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### Parametric Sensitivity Study of Multicomponent Adsorption in Agitated Tanks

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## Parametric Sensitivity Study of Multicomponent Adsorption in Agitated Tanks

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### Abstract

A comprehensive computer study of the most important physical, chemical, and geometric parameters on which the design of any multicomponent adsorption system relies was performed. In the analysis, the sensitivity of an adsorption model with respect to the model parameters was evaluated. The mathematical model utilized was developed by Mansour. The model takes into account internal and external diffusional resistances, and film resistance. The equilibrium between liquid and solid phases was described by a nonlinear Fritz-Schluender isotherm. The theoretical transient bath concentration profiles were obtained for the cases of adsorption of single, binary, and ternary systems. The numerical solution for the binary solute system was found to be in a very good agreement with previously published experimental results. The parametric study was applied to a binary solute system which has been shown to match corresponding experimental results. The parameters studied were: effect of competitive adsorption, size and porosity of carbon particles, porosity of carbon bath, adsorption rate constants, pore and solid diffusivities, film mass transfer coefficients, and fluctuations in the initial solutes concentration. Results obtained in this study were in agreement with those obtained by other investigators. The computer programs used in this study are flexible enough to be easily used for any number of components of any adsorption system in future studies.

## INTRODUCTION AND LITERATURE REVIEW

Adsorption on activated carbon has received widespread application in the treatment of municipal and industrial wastewaters. It is now recognized as a significant operation in the physicochemical treatment of waters and wastewaters (22). It is one of the applicable and attractive treatment concepts in the Best Available Treatment Economically Achievable (BATEA) process modes to be used to produce the 1983 quality level suggested for United States treatment plant effluents (7).

For the design of adsorbers it is necessary to know the concentration distribution of solutes in both the water and the adsorbing media. Reliable mathematical and experimental procedures are necessary to obtain design criteria for full-scale plants.

Numerical solutions for reliable and representative mathematical models must precede any design decision and should be performed prior to any experimental work for the following reasons:

1. A theory of multicomponent adsorption and factors affecting the process are lacking.
2. The time needed to perform an experiment is much greater than that usually needed to solve the engineering problem by numerical techniques.
3. It is much easier to get a numerical solution to a problem than to perform the experimental work.
4. The cost of labor and equipment required to perform experimental procedures is high.
5. Human and experimental errors encountered in the experimental work are minimized when numerical solutions are used. Adsorption theory is rigorous for single solutes, but becomes less definitive when applied to wastewaters containing multiple components with varying physical and chemical characteristics.

Unfortunately, most of the previous work regarding carbon treatment of industrial wastewaters centered around systems having single solutes. Therefore, it is hoped that the present study will contribute to the building of the theory of multicomponent adsorption.

A few investigators (11, 15, 23) have studied the effects of variation of the parameters influencing the process, and these workers used single-solute systems only.

The experimental factors influencing the adsorption process were studied by Martin and Al-Bahrani (15) using both batch (agitated flask) and column (flow through packed bed) systems. Carbon particle size, carbon

bed depth, flow rate, solution pH, and concentration were studied. They utilized gas-liquid chromatography in their adsorption experiments.

A mathematical model was developed by Wilson and Clarke (23) to describe a binary system of adsorption. The so-called lumped model was used to study the following parameters: solute diffusion constants, solute Langmuir isotherm parameters, pore depth, radius, and variability of radius.

A comprehensive mathematical model for multicomponent adsorption from a stirred bath was developed by Mansour (11, 14). Partial differential equations representing the adsorption model were numerically solved using finite difference techniques (14). Mansour's work included the investigation of the effects of the adsorption rate constant for a single-solute system.

The effective and reliable model developed by Mansour (14) has been used to investigate the effects of various parameters on the adsorption process of a binary mixture of butanol-2 and *t*-amyl alcohol.

## MATHEMATICAL MODEL

For any solute *i*, two differential equations result from mass balances in the pore fluid and on the adsorbent surface used to describe the pore and the surface concentrations inside the particles as functions of radius and time. These equations are

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

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

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:

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

at  $r = 0$ ,  $\frac{\partial C_{si}}{\partial r} = 0$  for any  $t$

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

and

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

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

In finite-bath models,  $C_{di}$  varies with time according to the following mass-transport equation:

$$\frac{dC_{di}}{dt} = \frac{3K_{fi}}{R} \left( \frac{1 - \varepsilon_B}{\varepsilon_B} \right) (C_{pi} - C_{di})_{r=R} \quad (3)$$

where  $\varepsilon_B$  is the void fraction of the bath.

The initial condition that completes the definition of Eq. (3) is  $C_{di}(t) = C_{di0}$  at  $t = 0$ .

Equilibria between fluid and solid phases are described by the following nonlinear general isotherm (8):

$$C_{si}^* = \frac{a_{i0} C_{pi}^{bi0}}{c_i + \sum_{j=1}^n a_{ij} C_{pj}^{bij}} = f_i(C_{p1}, C_{p2}, \dots, C_{pn}) \quad (4)$$

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.

For single-solute systems Eq. (4) reduces to the following Freundlich isotherms (10):

For Component 1 (butanol-2):

$$C_{s1}^* = 1.06 C_{p1}^{0.405} = f_1(C_{p1}) \quad (5)$$

For Component 2 (*t*-amyl alcohol):

$$C_{s2}^* = 1.07 C_{p2}^{0.348} = f_2(C_{p2}) \quad (6)$$

For Component 3 (phenol):

$$C_{s3}^* = 0.79 C_{p3}^{0.222} = f_3(C_{p3}) \quad (7)$$

For the binary system of butanol-2 (Component 1) and *t*-amyl alcohol (Component 2), Eq. (4) becomes (3)

$$C_{s1}^* = \frac{1.06C_{p1}^{1.217}}{C_{p1}^{0.812} + 0.626C_{p2}^{0.764}} = f_4(C_{p1}, C_{p2}) \quad (8)$$

$$C_{s2}^* = \frac{1.07C_{p2}^{1.254}}{C_{p2}^{0.906} + 0.045C_{p1}^{0.634}} = f_5(C_{p1}, C_{p2}) \quad (9)$$

For the ternary system of butanol-2, *t*-amyl alcohol, and phenol (Component 3), Eq. (4) becomes (3)

$$C_{s1}^* = \frac{1.05C_{p1}^{1.134}}{C_{p1}^{0.73} + 1.44C_{p2}^{0.793} + 0.53C_{p3}^{0.467}} = f_6(C_{p1}, C_{p2}, C_{p3}) \quad (10)$$

$$C_{s2}^* = \frac{1.09C_{p2}^{1.182}}{C_{p2}^{0.831} + 0.52C_{p1}^{0.884} + 0.30C_{p3}^{0.536}} = f_7(C_{p1}, C_{p2}, C_{p3}) \quad (11)$$

$$C_{s3}^* = \frac{0.79C_{p3}^{0.224}}{C_{p3}^{0.002} + 1.07C_{p1}^{0.286} + 0.79C_{p2}^{0.235}} = f_8(C_{p1}, C_{p2}, C_{p3}) \quad (12)$$

## METHOD OF NUMERICAL SOLUTION

It can be easily shown that the multicomponent model describing the behavior of *n* solutes consists of  $3n$  nonlinear partial differential equations, *n* isotherms,  $4n$  boundary conditions, and  $3n$  initial conditions.

For any component *i*, Eqs. (1) and (2) were coupled through Eq. (4) for different systems and successfully and iteratively solved using the backward-difference technique and a bi-tridiagonal algorithm (19). At the end of each time step of the solution of the above equations, Eq. (3) is numerically integrated. (Full details of the numerical solution are presented by Mansour (11, 14).)

## RESULTS AND DISCUSSION

### Comparison between Theoretical and Experimental Results

Regression analysis was used to test the degree of fitness of the results of the numerical solution on which this study was based with the experimental data. Numerical results obtained from the mathematical model for the

simultaneous adsorption of butanol-2 and *t*-amyl alcohol have been found to fit the experimental data obtained by Balzli (2) to accuracies of 92.4 and 90.9%, respectively.

### Parametric Analysis

There are many factors which influence both the rate and magnitude of adsorption. Detailed results and discussion of the most important factors affecting the performance of multicomponent adsorption process are presented herein. Each one of the eight parameters considered in this study was varied independently over its literature range while the other parameters were held constant at their average values. Table 1 shows parameter values as reported in the literature. The base case taken as a reference for all parameter values is shown in Table 2. These values were taken from the experimental work of Balzli (2).

### Effect of Number of Solutes on Adsorption (Competitive Adsorption)

Figures 1, 2, and 3 show data predicted for the adsorption of butanol-2, *t*-amyl alcohol, and phenol, each from its pure solution, calculated for simultaneous adsorption of butanol-2 and *t*-amyl alcohol from a mixture of both solutes (Fig. 4). Parameter values are given in Table 2.

A comparison of Figs. 1 and 2 with Fig. 4 shows that both the rate of adsorption and the steady-state concentration for each solute were adversely affected by the presence of the other solute. The steady-state

TABLE 1

Investigator	$K_1$ (s <sup>-1</sup> )	$K_f$ (cm/s)	$D_s$ (cm <sup>2</sup> /s)
Susuki and Kawazoe (18) <sup>a,b</sup>	—	—	—
Sphan and Schlunder (17) <sup>a,b</sup>	—	$2.3-5.2 \times 10^{-3}$	—
Liapis and Rippin (10) <sup>a</sup>	—	$2.2-2.54 \times 10^{-4}$	$1.25-2.2 \times 10^{-7}$
Balzli et al. (3) <sup>b</sup>	4248-6912	$4.132-4.472 \times 10^{-3}$	—
Martin and Al-Bahrani (15) <sup>b</sup>	—	—	—
Peel and Benedek (16) <sup>a,b</sup>	—	$6.8-9.9 \times 10^{-3}$	$1.7-2.5 \times 10^{-6}$

<sup>a</sup>Numerical work.

<sup>b</sup>Experimental work.

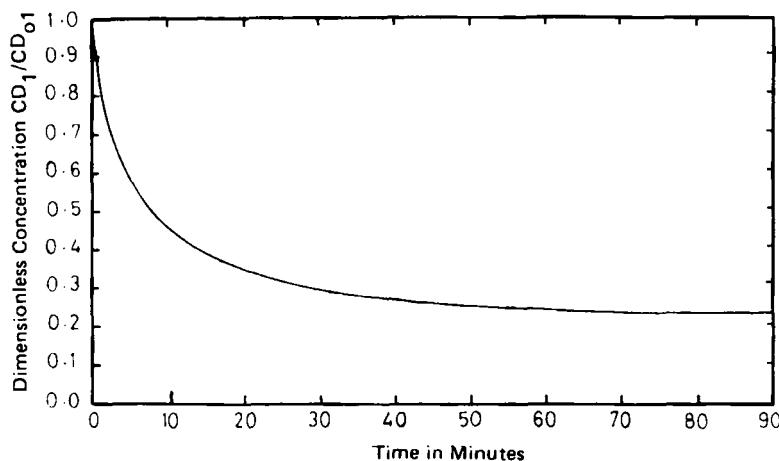


FIG. 1. Mathematical data for butanol-2.

value reached by each solute was about 50% of that when it was present alone in its solution.

When a ternary mixture of butanol-2, *t*-amyl alcohol, and phenol was used (i.e., phenol was added to the binary mixture described above), the same effect was observed; the steady-state concentration of butanol-2 was higher (less adsorption occurred) while a smaller effect was encountered for the adsorption of *t*-amyl alcohol. It was also observed that phenol was almost unaffected by the presence of other compounds as shown in Figs. 3 and 5. This was expected because phenol is known to have a higher

#### Parameters in Literature

$D_p$ (cm <sup>2</sup> /s)	$\epsilon_p$	$\epsilon_B$	$r$ (mm)	$C_0$ (g/cm <sup>3</sup> )
$0.94-5.9 \times 10^{-7}$	0.82-0.91	0.22-0.34	0.127-0.508	$2-4 \times 10^{-4}$
$0.28-1.25 \times 10^{-5}$	0.27-0.96	0.29	1.24-4.0	—
$7.4-13.0 \times 10^{-6}$	0.7	0.5	1.0	$10^{-3}$
$7.4-13.0 \times 10^{-6}$	0.94	0.9859	0.5	$5 \times 10^{-4}$
—	—	—	0.3-1.2	$5.6 \times 10^{-5}$
—	0.70	—	—	$10^{-4}$

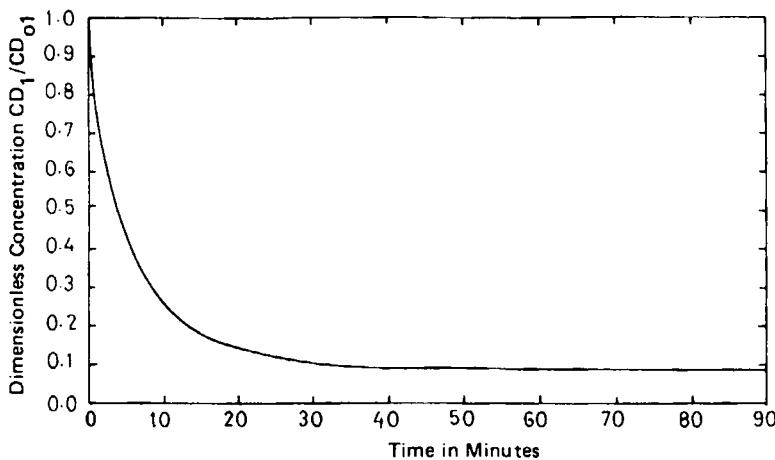


FIG. 2. Mathematical data for *t*-amyl alcohol.

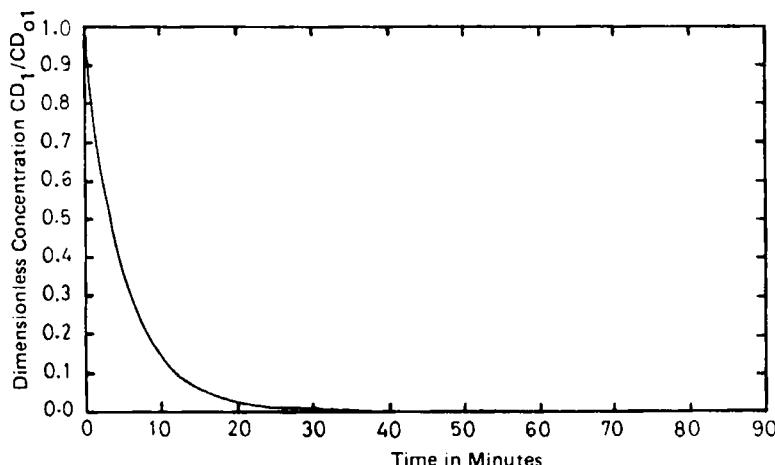


FIG. 3. Mathematical data for phenol.

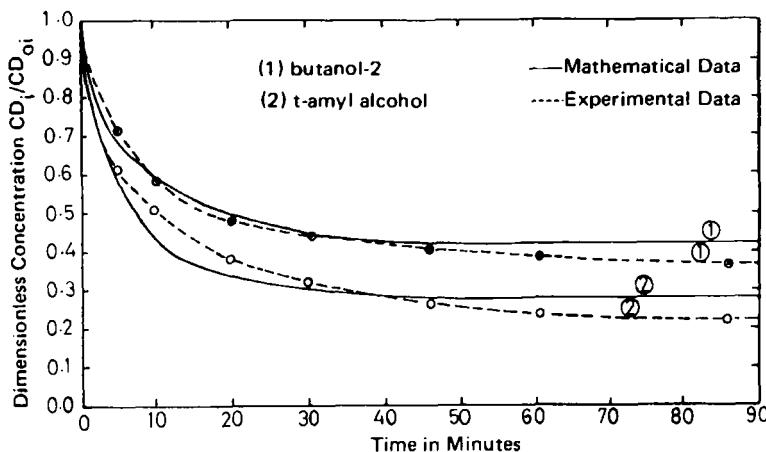


FIG. 4. Simultaneous adsorption of butanol-2 and *t*-amy1 alcohol in a finite bath.

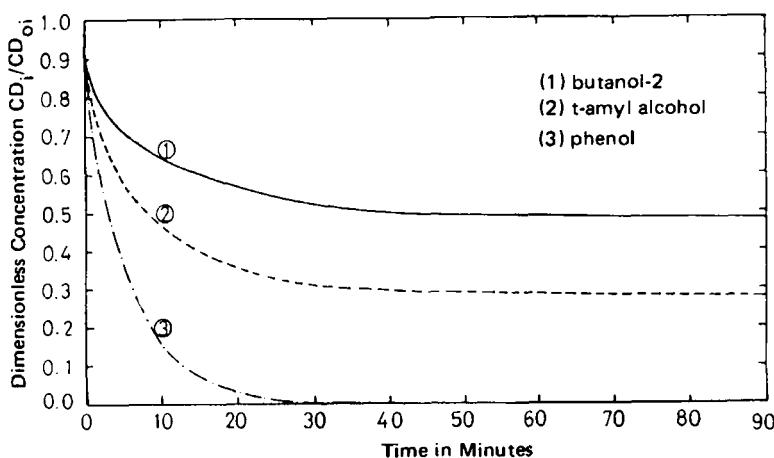


FIG. 5. Simultaneous adsorption of butanol-2, *t*-amy1 alcohol, and phenol in a finite bath.

TABLE 2  
Base Case Values

Component 1:	Component 2:
$C_{01} = 5 \times 10^{-4} \text{ g/cm}^3$	$C_{02} = 5 \times 10^{-4} \text{ g/cm}^3$
$K_1 = 1.92 \text{ h}^{-1}$	$K_2 = 1.76 \text{ h}^{-1}$
$K_{f1} = 4.472 \times 10^{-3} \text{ cm/s}$	$K_{f2} = 4.132 \times 10^{-3} \text{ cm/s}$
$D_{p1} = 7.4 \times 10^{-6} \text{ cm}^2/\text{s}$	$D_{p2} = 13.03 \times 10^{-6} \text{ cm}^2/\text{s}$
$D_{s1} = 1.25 \times 10^{-7} \text{ cm}^2/\text{s}$	$D_{s2} = 2.20 \times 10^{-7} \text{ cm}^2/\text{s}$
Component 3:	Parameters of the bath:
$C_{03} = 5 \times 10^{-4} \text{ g/cm}^3$	$R = 0.05 \text{ cm}$
$K_3 = 1.18 \text{ h}^{-1}$	$c_p = 0.94$
$K_{f3} = 4.380 \times 10^{-3} \text{ cm/s}$	$\epsilon_B = 0.9859$
$D_{p3} = 19.2 \times 10^{-6} \text{ cm}^2/\text{s}$	
$D_{s3} = 3.2 \times 10^{-7} \text{ cm}^2/\text{s}$	

adsorption affinity and larger diffusion coefficients.

The differences in the amounts of adsorption of each solute, due to the addition of other solutes, are caused by the competition occurring among solutes to occupy vacant sites on the available surface of particles, and since the capacity of carbon is fixed, the amounts adsorbed decrease as the number of solutes increases. Also, differences in molecular size among solutes compared to the size of the pore mouths of particles may cause different rates of diffusion inside particles. Another important factor is the presence of different kinds of sites on the internal surfaces of pores, some of which are only available for specific solutes (9).

These observations are in accord with the studies of Martin and Al-Bahrani (15) and of Fritz et al. (8). They reported that competitive effects increased noticeably with an increase in the number of solutes in solution. This could have a significant influence on the performance of activated carbon for the removal of dissolved solutes from polluted water.

### Effect of Porosity of Carbon Particles on Multisolute Adsorption

Several computer runs have been made with values of porosity ranging between 0.6 and 0.94. As Fig. 6 indicates, the variation of particle porosity shows almost no effect on the concentration profiles. This may be due to the low concentrations of both solutes, so that the available volume of pores inside the carbon particles is sufficient to accommodate these dilute solutions. It has been found that as the porosity of a carbon particle increases, the solute storage capacity of pores in the fluid and solid phases

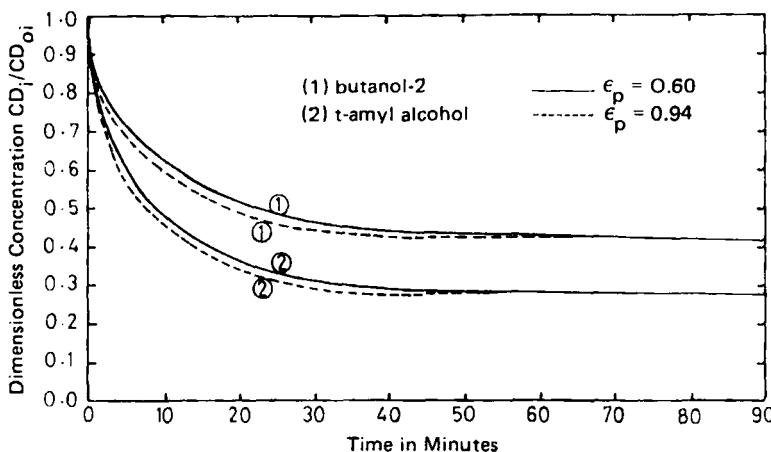


FIG. 6. Effect of particle porosity on bath concentrations.

becomes more due to the increase in the total surface available to the pores for adsorption (23). However, this does not mean that all the internal surface area will be available for all molecular sizes. It has been reported that the activated carbon particles consist of two regions, the macropores and the micropores (16). The macropores have radii significantly larger than the size of the diffusing solute molecules, and in these the rates of diffusion are rapid. The micropore region has sizes comparable to the diffusing molecules, and within these the rates of diffusion are restricted because of the roughness of the wall and the multidirectional bonding forces.

### Effect of the Voidage of the Bath on Multisolute Adsorption

Several computer runs have been made with values of voidage  $\epsilon_B$  ranging between 0.4 and 0.9. It can be seen from Fig. 7 that rapid adsorption of both solutes takes place for low values of  $\epsilon_B$ . It is expected that as the voidage of the bath increases, the available surface area of the carbon particles will be smaller, resulting in slower adsorption for both solutes. Also, the volume of solution surrounding the carbon particles will be larger, so that a longer contact time is required for solute molecules to be transported through the solution and diffuse into the thin film surrounding the particle.

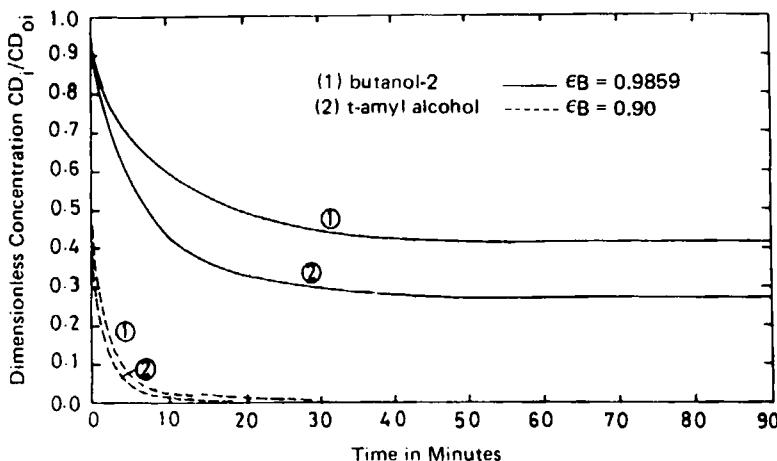


FIG. 7. Effect of the voidage of the bath on bath concentrations.

### Effect of Carbon Particle Size on Multisolute Adsorption

As shown in Fig. 8, rapid adsorption occurs when small particles are used, so lower concentration profiles result for small-sized particles. Two factors are believed to cause this behavior (4). The first concerns the mass transfer coefficients and the outside area per unit volume. When particles are contacted by the solution, the rate of mass transfer is controlled by the outside film resistance, and since all computer runs have the same initial concentration, the effect of this factor on the driving force for mass transfer is the same in all cases. Therefore, the rate of mass transfer is proportional to the product of the mass transfer coefficients and the outside area of the activated carbon particles per unit volume. Since this product is the smallest for 1.3 mm particles, the steady-state concentration for the two solutes will be the highest and the rate of adsorption will be the smallest. The second factor behind this phenomenon is that for a given particle, as its radius increases, the time required to reach steady-state concentration will be greater since it has a longer diffusional path (23).

Therefore, there is an increase in the reduction of bath concentration and rate of adsorption with decreasing carbon particle size, and this may be partly explained as being due to the opening of new pores when the carbon is crushed to a smaller particle size (22).

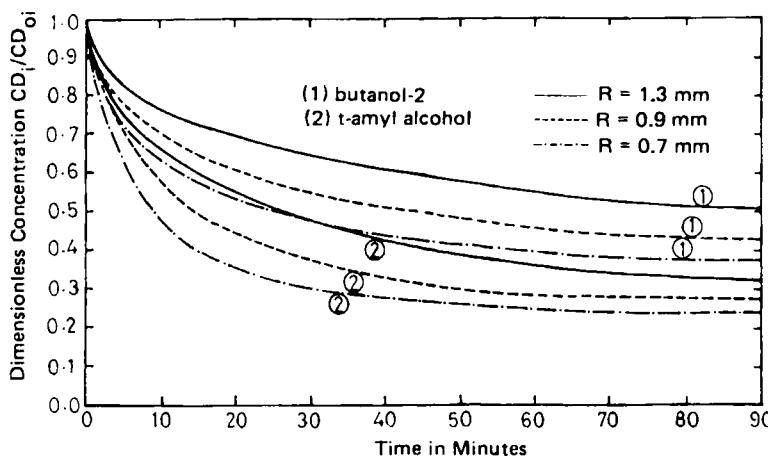


FIG. 8. Effect of particle size on bath concentrations.

### Effect of the Adsorption Rate Constant on Multisolute Adsorption

The effect of the adsorption rate constant,  $K$ , is shown in Fig. 9 which indicates that as  $K$  increases, the steady-state value of both solutes is reached earlier, since for large values of  $K$  the resistance to mass transfer will not slow down the rate of adsorption, and equilibrium at all points on the carbon particles will be readily attained. For small values of  $K$  the resistance to mass transfer is relatively large and the rate of adsorption will be slower (24).

Since the large values of  $K$  used to predict bath concentration values from the mathematical model proved to be in good agreement with experimental results, it is concluded that physical adsorption is relatively fast, so the rate of adsorption itself is rapid, and local equilibrium between solutes in pore liquid and solid phases can be assumed.

### Effect of Pore-Diffusion Coefficients on Multisolute Adsorption

Figure 10 shows the negligible effects on the bath concentration of Solute 2 as  $D_{p1}$  changes, while larger effects are noticed in the concentration profile of Solute 1. This implies that mutual diffusional effects resulting from

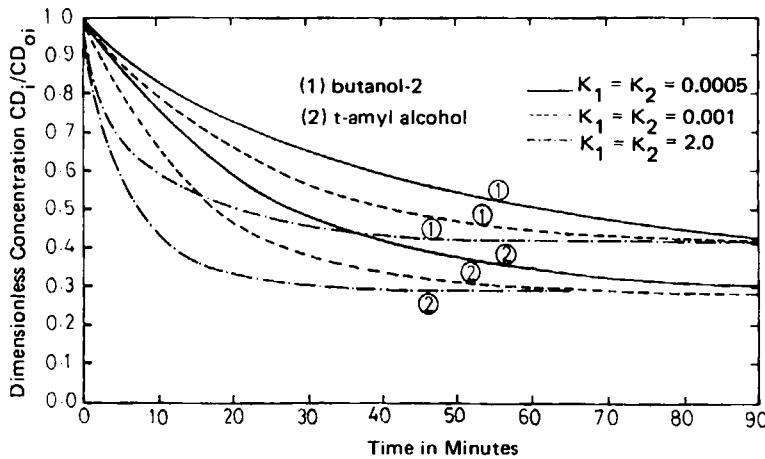


FIG. 9. Effect of adsorption rate constant on bath concentrations.

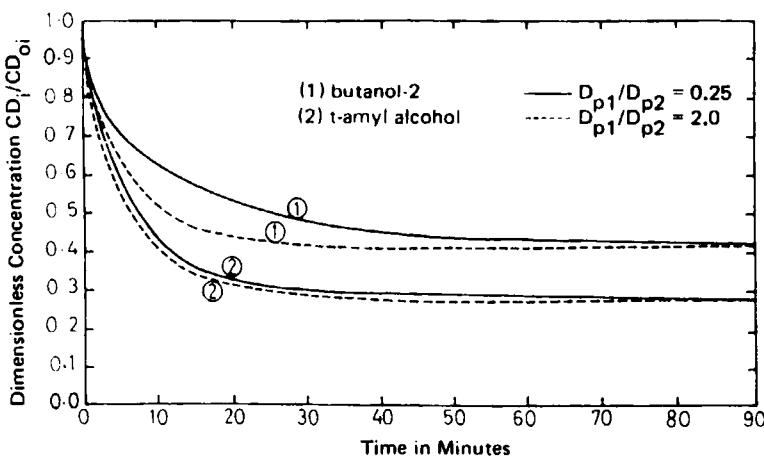


FIG. 10. Effect of pore diffusion coefficient on bath concentrations.

changes of  $D_p$ 's of different species (for this diluted mixture) are negligible. As expected, faster adsorption of Solute 1 occurs for higher values of  $D_{p1}$ .

### Effect of Solid-Diffusion Coefficients on Multisolute Adsorption

The effect of varying  $D_{s1}/D_{s2}$  ( $D_{s2}$  held constant) is shown in Fig. 11. In general, as Crittenden (5) found, the surface diffusion coefficients ( $D_s$ 's) depend on solute surface affinity. The more strongly adsorbed a molecule (a species) is, the less likely the molecule will migrate on the surface, i.e., the surface  $D_s$  decreases with increasing surface affinity. Hence, the surface flux ( $-D_s(\partial C_s/\partial r)$ ) did increase with increasing solute surface affinity. This phenomenon explains, as shown in Fig. 11, why varying  $D_{s1}$  influenced the concentration profile of Component 1 only, while negligible changes occurred in that of Component 2. It implies that the effects of the mutual diffusional interactions are much less than self-diffusion effects. As Fig. 11 indicates, for small values of  $D_{s1}$  there is little transfer of Component 1 into the particles and the concentrations in the pores are small; thus, few molecules are subject to adsorption and the total surface available to components is also small. Therefore, a slower adsorption is expected.

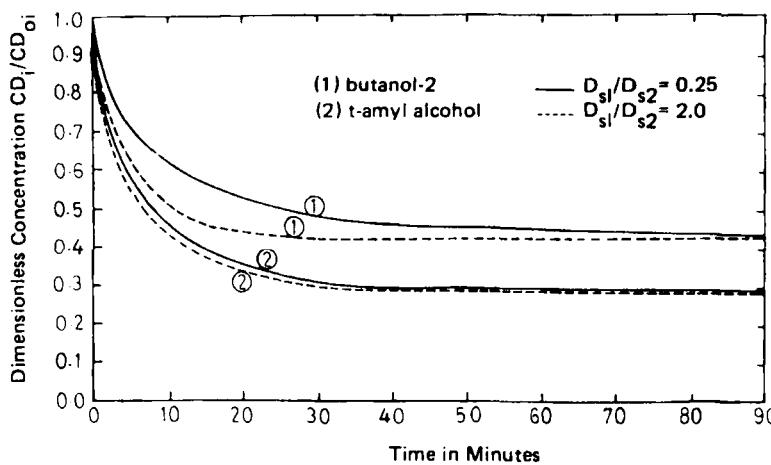


FIG. 11. Effect of surface diffusion coefficient on bath concentrations.

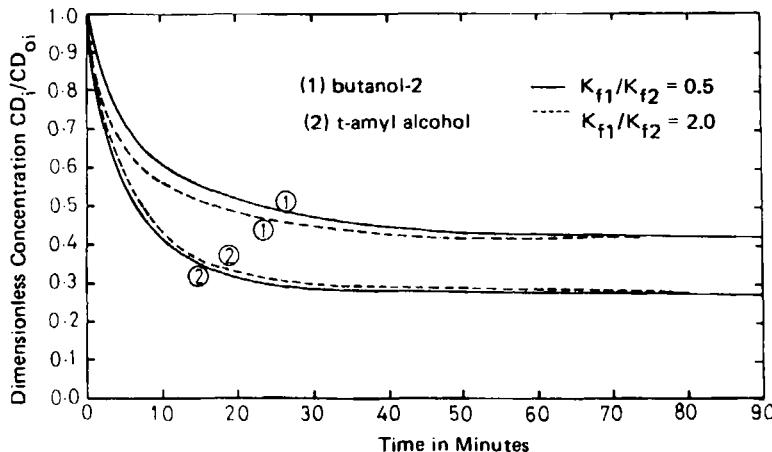


FIG. 12. Effect of mass transfer coefficient on bath concentrations.

### Effect of Film-Mass Transfer Coefficient of Multisolute Adsorption

The effect of  $K_f$  is shown in Fig. 12 for two values of  $K_{f1}/K_{f2}$ , where  $K_{f2}$  was held constant. It is seen that as the value of  $K_{f1}$  increases (i.e., the resistance to mass transfer through the thin film surrounding each particle decreases), the rate of adsorption of Solute 1 increases, while the rate of adsorption of Solute 2 decreases. However, the steady-state values for the bath concentration of both solutes are the same. Also, since the rate of adsorption of Solute 1 increases, equilibrium is reached earlier.

This behavior is expected, since at fixed values of pore diffusion constant  $D_{p1}$  and particle size  $R$ , the Biot number  $Bi$  will increase due to an increase in  $K_f$  caused by increasing the stirring speed in the bath. This results in a decrease in particle boundary layer thickness, which in turn results in increased mass transfer efficiency if the other parameters are held constant (18).

It is well known that as the degree of agitation increases, the external mass transfer resistance is reduced, hence the adsorption process will be controlled mostly by pore diffusion (6).

### Effect of the Initial Concentration of Multisolute Adsorption

The effect of varying the initial concentration in the bath is shown in Fig. 13 for three values of  $C_{01}/C_{02}$ , where  $C_{02}$  was held constant. As the initial

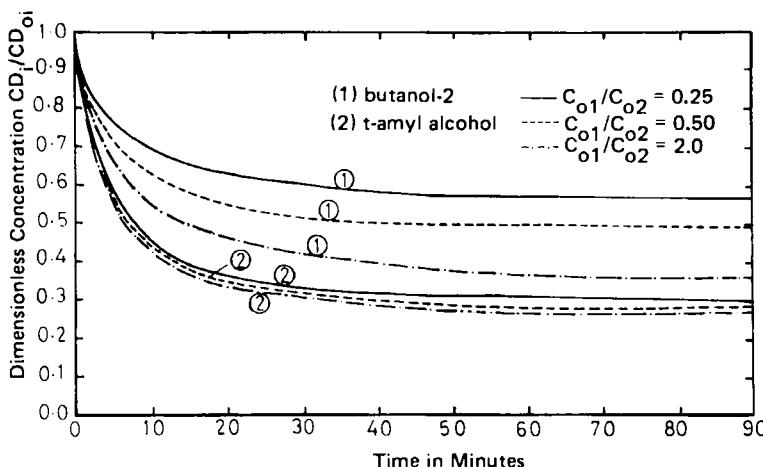


FIG. 13. Effect of initial concentration on bath concentrations.

concentration of Solute 1 increases, the rate of adsorption of Component 1 increases and the steady-state value for the bath concentration of Solute 1 will decrease. Also, as  $C_{01}$  increases, the difference between the steady-state values for bath concentration of Solute 1 for the three cases will be more affected than those for Solute 2. Thus the steady-state capacity of the activated carbon particles for each solute will be adversely affected by the presence of the other solute (15).

This difference of behavior of the two solutes in the adsorption process may be due to the relative competition for the surface area of particles. The extent of adsorption of each solute is a function of the relative pure solute affinities as well as the relative concentrations (12).

## CONCLUSIONS

A fairly comprehensive parametric study has been made on eight important parameters that are reported to influence the multicomponent adsorption process performance and design.

The conclusions that can be drawn from this study are summarized as follows:

1. The variation of the particle porosity has a small effect on the rate of adsorption of all solutes present in the organic mixture.
2. An increase in the voidage of the bath leads to an increase in the

remaining bath concentrations while low voidage leads to rapid solute adsorption.

3. Reduction in the particle size leads to a reduction in the remaining bath concentration and an increase in the rate of adsorption of solute.
4. The adsorption rate constant has a great effect on the adsorption process because, as  $K$  increases, the contact time required to achieve steady-state conditions is reduced. For large values of  $K$  the adsorption process is so rapid that equilibrium can be assumed between liquid and solid phases for all solutes.
5. An increase in the pore diffusion constant leads to an increase in the rate of adsorption which shortens the time to reach equilibrium concentration. Small changes in the value of  $D_p$  result in small effects on the concentration profile.
6. The effect of the solid diffusion constant is the same as that of  $D_p$  but to a lesser extent.
7. An increase in the film transfer coefficient caused by increasing the stirring speed leads to an increase in the rate of adsorption so equilibrium will be reached earlier while the equilibrium bath concentration will remain the same. For large values of  $K_f$ , adsorption can be assumed to be pore diffusion-controlled.
8. An increase in the initial bath concentration of solute leads to an increase in the rate of adsorption and in the equilibrium batch concentration.
9. The presence of more than one solute in solution will cause an increase in the equilibrium bath concentrations and a reduction in the rate of adsorption of each solute. Mutual effects have a great influence on the performance of multicomponent adsorption processes.
10. For dilute systems, mutual interactions resulting from changing convective and diffusive transfer coefficients are of negligible effect.

## SYMBOLS

$a_{i0}$ , $a_{ij}$	coefficients in Eq. (4)
$b_{i0}$ , $b_{ij}$	exponents in Eq. (4)
$C_d$	concentration of solute in fluid phase of the bed (g/cc)
$C_0$	the value of $C_d$ at the beginning of adsorption
$C_p$	concentration of solute in the pore fluid phase (g/cc)
$C_s$	concentration of solute in the solid phase (per unit volume of particles), (g/cm <sup>3</sup> )

$D_p$	effective diffusivity in the pore fluid (cm <sup>2</sup> /s)
$D_s$	effective diffusivity in the particle solid phase (cm <sup>2</sup> /s)
$K_f$	mass transfer coefficient for liquid–particle transfer (cm/s)
$K$	adsorption rate coefficient (h <sup>-1</sup> )
$r$	radius of particle (cm)
$t$	time (s)

### Greek

$\varepsilon_B$	bed void fraction
$\varepsilon_p$	particle void fraction

### Superscripts

*	Equilibrium value
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### Subscripts

$i$	index for the solute number
$j$	index for the solute number
$p$	pore
$s$	solid

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