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A General Nonequilibrium Multicomponent Adsorption Model: Numerical Solution

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Abstract

A comprehensive mathematical model has been developed to describe the process of multicomponent adsorption from a well-stirred bath. Both internal and external diffusional resistances were included in the physical model. A nonlinear Fritz-Schluender isotherm was used to describe the adsorption equilibrium. An infinite bath, one-component, non-equilibrium model was compared with an equilibrium model. A numerical solution for a binary system in an infinite bath was obtained. The numerical solution for a two-component model in a stirred finite bath was shown to satisfactorily match previously published experimental data. Its extension to an n-component system was shown. It was shown that the solution of nonequilibrium model is easier and more efficient than that of the equilibrium model. The nonequilibrium model is especially advantageous for a large number of solutes.

INTRODUCTION

The separation of solutes from a fluid stream by adsorption onto a solid surface is an important process and is especially important in advanced wastewater treatment processes. The limitations of theoretical concepts relative to the practicalities of treatment for industrial wastewater necessitates that comprehensive process simulation studies precede the final design decision.

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TABLE 1
Previous Work

Investigator	Film resistance	Type of equilibrium isotherm	Number of components considered	Type of treatment
DiGiano and Weber (*4*)	Yes	Langmuir	1	Experimental and analytical
Suzuki and Kawazoe (*11*)	No	Linear	1	Experimental and analytical
Liapis and Rippin (*6*)	Yes	Fritz-Schluender	2	Numerical
Weber (*13*)	Yes	Irreversible	1	Analytical
Peel and Benedek (*10*)	Yes	Linear and quadratic	1	Experimental and analytical

Many investigators have studied multicomponent adsorption as shown in Table 1. None of the existing models has accounted for all the following factors:

1. Intraparticle diffusional resistance
2. Interparticle diffusional resistance
3. Nonequilibrium conditions
4. Nonlinear equilibrium relationship
5. Interphase film resistance
6. Capability of models to be used for n-component systems

In the present study, all of these factors are taken into account.

MATHEMATICAL ANALYSIS

Physical Model

The present work is concerned with removal of solutes from a fluid stream by adsorption onto a solid surface of spherical particles. The solute to be removed is transferred from the fluid phase to the solid phase according to the following steps:

1. Mass transport from bulk fluid to pore fluid at the particle surface
2. Diffusion into the porous solid
3. Adsorption onto the solid surface

The equilibrium existing between the fluid and the solid concentration is assumed to be given by Fritz-Schluender (5) isotherm:

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

where C_{si}^* is the amount of solute i adsorbed per unit volume of particle at equilibrium with a liquid-phase concentration C_{pi}, in a solution containing n solutes. The equilibrium isotherms for the bisolute system used in this study were taken from Liapis and Rippin (*6*), and these are

$$C_{s1}^* = \frac{1.06 C_{p1}^{1.217}}{C_{p1}^{0.812} + 0.626 C_{p2}^{0.764}} \tag{1a}$$

$$C_{s2}^* = \frac{1.07 C_{p2}^{1.254}}{C_{p2}^{0.906} + 0.045 C_{p1}^{0.634}} \tag{1b}$$

where butanol-2 is taken as Component 1 and *t*-amyl alcohol as Component 2; b_{i0} and b_{ij} are empirical constants.

In this process the radial concentration profiles of solutes inside the particles as well as the bulk concentration in the bath are to be determined as functions of time.

Mathematical Models

1. Infinite-Bath Nonequilibrium Model

For any solute i, two differential equations result from mass balances in the pore liquid and on the adsorbent surface to describe the pore and the surface concentrations inside the particles. These equations are:

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

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

for $i = 1, 2, \ldots.\ n$.

Equations (2) and (3) contain three dependent variables since C_{si}^* is also unknown. C_{si}^* is expressed in terms of C_{pi} by Eq. (1). The initial and boundary conditions needed for Eqs. (2) and (3) are

$$C_{pi}(r,\ 0) = 0 \tag{4}$$

$$\frac{\partial C_{pi}}{\partial r}(0,\ t) = 0 \tag{5}$$

$$\varepsilon_p D_{pi} \frac{\partial C_{pi}}{\partial r}(R,\ t) = K_{fi}(C_{di} - C_{pi}(R,\ t)) \tag{6}$$

$$C_{si}(r,\ 0) = 0 \tag{7}$$

$$\frac{\partial C_{si}}{\partial r}(0,\ t) = 0 \tag{8}$$

$$\frac{\partial C_{si}}{\partial r}(R,\ t) = 0 \tag{9}$$

It can be easily shown that the multicomponent model composed of n solutes consists of $2n$ partial differential equations, n isotherms, $4n$ boundary conditions, and $2n$ initial conditions.

2. Finite-Bath Nonequilibrium Model

The finite-bath model is similar to the infinite bath model except that the concentration of solutes in the surrounding fluid, C_{di}, varies with time for a finite bath. Variation of this concentration with time is described for any solute i by the following differential equation:

$$\frac{dC_{di}}{dt} = \frac{3K_{fi}(1 - \varepsilon_B)}{R\varepsilon_B}(C_{pi} - C_{di})|_{r=R} \tag{10}$$

where ε_B is the void fraction of bath.

The initial condition needed to complete the definition of Eq. (10) is

$$C_i(t) = C_{di0} \qquad \text{at } t = 0 \tag{11}$$

The set of Eqs. (1)–(3) is used for each solute. Equations (2) and (3) are coupled in C_{pi}^* and C_{si} for solute i through the interphase adsorption term, $K_{1,i}(C_{si}^* - C_{si})$. The pairs for all solutes are also coupled through the equilibrium relation of Eq. (1). Also, each pair for a specific solute is coupled with Eq. (10) through the interphase term, $K_{fi}(C_{di} - C_{pi})$. Since the equations are highly nonlinear, an iterative numerical procedure was followed to solve each set of equations.

3. Equilibrium Model

One purpose of using this model was to study the possibility of simulating adsorption equilibrium with the nonequilibrium model by using large values for K_1. Therefore Eqs. (2) and (3) do not contain the adsorption term, $K_{1,i}$ $(C_{si}^* - C_{si})$. For this case $C_{si}^* = C_{si} = f_i(C_{p1}, C_{p2}, \ldots, C_{pn})$, and thus Eqs. (2) and (3) have only one dependent variable each. The governing equation is:

$$\varepsilon_p \frac{\partial C_{pi}}{\partial t} + \frac{\partial C_{si}}{\partial t} = \varepsilon_p D_{pi} \frac{1}{r^2} \frac{\partial}{\partial r} \frac{(r^2 \partial C_{pi})}{\partial r} + D_{si} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial C_{si}}{\partial r} \right) \tag{12}$$

where $C_{si} = f_i(C_{p1}, C_{p2}, \ldots, C_{pn})$.

METHOD OF NUMERICAL SOLUTION

Linearization of Equations

Equations (2) and (3) are highly nonlinear partial differential equations. To eliminate the nonlinearity arising from the term C_{si}^* which is defined in Eq. (1), an iterative procedure from the finite-difference equations is followed. The denominator of this expression is evaluated with values computed from the previous iteration. The nonlinear term C_{si}^* is put in the form $C_s^* = C_p F(C_{pA})$, which is linear in C_p since C_{pA} is the value obtained from the previous iteration. At the end of each iteration the absolute difference between C_p and C_{pA} is compared with a set tolerance. If it does not match, the computed values of C_p are used as C_{pA}, and another set of values is computed.

Finite-Difference Equations

For any component i, both the backward and Crank-Nicolson methods are suitable to solve the set of Eqs. (2) and (3) since they are unconditionally stable (*3, 12*). Also, the same system has been solved by Mansour (*9*) and shown to be unconditionally stable. Since Crank-Nicolson method may cause some oscillations at the boundries, the backward method was used in this study. Details of the finite-difference equations are described in the Appendix.

Scheme of Numerical Solution

The finite-difference equations obtained from Eqs. (2) and (3) form a bi-tridiagonal system. This system is solved by the algorithm for bi-tridiagonal matrices (*12*) using the subroutine BTD which has been written by Mansour (*7*). This algorithm is used to solve for the variables C_s's and C_p's during each iteration at a given time step. After convergence is obtained, the coefficients of the matrices are updated, and the procedure is repeated for the next time step.

Solution of Finite-Bath Model

In the infinite-bath model described above, the bulk concentration C_{di}, in the boundary condition described by Eq. (6), is taken as a constant, and it appears in the right-hand side matrices of the difference equations.

For the finite-bath model, all the difference equations are exactly the same for the infinite-bath model except for Eq. (10) which describes the variation of C_{di} with time. Therefore the difference equation obtained from Eq. (10) is substituted into the difference equation of Eq. (6). After some manipulation processes, the variable C_{di} is expressed as a function of C_p at the boundary and its value in the previous time step. At the end of each time step the value of C_{di} is updated and the process is repeated.

Solution of Equilibrium Model

The finite-difference equation arising from Eq. (12) forms a tridiagonal system which can be iteratively solved by using the Thomas algorithm (*12*).

Solution of Multicomponent Model

This model consists of a pair of coupled partial differential equations and an equilibrium relationship for each component. The equilibrium-solid concentration of each component is expressed as a function of the pore concentration of all components. The initial and boundary conditions are similar to those for the one- and two-component cases. Values of the pore concentrations are assumed for use in the denominators of the equilibrium relations. By use of these values, the pair of equations for each component is uncoupled from the pairs for the other components, and all the finite-difference equations are linearized. As in the other models, these equations fit bi-tridiagonal algorithm and are readily solved for each component.

RESULTS AND DISCUSSION

Comparison of Equilibrium and Nonequilibrium One-Component Models

The purpose of this comparison is to determine whether the nonequilibrium model, with large value of K_1, gives the same results as the equilibrium model. Test runs for different values of K_1 were made, and the results show that when K_1 is 2 or larger, equilibrium between C_{pi} and C_{si} is attained. Results obtained from the solution of the nonequilibrium model described by Eqs. (2) and (3), as shown in Table 2, are in an excellent agreement with those obtained from the solution of the equilibrium model described by Eq. (12), provided equilibrium between C_{pi} and C_{si} is described by the following Langmuir isotherm:

$$C_{si} = \frac{a_{10} C_{pi}}{1 + a_{11} C_{pi}}$$

The values of parameters used are:

$a_{10} = 171.07$ $\quad a_{11} = 1400$ $\quad \varepsilon_p = 0.7$

$R = 0.1$ $\quad C_{d0} = 0.001$ $\quad K_f = 2.205 \times 10^{-4}$

$D_p = 7.4 \times 10^{-6}$ $\quad D_s = 1.25 \times 10^{-7}$

As shown in Table 2, for large value of K_1 the equilibrium and the nonequilibrium models are equivalent. In addition to this, there are two total

TABLE 2
Comparison of Equilibrium and Nonequilibrium One-Component Models

r/R	0.0	0.2	0.4	0.6	0.8	1.0
			Time = 20 s			
C_{peq}	0.238×10^{-26}	0.205×10^{-22}	0.166×10^{-17}	0.163×10^{-12}	0.145×10^{-7}	0.100×10^{-2}
C_{pneq}	0.227×10^{-26}	0.194×10^{-22}	0.154×10^{-17}	0.151×10^{-12}	0.132×10^{-7}	0.100×10^{-2}
C_{seq}	0.407×10^{-24}	0.350×10^{-20}	0.284×10^{-15}	0.279×10^{-10}	0.248×10^{-5}	0.712×10^{-1}
C_{sneq}	0.388×10^{-24}	0.332×10^{-20}	0.263×10^{-15}	0.258×10^{-10}	0.226×10^{-5}	0.712×10^{-1}
			Time = 60 s			
C_{peq}	0.408×10^{-23}	0.172×10^{-19}	0.560×10^{-15}	0.253×10^{-11}	0.274×10^{-6}	0.100×10^{-2}
C_{pneq}	0.395×10^{-23}	0.161×10^{-19}	0.549×10^{-15}	0.244×10^{-11}	0.266×10^{-6}	0.100×10^{-2}
C_{seq}	0.698×10^{-21}	0.294×10^{-17}	0.958×10^{-13}	0.433×10^{-9}	0.468×10^{-4}	0.712×10^{-1}
C_{sneq}	0.675×10^{-21}	0.275×10^{-17}	0.934×10^{-13}	0.417×10^{-9}	0.455×10^{-4}	0.712×10^{-1}
			Time = 100 s			
C_{peq}	0.526×10^{-21}	0.122×10^{-17}	0.190×10^{-13}	0.231×10^{-9}	0.120×10^{-5}	0.100×10^{-2}
C_{pneq}	0.518×10^{-21}	0.117×10^{-17}	0.182×10^{-13}	0.224×10^{-9}	0.114×10^{-5}	0.100×10^{-2}
C_{seq}	0.899×10^{-19}	0.209×10^{-15}	0.325×10^{-11}	0.359×10^{-7}	0.204×10^{-3}	0.712×10^{-1}
C_{sneq}	0.886×10^{-19}	0.200×10^{-15}	0.311×10^{-11}	0.383×10^{-7}	0.195×10^{-3}	0.712×10^{-1}

derivatives containing C_{pi} and C_{si} to be determined from the equilibrium relation when the equilibrium model is used. In the case of a two-component system, there are 10 partial derivatives containing C_{pi}'s and C_{si}'s to be determined. For three-component systems, there are 27 partial derivatives. Therefore, it is obvious that partial differential equations become very complex when the number of sorbates becomes large. Moreover, the nonequilibrium model could be extended to be used for any number of sorbates, while a new computer program must be written as a new sorbate is added to the system when equilibrium model is used.

Pore and Surface Concentration Profiles Inside Particles (Infinite-Bath Model)

Figure 1 through 4 illustrate the increase in sorbate concentration within the particle. Although the pore diffusivities were larger than the surface ones, the surface concentrations were 30 to 70 times greater than the pore

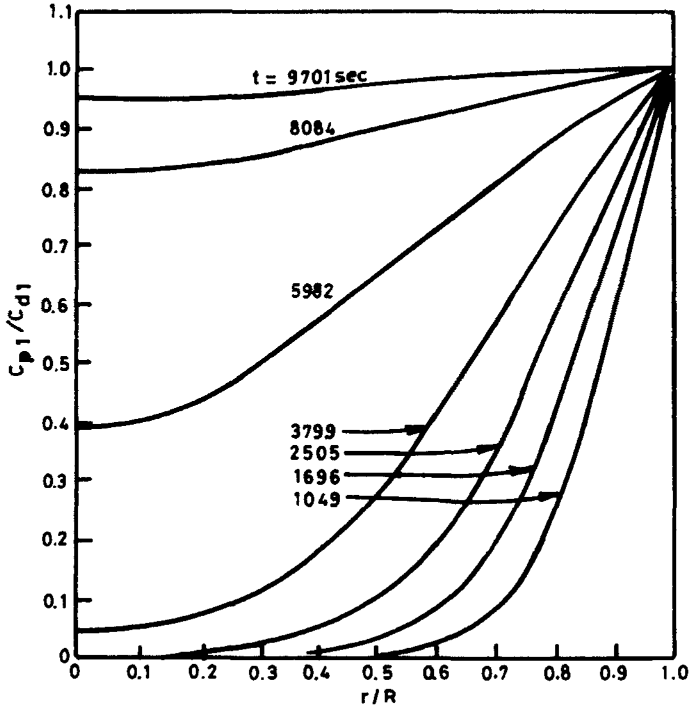

FIG. 1. Pore-concentration profile of Component 1.

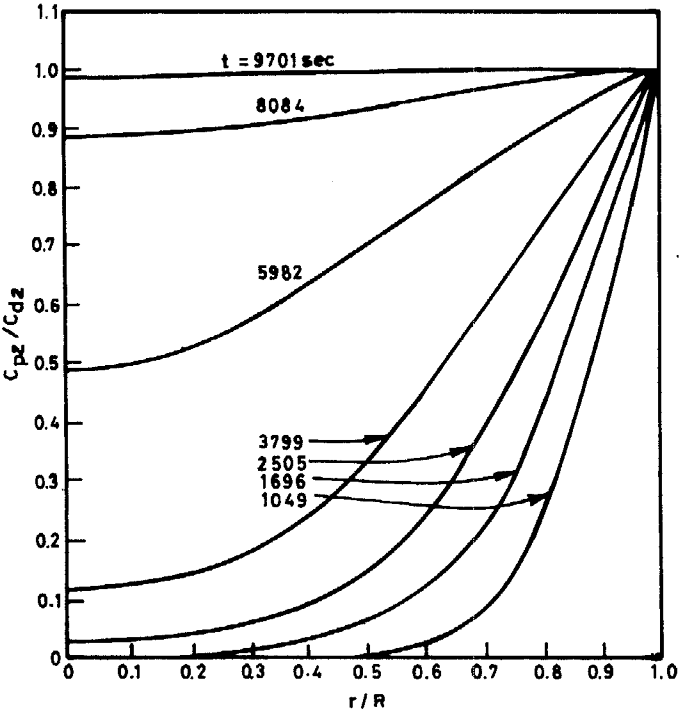

FIG. 2. Pore-concentration profile of Component 2.

concentrations by nature of the equilibrium. Adsorbate 2 diffuses more rapidly into the particle than Sorbate 1 since both its diffusivities are larger than those for Adsorbate 1. The surface becomes saturated with the adsorbates much faster than the pore liquid since the denominators in the equilibrium relations compensate for the lower values of the pore concentrations in the numerators. Notice that, at 5982 s, the surface concentrations are much nearer to the values at the outer radius than are the pore concentrations. Finally, at a time of 9701 s, all four concentrations have nearly reached the values at the outer radius of the particle.

Results for the Two-Component Finite Bath Model

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

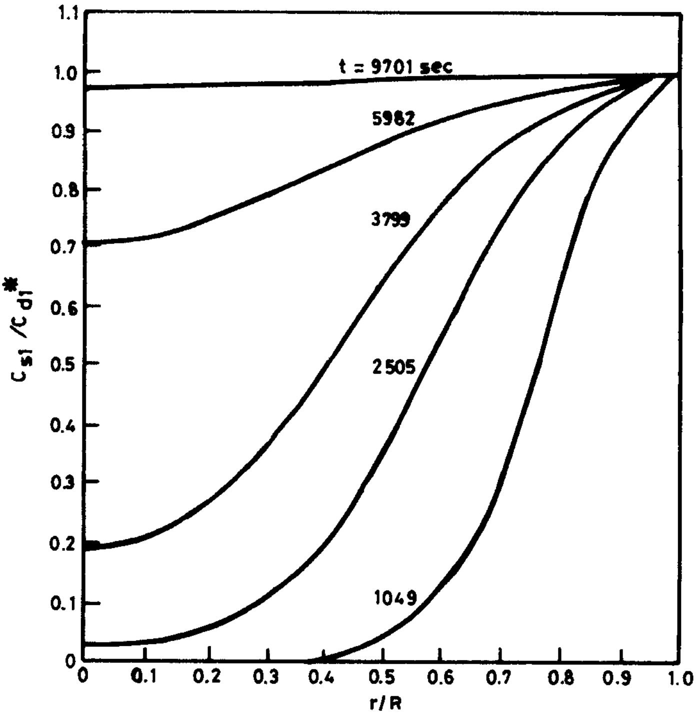

FIG. 3. Surface-concentration profile of Component 1.

$\varepsilon_p = 0.94$ $\varepsilon_B = 0.9859$ $C_{01} = 0.0005$

$C_{02} = 0.0005$ $K_{f1} = 4.472 \times 10^{-3}$ $K_{f2} = 4.132 \times 10^{-3}$

$K_{1,1} = 1.92$ $K_{1,2} = 1.76$ $D_{p1} = 7.4 \times 10^{-6}$

$D_{p2} = 13.0 \times 10^{-6}$ $D_{s1} = 1.25 \times 10^{-7}$ $D_{s2} = 2.2 \times 10^{-7}$

$R = 0.05$

The coefficients in the isotherms were given in Equations (1a) and (1b). Figure 5 shows a good agreement between the theoretical predictions of this study and experimental data obtained by Balzli (*2*). However, the deviations noticed in the initial times of adsorption are due to the uncertainties in the values of diffusion rate constants which were used by Liapis and Rippin (*6*) since they used them for a little bit different model.

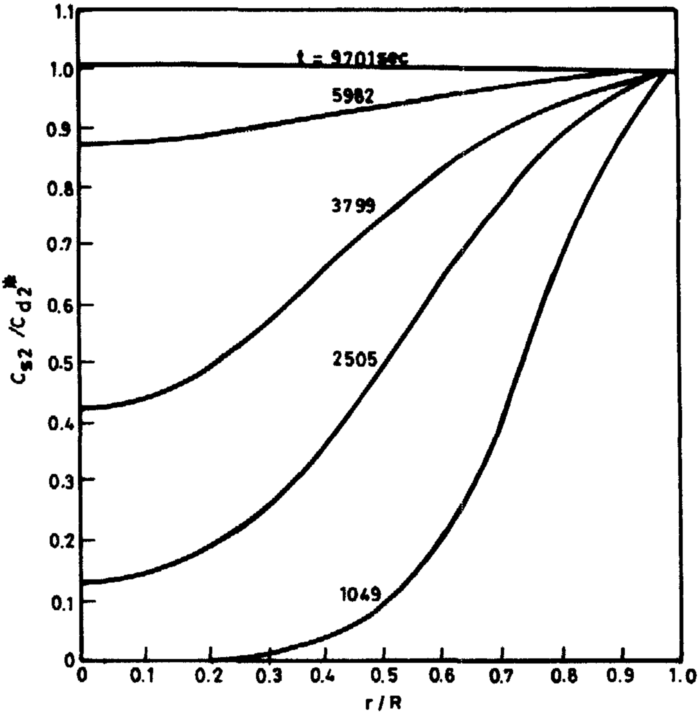

FIG. 4. Surface-concentration profile of Component 2.

With the backward-difference method, which is unconditionally stable, it was easy to start with a small time step and increase it successively for the remainder of the solution, which implies that the computer time will be shorter than that consumed in other methods. (The computer time consumed for binary adsorption in a finite bath using orthogonal collocation was in the range of 105–170 s (*6*), while it is only 68 s for the same system when the difference method is used.)

CONCLUSIONS

A comprehensive computer simulation program for multicomponent adsorption from a finite bath has been successfully used to predict theoretical results that have been shown to satisfactorily match experimental results.

The advantages of the computer program can be summarized as follows:

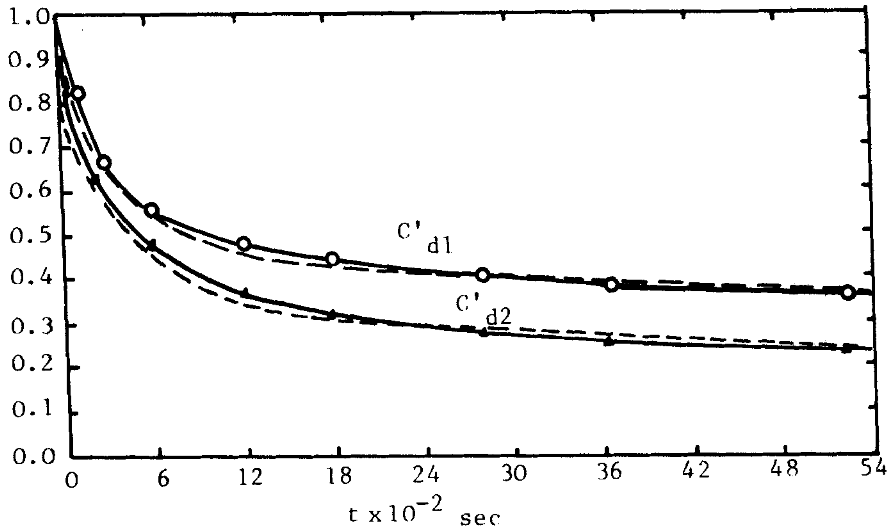

FIG. 5. Simultaneous adsorption of butanol-2 and 1-amyl alcohol in a finite bath. (- -) Mathematical data, (○) experimental data of butanol-2, (▲) experimental data of 1-amyl alcohol.

1. It is applicable to both equilibrium and nonequilibrium conditions.
2. It is a general program that can be used for any number of sorbates.
3. It can be used for any type of equilibrium isotherm without the need of any modifications in the program since the most general type of isotherms was used.
4. It is more comprehensive than other programs since it yields radial concentration variations and takes into account internal, external, and interfacial resistances.
5. Although the general model is very complex, the program has been structured to be flexible and easy to use.
6. Moreover, with the backward-difference method used, which is unconditionally stable, one can use a variable and large time step for the solution, which implies that the computer time is considerably shorter than that consumed in other methods.

APPENDIX

The backward-finite difference form of Eq. (2) for one solute is

$$\varepsilon_p D_p \left(\frac{C_{pi-1,j+1} - 2C_{pi,j+1} + C_{pi+1,j+1}}{(\Delta r)^2} \right) + \frac{2\varepsilon_p D_p}{r_i} \left(\frac{C_{pi+1,j+1} - C_{pi-1,j+1}}{2\Delta r} \right)$$
$$+ K_1(C_{si,j+1} - F(C_{pAi})C_{pi,j+1} = \varepsilon_p \left[\frac{C_{pi,j+1} - C_{pi,j}}{\Delta t} \right] \qquad \text{(A1)}$$

for $2 \le i \le N$ and $i \le j \le$ JMAX.

The above equation can be written in the form of bi-tridiagonal matrices as

$$A_i^{(1)} C_{si-1,j+1} + A_i^{(2)} C_{pi-1,j+1} + B_i^{(1)} C_{si,j+1} + B_i^{(2)} C_{pi,j+1}$$
$$+ C_i^{(1)} C_{si+1,j+1} + C_i^{(2)} C_{pi+1,j+1} = D_i^{(1)} \qquad \text{(A2)}$$

where $A_i^{(1)} = 0$

$$A_i^{(2)} = -\varepsilon_p D_p \Delta t + \varepsilon_p D_p \Delta t \Delta r / r_i$$
$$B_i^{(1)} = -K_l \Delta t (\Delta r)^2$$
$$B_i^{(2)} = 2\varepsilon_p D_p \Delta t + K_1 \Delta t (F(C_{pAi})(\Delta r)^2 + \varepsilon_p (\Delta r)^2$$
$$C_i^{(1)} = 0$$
$$C_i^{(2)} = -\left(\varepsilon_p D_p \Delta t + \frac{\varepsilon_p D_p \Delta t \Delta r}{r_i} \right)$$
$$D_i^{(1)} = \varepsilon_p (\Delta r)^2 C_{pi,j}$$

Equation (4) does not apply at $r = 0$ since the term $(\partial C_p / \partial r)/r$ becomes indeterminant. Therefore L'Hospital's rule is used to evaluate the term. Taking the

$$\lim_{r \to 0} \frac{\partial C_p / \partial r}{r} = \frac{\partial^2 C_p / \partial r^2}{1}$$

Thus Eq. (2) at this boundary becomes

$$3\varepsilon_p D_p \frac{\partial^2 C_p}{\partial r^2} + K_1(C_s - C_p F(C_{pA})) = \varepsilon_p \frac{\partial C_p}{\partial t} \qquad \text{(A3)}$$

The finite difference equation resulting from Eq. (A5) is

$$3\varepsilon_p D_p \left[\frac{C_{p0,j+1} - 2C_{p1,j} + C_{p2,j+1}}{(\Delta r)^2}\right] + K_1(C_{s1,j+1} - F(C_{pA1})(C_{pi,j+1})) = \varepsilon_p \left[\frac{C_{p1,j+1} - C_{p1j}}{\Delta t}\right] \tag{A4}$$

The fictitious value contained in Eq. (A4) is eliminated by using the difference Eq. (A5) which results from Eq. (5) as follows:

$$\frac{C_{p2,j+1} - C_{p0,j+1}}{2\Delta r} = 0 \tag{A5}$$

which implies that $C_{p0,j+1} = C_{p2,j+1}$.

Thus the resulting finite difference equation at this point is

$$A_1^{(1)} C_{s0,j+1} + A_1^{(2)} C_{p0,j+1} + B_1^{(1)} C_{si,j+1} + B_1^{(2)} C_{p1,j+1} + C_1^{(1)} C_{s2,j+1} + C_1^{(2)} C_{p2,j+1} = D_1^{(1)} \tag{A6}$$

where $A_1^{(1)} = 0$

$A_1^{(2)} = 0$

$B_1^{(1)} = K_1 \Delta t (\Delta r)^2$

$B_1^{(2)} = -(6\varepsilon_p D_p \Delta t + K_1 \Delta t (\Delta r)^2 F(C_{pA1}) + \varepsilon_p (\Delta r)^2)$

$C_1^{(1)} = 0$

$C_1^{(2)} = 6\varepsilon_p D_p \Delta t$

$D_1^{(1)} = -\varepsilon_p (\Delta r)^2 C_{p1,j}$

Equation (A6) gives another fictitious point at the boundary $r = R$ which is eliminated by using Eq. (A7) which results from Eq. (6):

$$\varepsilon_p D_p \left(\frac{C_{pN+1,j+1} - C_{pN-1,j+1}}{2\Delta r}\right) = K_f(C_{dj+1} - C_{pN+1,j+1}) \tag{A7}$$

Thus the fictitious point $C_{pN+1,j+1}$ is expressed in terms of the interior point $C_{pN-1,j+1}$.

The finite difference equation at this boundary becomes

$$A^{(1)}_{N+1}C_{sN-1,j+1} + A^{(2)}_{N+1}C_{pN-1,j+1} + B^{(1)}_{N+1}C_{sN,j+1} + B^{(2)}C_{pN,j+1} + C^{(1)}_{N+1}C_{sN+1,j+1} + C^{(2)}_{N+1}C_{pN+1,j+1} = D^{(1)}_{N+1} \tag{A8}$$

where $A^{(1)}_{N+1} = 0$

$$A^{(2)}_{N+1} = 2\varepsilon_p D_p \Delta t$$

$$B^{(1)}_{N+1} = K_1 \Delta t(\Delta r)^2$$

$$B^{(2)}_{N+1} = 2\varepsilon_p D_p \Delta t + K_1 \Delta t(\Delta r)^2 F(C_{pAN+1}) + \varepsilon_p(\Delta r)^2 + 2K_f \Delta t \Delta r + \frac{2K_f \Delta t \Delta r}{N}$$

$$C^{(1)}_{N+1} = 0$$

$$C^{(2)}_{N+1} = 0$$

$$D^{(1)}_{N+1} = -\varepsilon_p(\Delta r)^2 C_{pN+1,j} - \left(2K_f \Delta t \Delta r + \frac{2K_f \Delta t \Delta r}{N}\right) C_{dj+1}$$

Similarly, the finite difference of Eq. (3) and the finite difference equations using the boundary conditions (8) and (9) can be written, respectively, as

$$A^{(3)}_{i}C_{si-1,j+1} + A^{(4)}_{i}C_{pi-1,j+1} + B^{(3)}_{i}C_{si,j+1} + B^{(4)}C_{pi,j+1} + C^{(3)}_{i}C_{si+1,j+1} + C^{(4)}_{i}C_{pi+1,j+1} = D^{(2)}_{i} \tag{A9}$$

for $2 \leq i \leq N$ and $1 \leq j \leq \text{JMAX}$.

$$A^{(3)}_{1}C_{s0,j+1} + A^{(4)}_{1}C_{p0,j+1} + B^{(3)}_{1}C_{s1,j+1} + B^{(4)}_{1}C_{p1,j+1} + C^{(3)}_{1}C_{s2\,j+1} + C^{(4)}_{1}C_{p2,j+1} = D^{(2)}_{1} \tag{A10}$$

$$A^{(3)}_{N+1}C_{sN-1,j+1} + A^{(4)}_{N+1}C_{pN-1,j+1} + B^{(3)}_{N+1}C_{sN,j+1} + B^{(4)}C_{pN,j+1} + C^{(3)}_{N+1}C_{sN+1,j+1} + C^{(4)}_{N+1}C_{pN+1,j+1} = D^{(2)}_{N+1} \tag{A11}$$

SYMBOLS

a_{i0}, a_{ij}	coefficients in Eq. (1)
b_{i0}, b_{ij}	exponents in Eq. (1)
C_{di}	concentration of solute i in fluid phase of the bath (g/cc)
C_{0i}	initial value of C_{di}
C_p	concentration of solute in pore-fluid phase (g/cc)
C_{pA}	value of C_p assumed

C_s	concentration of solute phase (per unit volume of particles) (g/cc)
D_p	effective diffusivity in pore fluid (cm^2/s)
D_s	effective diffusivity in particle solid phase (cm^2/s)
K_f	mass-transfer coefficient between liquid and particle (cm/s)
$K_{1,i}$	adsorption rate constant for solute i (h^{-1})
n	number of adsorbed solutes
r	radial distance in particle (cm)
R	radius of particle (cm)
t	time (s)

Greek Letters

Δr	increment along the radius r
Δt	increment in time
ε_B	bath void fraction
ε_p	particle void fraction

Superscripts

*	equilibrium value

Subscripts

eq	equilibrium value
i	index for grid points along the radius
j	time-step index
JMAX	maximum number of time steps
N	number of increments along the radius
neq	nonequilibrium value
p	pore
s	solid

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