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Computer Prediction of Multicomponent Sorption with Variable Initial Concentrations Using a Complex Model

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Computer Prediction of Multicomponent Sorption with Variable Initial Concentrations Using a Complex Model

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Abstract

A generalized mathematical model describing the process of multicomponent adsorption on activated carbon in fixed beds has been used to study the influence of changes in feed concentrations for a ternary system by using an accurate computer solution.

INTRODUCTION

In industrial water and wastewater treatment systems (Fig. 1), it is rare that the inlet concentrations of pollutants to be removed will remain constant. Only a few investigators (*6*, *7*) have studied the effects of changes in feed concentrations for multisolute adsorption processes. Therefore, there is a need to study this important aspect.

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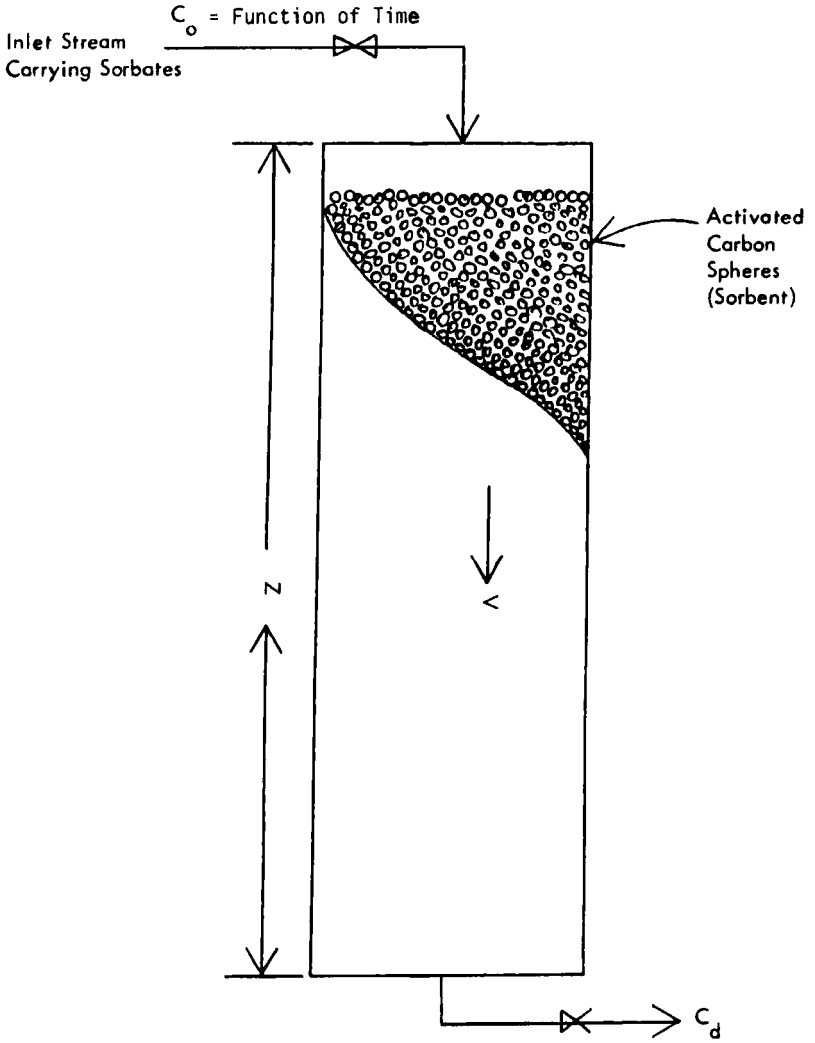

FIG. 1. Fixed-bed adsorber.

GENERAL MODEL

For the general case for any solute, the mathematical model (*6*) needed to define the pore and surface concentrations inside the particles (micro system) as functions of particle radius, r, and time, t, can be described as

$$\varepsilon_p D_p\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C_p}{\partial r}\right)\right] - K_1(C_s^* - C_s) = \varepsilon_p\frac{\partial C_p}{\partial r} \tag{1}$$

$$D_s\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C_s}{\partial r}\right)\right] + K_1(C_s^* - C_s) = \frac{\partial C_s}{\partial t} \tag{2}$$

where the equilibrium value of surface concentration, C_s^*, is defined by the general nonlinear isotherm (*3*)

$$C_{si}^* = \frac{a_{i0}C_{pi}^{b_{i0}}}{C_i + \sum_{i=1}^{n} a_{ij}C_{pi}^{b_{ij}}} = f_i(C_{p1}, C_{p2}, \ldots, C_{pn}) \tag{3}$$

The initial and boundary conditions needed to complete the definition of the micro system are

$$\text{at } t = 0, \qquad C_p = C_s = 0 \text{ for all } x \text{ and } r$$

$$\text{at } r = 0, \qquad \frac{\partial C_p}{\partial r} = \frac{\partial C_s}{\partial r} = 0 \text{ for all } t$$

$$\text{at } r = R, \qquad \frac{\partial C_s}{\partial r} = 0, \qquad \varepsilon_p D_p\frac{\partial C_p}{\partial r} = K_f(C_d - C_p) \text{ for all } t$$

The macro system describing the adsorbate distribution due to the fluid flow of the stream carrying pollutants can be described by the following partial differential equation (*5*, *6*):

$$\frac{\partial C_d}{\partial t} + \left(\frac{1-\varepsilon_B}{\varepsilon_B}\right)\left(\frac{3K_f}{R}\right)(C_d - C_p)_{r=R} + \frac{V}{\varepsilon_B}\frac{\partial C_d}{\partial x} = 0 \tag{4}$$

The boundary and initial conditions needed for Eq. (4) are

$$C_d(t,x) = 0 \text{ for } t < 0 \text{ and all } 0 < x < z$$

$$C_d(t,x) = C_0 \text{ for } x = 0 \text{ and all } t$$

TRI-SOLUTE SYSTEM

It can be shown that the micro system for a tri-solute system consists of the following partial differential equations:

$$\frac{D_{s1}}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C_{s1}}{\partial r}\right) - K_{1,1}(C_{s1} - C_{s1}^*) = \frac{\partial C_{s1}}{\partial t} \tag{5}$$

$$\varepsilon_p\frac{D_{p1}}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C_{p1}}{\partial r}\right) + K_{1,1}(C_{s1} - C_{s1}^*) = \varepsilon_p\frac{\partial C_{p1}}{\partial t} \tag{6}$$

$$\frac{D_{s2}}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C_{s2}}{\partial r}\right) - K_{1,2}(C_{s2} - C_{s2}^*) = \frac{\partial C_{s2}}{\partial t} \tag{7}$$

$$\varepsilon_p\frac{D_{p2}}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C_{p2}}{\partial r}\right) + K_{1,2}(C_{s2} - C_{s2}^*) = \varepsilon_p\frac{\partial C_{p2}}{\partial r} \tag{8}$$

$$\frac{D_{s3}}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C_{s3}}{\partial r}\right) - K_{1,3}(C_{s3} - C_{s3}^*) = \frac{\partial C_{s3}}{\partial t} \tag{9}$$

$$\varepsilon_p\frac{D_{p3}}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C_{p3}}{\partial r}\right) + K_{1,3}(C_{s3} - C_{s3}^*) = \varepsilon_p\frac{\partial C_{p3}}{\partial t} \tag{10}$$

These six equations govern the three solutes and are related to each other by the three equilibrium relationships (*1*, *2*):

$$C_{s1}^* = \frac{1.05C_{p1}^{1.134}}{C_{p1}^{0.73} + 1.44C_{p2}^{0.793} + 0.53C_{p3}^{0.467}} \tag{11}$$

$$C_{s2}^* = \frac{1.09C_{p2}^{1.182}}{C_{p2}^{0.831} + 0.52C_{p1}^{0.884} + 0.30C_{p3}^{0.536}} \tag{12}$$

$$C_{s3}^* = \frac{0.79C_{p3}^{0.224}}{C_{p3}^{0.002} + 1.07C_{p1}^{0.286} + 0.79C_{p2}^{0.235}} \tag{13}$$

Boundary and initial conditions necessary for solution are

$$\left(\frac{\partial C_{s1}}{\partial r}\right)_{r=0} = \left(\frac{\partial C_{s1}}{\partial r}\right)_{r=R} = 0$$

$$\left(\frac{\partial C_{p1}}{\partial r}\right)_{r=0} = 0 \qquad \text{for all } t$$

$$\varepsilon_p D_{p1}\left(\frac{\partial C_{p1}}{\partial r}\right)_{r=R} = K_{f1}(C_{d1} - C_{p1})_{r=R}$$

$$C_{s1} = C_{p1} = 0 \qquad \text{at } t = 0 \text{ for all } r$$

Similarly,

$$\left(\frac{\partial C_{s2}}{\partial r}\right)_{r=0} = \left(\frac{\partial C_{s2}}{\partial r}\right)_{r=R} = 0$$

$$\left(\frac{\partial C_{p2}}{\partial r}\right)_{r=0} = 0 \qquad \text{for all } t$$

$$\varepsilon_p D_{p2}\left(\frac{\partial C_{p2}}{\partial r}\right)_{r=R} = K_{f2}(C_{d2} - C_{p2})_{r=R}$$

$$C_{s2} = C_{p2} = 0 \qquad \text{at } t = 0 \text{ for all } r$$

Also,

$$\left(\frac{\partial C_{s3}}{\partial r}\right)_{r=0} = \left(\frac{\partial C_{s3}}{\partial r}\right)_{r=R} = 0$$

$$\left(\frac{\partial C_{p3}}{\partial r}\right)_{r=0} = 0 \qquad \text{for all } t$$

$$\varepsilon_p D_{p3}\left(\frac{\partial C_{p3}}{\partial r}\right)_{r=R} = K_{f3}(C_{d3} - C_{p3})_{r=R}$$

The macro system for the three-component system can be described by the equations

$$\frac{\partial C_{d1}}{\partial t} + \frac{V}{\varepsilon_B}\frac{\partial C_{d1}}{\partial x} + \frac{1-\varepsilon_B}{\varepsilon_B}\frac{3}{R}K_{f1}(C_{d1} - C_{p1}|_{r=R}) = 0 \qquad (14)$$

$$\frac{\partial C_{d2}}{\partial t} + \frac{V}{\varepsilon_B}\frac{\partial C_{d2}}{\partial x} + \frac{1-\varepsilon_B}{\varepsilon_B}\frac{3}{R}K_{f2}(C_{d2} - C_{p2}|_{r=R}) = 0 \qquad (15)$$

$$\frac{\partial C_{d3}}{\partial t} + \frac{V}{\varepsilon_B}\frac{\partial C_{d3}}{\partial x} + \frac{1-\varepsilon_B}{\varepsilon_B}\frac{3}{R}K_{f3}(C_{d3} - C_{p3}|_{r=R}) = 0 \qquad (16)$$

The boundary conditions are

$$C_{d1}(t,x) = 0 \qquad \text{at } t < 0, \text{ for all } 0 < x < z$$

$$C_{d1}(t,x) = C_{01}(t) \qquad \text{at } x = 0, \text{ for all } t$$

$$C_{d2}(t,x) = 0 \qquad \text{at } t < 0, \text{ for all } 0 < x < z$$

$$C_{d2}(t,x) = C_{02}(t) \qquad \text{at } x = 0, \text{ for all } t$$

$$C_{d3}(t,x) = 0 \qquad \text{at } t < 0, \text{ for all } 0 < x < z$$

$$C_{d3}(t,x) = C_{03}(t) \qquad \text{at } x = 0, \text{ for all } t$$

NUMERICAL SOLUTION

The finite difference equations used for solving the set of nonlinear partial differential equations of the micro system (Eqs. 5-13) and the macro system (Eqs. 14-16) are described in details by Mansour (*5*, *6*).

RESULTS AND DISCUSSION

In a recent paper, numerical results for a tri-solute system consisting of a mixture of butanol, *t*-amyl alcohol, and phenol using the base case with the parameters given in Table 1 (*7*) have been shown to achieve excellent agreement with previously published experimental data (*1*, *2*). Therefore, the computer program used in the base case was used here with the convenient modifications that let the initial concentrations of the three solutes vary with time. The effects of two types of disturbances were studied: step change and sinusoidal disturbances.

RESULTS OF STEP CHANGE DISTURBANCES

The effect of increasing the inlet concentrations of the three components in the ternary system by 20% each 1 h after the adsorption process started is shown in Fig. 2. It is noted that the breakthrough curves of the key component (phenol) and the nonkey components (butanol and *t*-amyl alcohol) are earlier than when inlet concentrations were constant. This is the result of the relative competition for adsorbent surface

TABLE 1
Base Case Variables Values

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_p, fraction	0.45
Bulk velocity, V, cm/s	0.139
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 coefficient 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 constant, K_{1i}, s^{-1}:	
Component 1, $K_{1,1}$	5.333×10^{-4}
Component 2, $K_{1,2}$	4.917×10^{-4}
Component 3, $K_{1,3}$	3.278×10^{-4}

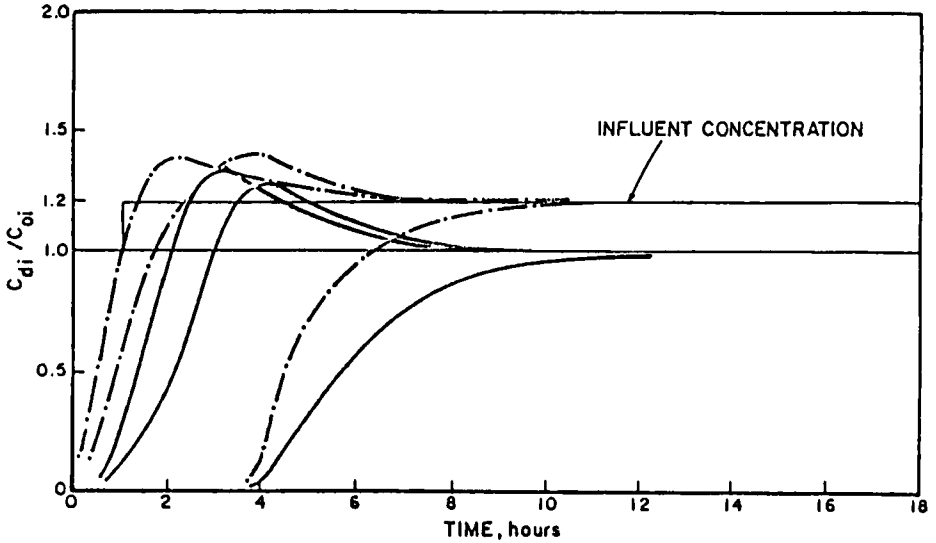

FIG. 2. Effect of positive step change on breakthrough curves of three-component system.

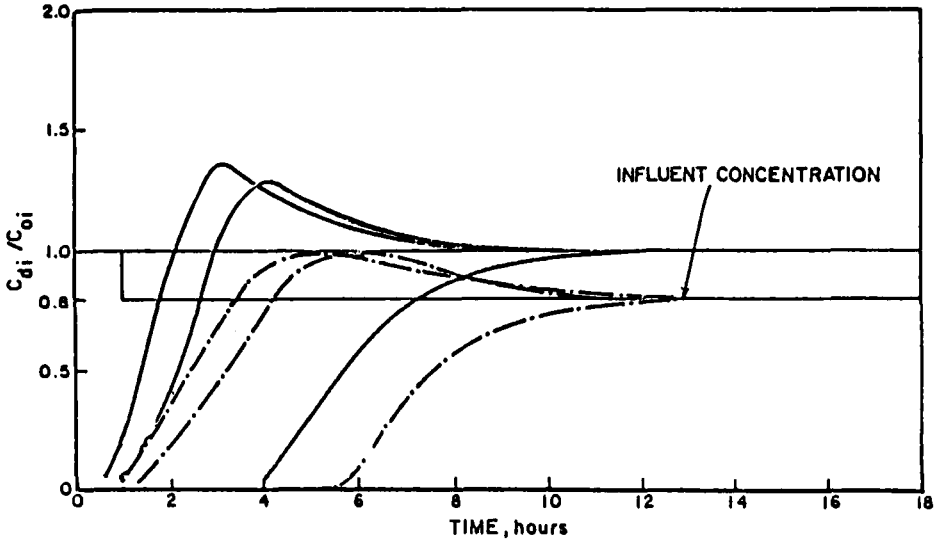

FIG. 3. Effect of negative step change on breakthrough curves of three-component system.

between the sorbates; the extent of the adsorption of each component is a function of the relative pure component affinities (which did not change) as well as the relative concentrations. Hence, the nonkey component adsorbability is increased with increasing composition, which means that less is displaced downstream. Higher peaks are also noted in Fig. 3, and this is expected since in order to satisfy the material balance the three components should return asymptotically to their original feed concentrations which have been changed to 1.2 dimensionlessly (see Fig. 2). Conversely, when inlet concentrations of the three components were decreased by 20% of their original feed concentrations, a similar behavior is noted but in the opposite direction; that is, the breakthrough curves are delayed and the peaks of the nonkey components are lower and all three profiles returned to their perturbed feed concentrations, 0.8, as shown in Fig. 3.

RESULTS OF SINUSOIDAL DISTURBANCES

For the sake of clarity, the influent concentration profile for the specified ternary system was plotted (Fig. 4) separately from the effluent concentration profiles (Fig. 5).

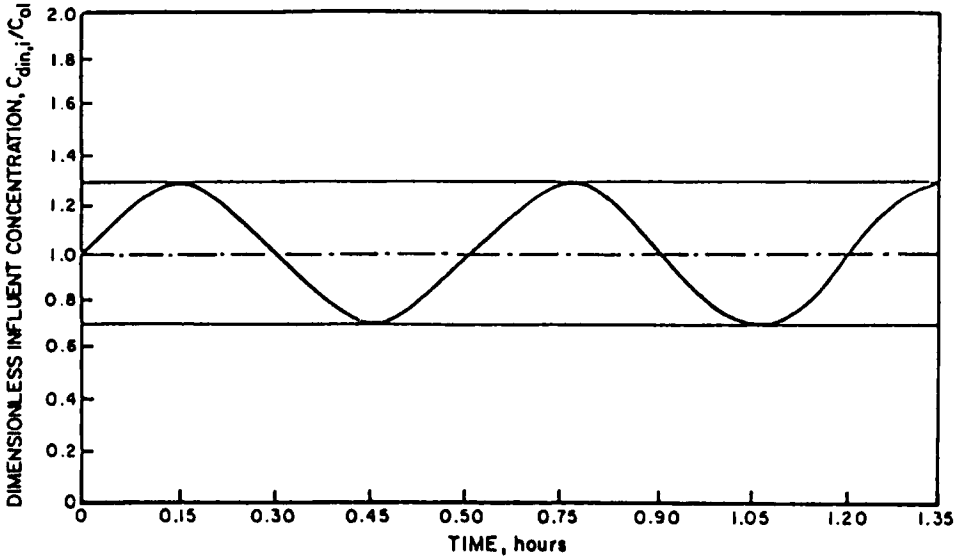

FIG. 4. Influent concentration of sinusoidal form applied to three-component system.

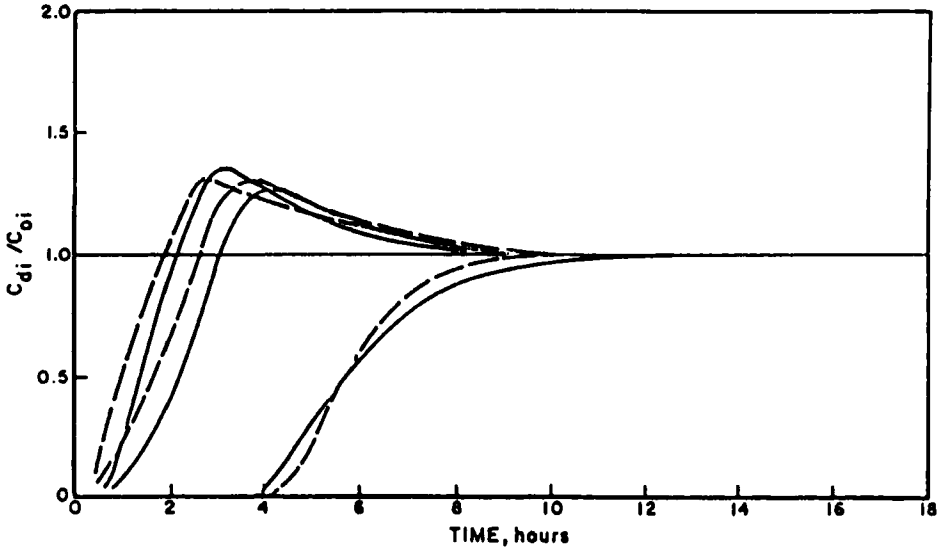

FIG. 5. Effect of sine wave change on breakthrough curves of ternary system.

This time the inlet concentration was expressed by a simple sine wave of the form $C_{d_{in}} = C_0 + A \sin \omega t$, where A = the amplitude of the wave (chosen to be as large as 30% of the constant feed concentration) and ω = frequency of the wave (10 times per minute, which is close to the figures encountered in practice). As shown in Fig. 5, earlier breakthrough curves for the nonkey components with lower peak heights is intuitively expected since the sine wave can be imagined to be approximately expressed by a consecutive series of positive and negative step changes. Therefore, the effect of a sine wave would be (also approximately) a combination of the effects of the two kinds of step changes discussed in the previous section. Accordingly, the breakthrough curve of the key component was later at the beginning and earlier at longer times. Of course, this behavior cannot be generalized for all types of input functions, so more cases need to be studied.

CONCLUSIONS

It is concluded that feed composition is one of the most important factors affecting the design of multisolute adsorbers. This is because, in actual sorption processes, we expect to deal with feeds of varying concentrations and, as shown, the sharpness and broadness of the breakthrough curves for both key and nonkey components directly depend on the feed composition and concentrations.

SYMBOLS

a_{i0}, a_{ij}	coefficients in Eq. (3)
b_{i0}, b_{ij}	exponents in Eq. (3)
C_d	concentration of solute in fluid phase of the bed (g/cm^3)
C_0	value of C_d at the entrance of bed
C_p	concentration of solute in pore fluid phase (g/cm^3)
C_s	concentration of solute in solid phase (per unit volume of particles) (g/cm^3)
D_p	effective diffusivity in pore fluid (cm^2/s)
d_p	particle diameter (cm)
D_s	effective diffusivity in particle solid phase (cm^2/s)
K_f	mass transfer coefficient for liquid–particle transfer (cm/s)
K_1	adsorption rate coefficient (s^{-1})
r	radial distance in particle (cm)

R	radius of particle (cm)
t	time (s)
V	fluid velocity (cm/s)
x	distance along bed (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
ε_p	particle void fraction

Superscripts

*	equilibrium value

Subscripts

i	integer value
j	integer value
p	pore
s	solid

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