponent adsorption onto activated carbon is finding increasing application in the purification treatment of domestic and industrial water and wastewater. The prediction of the breadth and shape of breakthrough curves is of fundamental importance in the engineering design of fixed-bed adsorption systems. For the design of efficient adsorbers it is desirable to have a background of theory in order to know how various factors influence the sharpness of separation. Among these factors is axial dispersion, which plays an important role in many processes of chemical reaction and separation. The effect of axial dispersion on the performance of liquid-phase adsorption and other mass transfer processes has been extensively investigated for many years (*1–32*). Most investigators (*1*) ignored the dispersion effect in their theoretical works and in the analysis of experimental results. Other reseasrchers (*16*, *18*, *20*) showed that neglecting dispersion effects may cause considerable errors in the evaluation of transfer coefficients at low flow rates, particularly when the fluid is a gas.

In the present work a comprehensive mathematical model considering all the significant external and internal diffusion and mass transfer processes as well as the axial dispersion using a highly nonlinear equilibrium isotherm is numerically solved for binary and ternary systems and compared to previously published experimental and theoretical works.

MATHEMATICAL GENERAL MODEL

The mathematical model describing solutes distribution consists of three parts as follows: 1) sorbent phase, 2) liquid-stream phase, 3) equilibrium isotherms.

Sorbent-Phase Governing Equations

For any solute i the pore and surface concentrations are described by Eqs. (1) and (2) respectively:

$$\varepsilon_p D_{pi} \frac{1}{\partial r}\frac{\partial}{\partial r}\left(r^2 \frac{\partial C_{pi}}{\partial r}\right) - K_{1i}(C^*_{si} - C_{si}) = \varepsilon_p \frac{\partial C_{pi}}{\partial r} \tag{1}$$

$$D_{si}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial C_{si}}{\partial r}\right) + K_{1i}(C^*_{si} - C_{si}) = \frac{\partial C_{si}}{\partial t} \tag{2}$$

for $i = 1, 2, 3, \ldots, n$, where n is the number of solutes. (The symbols are defined in the Symbols section.) The initial and boundary conditions needed for Eqs. (1) and (2) are:

$$\text{at } t = 0,\ C_{pi} = C_{si} = 0 \text{ for all } 0 \leqslant r \leqslant R$$

$$\text{at } r = 0,\ \partial C_{si}/\partial r = 0 \text{ and } \partial C_{pi}/\partial r = 0 \text{ for any } t > 0$$

$$\text{at } r = R,\ \varepsilon_p D_{pi} \frac{\partial C_{pi}}{\partial r} = K_{fi}(C_{di} - C_{pi})$$

and

$$\partial C_{si}/\partial r = 0 \text{ for any } t > 0$$

where C_{di} is the concentration of solute in the bulk fluid.

Liquid-Stream Phase Governing Equations

The concentration distribution of solute i in the liquid stream flowing inside the fixed-bed is described by the following partial differential equation:

$$\frac{\partial C_{di}}{\partial t} + \left(\frac{1-\varepsilon_B}{\varepsilon_B}\right)\left(\frac{3K_{fi}}{R}\right)(C_{di} - C_{pi})_{r=R} + \frac{V\partial C_{di}}{\varepsilon_B \partial x} = D_{Li}\frac{\partial^2 C_{di}}{\partial x^2} \quad (3)$$

The initial and boundary conditions of Eq. (3) are given by

$$C_{di}(t,x) = 0 \text{ at } t \leqslant 0 \text{ for } 0 \leqslant x \leqslant z$$

$$\frac{V}{\varepsilon_B} C_{0i}(t) = \frac{V}{\varepsilon_B} C_{di}(t,x) - D_{Li}\frac{\partial C_{di}}{\partial x} \text{ at } x = 0, t > 0$$

$$\frac{\partial C_{di}}{\partial x} = 0 \text{ at } x = z, t > 0$$

Equilibrium Isotherms

For each solute i, the general nonlinear equilibrium isotherm is described by the following equation (*34*):

$$C_{si}^{*} = \frac{a_{i0}C_{pi}^{b_{i0}}}{c_i + \sum_{j=1}^{n} a_{ij} C_{pj}^{b_{ij}}} = f_i(C_{p1}, C_{p2}, \ldots, C_{pn}) \quad (4)$$

The Langmuir and Freundlich and other known isotherms are special cases of Eq. (4). This equation has been shown (*8*, *9*) to satisfactorily fit experimental data of two and three solute systems.

Equation (4) is used to couple Eqs. (1) and (2) for each solute i through the term $K_{1,i}(C_{si}^{*} - C_{si})$.

Since $C^*_{si} = f_i(C_{p1}, C_{p2}, \ldots, C_{pn})$, sorbent- and liquid-phase equations are linked together through the term $(C_{di} - C_{pi})_{r=R}$ applied at the outer surface of the sorbent particles.

NUMERICAL SOLUTION

An accurate stable scheme of backward-difference technique (*35*, *36*) has been successfully used (*1*) to solve the Eqs. (1)–(4) and is extended here to include the axial diffusion term on the right-hand side of Eq. (3). Details of the numerical solution are described elsewhere (*2*). The general flow chart describing the algorithmic logic of the computer program of the complex model is shown in Fig. 1.

RESULTS AND DISCUSSIONS

The purpose of this paper is to present a numerical solution of a generalized multicomponent adsorption model and to study the effect of axial diffusion on the performance of fixed-bed adsorbers.

Results for the Two-Component System

The values of parameters for this system were also experimentally used by Balzli (*9*) where butanol is taken as Component 1, and *t*-amyl alcohol as Component 2. These values are given in Table 1.

As shown in Fig. 2, our findings indicate that axial dispersion does not contribute significantly to the shapes of the breakthrough curves for the two-component system. These results are in agreement with those obtained by many investigators in recent works (*12*, *15*, *20*, *22*, *26*).

For $z \gg$ particle diameter and Pe > 1, and Re $\geqslant 10$, it has been shown (*15*, *22*) that axial dispersion is unlikely to be significant, since the axial diffusive term in the mass balance equation (Eq. 3) is much less than the convective term. Farkas and Byleveld (*15*) found by experiment that axial dispersion is insignificant even when Re < 10 and Re is in the range of 0.02 to 0.22. In the present work, the values of Re and Pe are, respectively, about 2 to 0.3. Moreover, the findings of Farkas and Byleveld (*15*) and Wilson (*12*) indicate that axial dispersion does not contribute significantly to the shapes of the breakthrough curves.

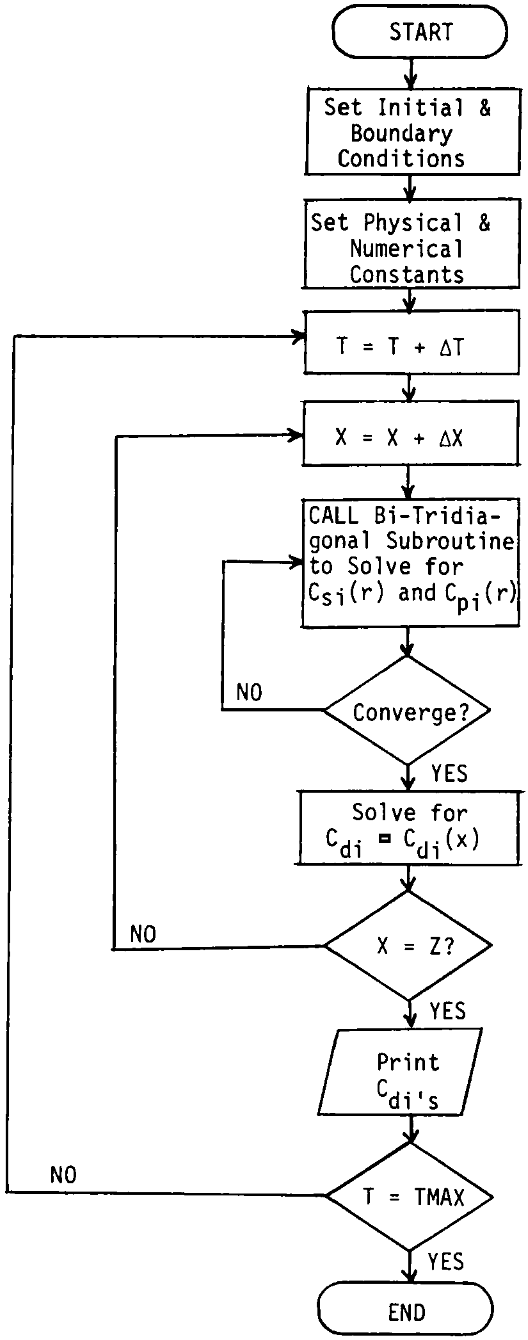

FIG. 1. Flow chart for complex model.

TABLE 1
Values of Binary System Parameters

Height of adsorber, z, cm	41.0
Radius of carbon particle, R, cm	0.05
Porosity of particles, ε_p, fraction	0.94
Voidage of bed, ε_B, fraction	0.45
Bulk velocity, V, cm/s	0.139
Initial concentration, C_{0i}, g/cm^3:	
Component 1	0.001
Component 2	0.001015
Mass transfer coefficient, K_{fi}, cm/s:	
Component 1	2.115×10^{-3}
Component 2	1.68×10^{-3}
Adsorption rate constant, K_{1i}, s^{-1}:	
Component 1	5.333×10^{-4}
Component 2	4.917×10^{-4}
Pore diffusion coefficient, D_{pi}, cm^2/s:	
Component 1	7.40×10^{-6}
Component 2	13.03×10^{-6}
Surface diffusion coefficient, D_{si}, cm^2/s:	
Component 1	1.25×10^{-7}
Component 2	2.2×10^{-7}
Axial diffusion coefficient, D_{Li}, cm^2/s:	
Component 1	0.04
Component 2	0.04
Equilibrium parameters for Component 1:	
$a_{10} = 1.06$ $b_{10} = 1.217$ $c_1 = 0$	
$a_{11} = 1$ $b_{12} = 0.626$ $b_{11} = 0.812$ $b_{12} = 0.764$	
Equilibrium parameters for Component 2:	
$a_{20} = 1.07$ $b_{20} = 1.254$ $c_2 = 0$	
$a_{21} = 1$ $a_{22} = 0.045$ $b_{21} = 0.906$ $b_{22} = .634$	

From Fig. 2, for a 41-cm adsorber, it is noted that the results with axial diffusion is a little bit closer to the experimental data than the results without axial diffusion. This difference in results is not noted in the longer adsorber (82 cm) as shown in Fig. 4 for the ternary system.

Results for the Thee-Component System

The parameters used in this model are shown in Table 2. Phenol is used here as Component 3.

As shown in Figs. 3 and 4 for the three-component system in both 41 and 82 cm adsorbers, it is noted that including axial diffusion in the

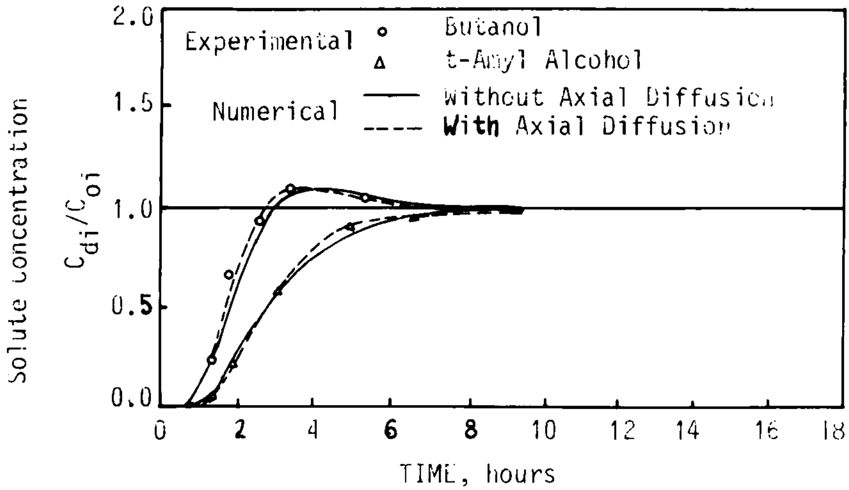

FIG. 2. Effect of axial diffusion on the simultaneous adsorption of butanol and *t*-amyl alcohol.

complex model does not affect the shape of the breakthrough curves for all components. It is also noted that the effect of axial diffusion is less for the longer adsorber, and this result has been reported in a recent paper by Raghavan and Ruthven (*17*), who showed that the effect of axial diffusion is minimal except when the bed is very short (less than 20 particle diameters), and in our study this ratio is 820. Therefore the neglect of axial dispersion is reasonable for long adsorbers.

CONCLUSIONS

It is concluded that axial dispersion has a minimal effect on the shape and sharpness of breakthrough curves in multicomponent sorption processes, and this effect becomes less for relatively long fixed-bed adsorbers. Hence, axial dispersion can be neglected in the simulation and the design of multicomponent adsorbers.

SYMBOLS

a_{i0}, a_{ij}	coefficients in Eq. (4)
b_{i0}, b_{ij}	coefficients in Eq. (4)

TABLE 2
Values of Parameters for the Ternary System

Height of adsorbers, z, cm:	41.0, 82.0
Initial concentration, C_{0i}, g/cm^3:	
Component 1, C_{01}	9.150×10^{-4}
Component 2, C_{02}	9.120×10^{-4}
Component 3, C_{03}	9.970×10^{-4}
Mass transfer coefficients, K_{fi}, cm/s:	
Component 1, K_{f1}	2.120×10^{-3}
Component 2, K_{f2}	1.950×10^{-3}
Component 3, K_{f3}	2.170×10^{-3}
Adsorption rate constants, K_{1i}, s^{-1}:	
Component 1	5.333×10^{-4}
Component 2	4.917×10^{-4}
Component 3	3.278×10^{-4}
Pore diffusion coefficient, D_{pi}, cm2/s:	
Component 1	7.4×10^{-6}
Component 2	13.03×10^{-6}
Component 3	19.2×10^{-6}
Surface diffusion coefficient, D_{si}, cm^2/s:	
Component 1	1.25×10^{-7}
Component 2	2.20×10^{-7}
Component 3	3.20×10^{-7}
Axial diffusion coefficient, D_{Li}, cm^2/s:	
Component 1	0.04
Component 2	0.04
Component 3	0.04
Parameters of the equilibrium isotherm:	

$a_{10} = 1.05$	$a_{11} = 1.00$	$a_{12} = 1.44$	$a_{13} = 0.53$	$c_1 = 0$
$b_{10} = 1.134$	$b_{11} = 0.73$	$b_{12} = 0.793$	$b_{13} = 0.467$	
$a_{20} = 1.09$	$a_{21} = 0.52$	$a_{22} = 1.00$	$a_{23} = 0.30$	$c_2 = 0$
$b_{20} = 1.182$	$b_{21} = 0.884$	$b_{22} = 0.831$	$b_{23} = 0.536$	
$a_{30} = 0.79$	$a_{31} = 1.07$	$a_{32} = 0.79$	$a_{33} = 1.00$	$c_3 = 0$
$b_{30} = 0.224$	$b_{31} = 0.286$	$b_{32} = 0.235$	$b_{33} = 0.002$	

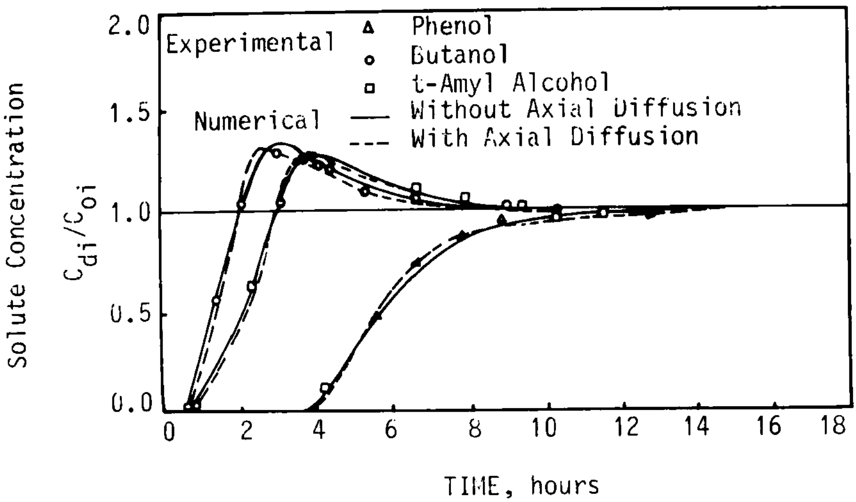

FIG. 3. Effect of axial diffusion on the simultaneous adsorption of butanol, *t*-amyl alcohol, and phenol in a 41-cm bed.

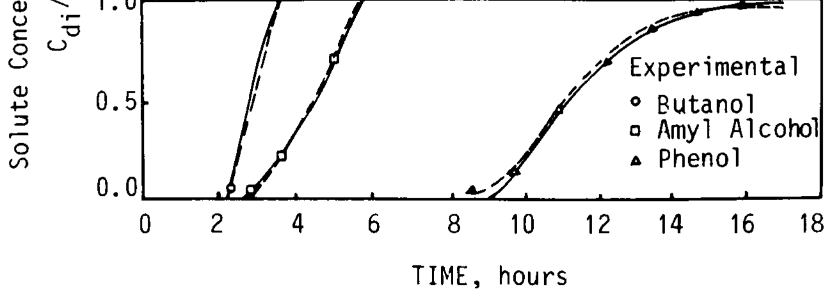

FIG. 4. Effect of axial diffusion on the simultaneous adsorption of butanol, *t*-amyl alcohol, and phenol in a 82-cm bed.

C_{di}	concentration of solute i in fluid phase of the bed (g/cm^3)
C_{0i}	value of C_{di} at the entrance of bed
C_{pi}	concentration of solute i in pore fluid phase (g/cm^3)
C_{si}	concentration of solute i in solid phase (g/cm^3)
D_{Li}	axial diffusion coefficient of solute i (cm^2/s)
D_{pi}	pore diffusion coefficient of solute i (cm^2/s)
d_p	particle diameter (cm)
D_{si}	surface diffusion coefficient of solute i (cm^2/s)
K_{fi}	mass transfer coefficient of solute i (cm/s)
K_{1i}	adsorption rate constant of solute i (s^{-1})
Pe	Peclet number = d_pV/D_L (dimensionless)
r	radial distance in particle (cm)
R	particle radius (cm)
Re	Reynolds number = $\rho V d_p/\mu$
t	time (s)
V	fluid velocity (cm/s)
X	distance along adsorber (cm)
Z	length of adsorber (cm)

Greek Letters

ρ	fluid density (g/cm^3)
μ	fluid viscosity (g/cm · s)
ε_B	bed void fraction (dimensionless)
ε_P	particle porosity (dimensionless)

Superscripts

*	equilibrium value

Subscripts

i	integer value
j	integer value
p	pore
s	solid

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