k = wavenumber
k_d = Kolmogoroff dissipation wavenumber, $(= \epsilon^{1/4}/\nu^{3/4})$
r = radial coordinate
R = pipe radius
Re = Reynolds number
$R_{11}(\tau)$ = autocorrelation of streamwise fluctuating velocity
T_B = mean time between bursts
u^* = friction velocity
u' = root-mean-square fluctuating velocity
U, U^+ = mean velocities, $(U^+ = U/u^*)$
x = downstream distance ($x = 0$ at point of injection)
y, y^+ = distance from wall $(y^+ = yu^*/\nu)$

Greek Letters

ϵ = rate of energy dissipation
η_d = dissipation length scale, $(= \nu^{3/4}/\epsilon^{1/4})$
ν = kinematic viscosity
τ = delay time in autocorrelation
τ_d = dissipation time scale $(= \nu^{1/2}/\epsilon^{1/2})$

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Manuscript received April 6, 1981; revision received September 22, and accepted October 13, 1981.

Further Work on Multicomponent Liquid Phase Adsorption in Fixed Beds

The problem of multicomponent liquid phase adsorption in fixed beds was studied further. In contrast to the earlier work (Hsieh et al., 1977), the method developed in this work is more efficient and also has a greater scope of applicability as it incorporates the use of the IAS (Ideal Adsorbed Solution Theory) method for the estimation of multicomponent adsorption equilibrium data. It was shown that the use of the more complex IAS method for the prediction of the isotherm data does not present insurmountable obstacles as once feared (DiGiano, 1978) but provides much better prediction of carbon adsorption. An extension of the method to batch adsorption was shown to be straightforward and presented no special difficulty.

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SCOPE

This study further develops the numerical technique necessary for the solution of multicomponent liquid phase adsorption in fixed beds. Although a general method for the solution of this problem is already available (Hsieh et al., 1977) this earlier developed method was found to experience convergence difficulty if the number of adsorbable species involved is large and/or if the rate controlling step of the adsorption process is a combination of the liquid and particle phase mass transfer resistances. Furthermore, it was limited to systems whose equilibrium relationships are of the Langmuir type.

The method developed in this work is free of the convergence difficulty. Furthermore, it is developed to incorporate the use of the IAS method for the prediction of the isotherm data, which

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0001-1541-82-5764-0565-$2.00

is suited for adsorbents with heterogeneous surfaces (such as activated carbon). The availability of a computation algorithm which can be used for the calculation of the simultaneous adsorption of a large number of adsorbates with activated carbon is particularly relevant to the study of the carbon process for water and waste treatment.

CONCLUSIONS AND SIGNIFICANCE

The numerical method developed in this work represents a more general and also more practical alternative to previous ones for the calculation of liquid phase adsorption involving a large number of adsorbable species. The comparative study on the choice of the expression of the equilibrium relationship between the solution and adsorbed phases, indicates that in spite of the apparent complexities of the IAS method for isotherm prediction, the increase in CPU time for a given calculation with the use of the IAS method is not excessive. On the other hand, much better agreement with experiment was achieved when the IAS method was employed.

Fixed bed adsorption has been used extensively in industrial processes for the purposes of separation and purification. Although a significant number of these applications are concerned with multicomponent systems, most of the studies and analyses of fixed bed processes are confined to single species adsorption. Only in recent years has there been any significant effort directed toward the study of fixed bed multicomponent adsorption under nonequilibrium conditions.

The first analytical study of fixed bed sorptive processes involving more than one species was made by Dranoff and Lapidus (1958) who considered the ion exchange problem with two exchanging species. Their results are directly applicable to bi-solute adsorption if the rate of adsorption is of the chemical-reaction type. An approximate procedure for the solution of multicomponent fixed bed adsorption was proposed by Cooney and coworkers (1966, 1972) based on an earlier work of Cooney and Lightfoot (1965). The procedure was found to give reasonable accuracy (Hsieh et al., 1977). It is not clear how this procedure can be extended to situations when the number of adsorbable species exceed two.

In more recent years, the use of granular activated carbon for water and waste treatment has become widely spread. This has stimulated considerable interest in the study of multiple species carbon adsorption including those by Crittenden, (1976); Crittenden and Weber, (1978); Liapis and Rippin, (1977, 1978) and Balzli et al., (1978). These studies, in general, dealt with bi-solute adsorption and the use of specially derived adsorption isotherm expressions. The usefulness of these results therefore are limited.

A more general method for the numerical solution of fixed bed multicomponent adsorption was formulated by Hsieh, Turian and Tien (1977). The general rate controlling step was considered to be confined either in the liquid phase, particle phase or a combination of both. The equilibrium relationship was assumed to be of the Langmuir type. However, the method becomes less efficient when mass transfer resistances in both phases become comparable. (For instance, see example problems given in Tables 1 and 2 of Hsieh et al., 1977.)

The thermodynamic relationship between a solution containing adsorbable species and adsorbents in contact with the solution at equilibrium is the absorption isotherm which relates the concentrations in the solution phase with those in the adsorbed phase. It is one piece of information necessary to the calculation of adsorption kinetics. In fixed bed processes with the local equilibrium assumption, isotherm data, together with stoichiometric consideration, define fixed bed performance. For the more realistic consideration of including mass transfer effects, the knowledge of isotherm expression is needed for the calculation of the interphase concentrations of adsorbable species.

For systems involving a single adsorbable species, the necessary equilibrium relationship can best be determined from experimentation. The choice of the isotherm functional form is dictated largely by its ability to represent the data. Although the specific isotherm functional form used may determine whether or not an analytical solution of the relevant adsorption problem can be obtained, numerical methods which are often required for the more general rate expression are insensitive to isotherm functional forms. The important consideration is that the chosen function fits the data accurately.

Such convenience however does not exist in the case of multicomponent adsorption. Experimental determination of isotherm data becomes difficult and even impractical if the number of adsorbable species becomes greater then four or five. Even when the data become available, there also exists the difficulty of fitting the data into analytic form since more species means more variables to be considered. Furthermore, in many cases such as liquid wastes, a complete identification of all of all the species is impossible.

For problems dealing with multicomponent adsorption, the practical way of obtaining the equilibrium relationship is to rely on methods which express the equilibrium relationship of a multicomponent system in terms of the single species isotherm data of the individual species. The Langmuir isotherm expression represents such a possibility and was, therefore, used in the earlier study (Hsieh et al., 1977). The Langmuir expression, however, does not always provide accurate predictions, especially for adsorbents with inhomogeneous surfaces (Jain and Snoeyink, 1973; Fritz and Schluender, 1974; Huang and Steffens, 1976). In more recent years, an alternative way of predicting multicomponent isotherms from isotherm data of individual species based on the ideal adsorbed solution theory (Myers and Prausnitz, 1965; Radke and Prausnitz,

TABLE 1. ISOTHERM PARAMETERS

	Langmuir* $\left(q = \dfrac{ac}{1+bc}\right)$		Freundlich ($q = AC^{1/n}$)	
Substance	a	b	A	$1/n$
PNP	115	34.7	3.3	0.15
PCP	86.3	27.7	3.1	0.16
PA	0.264†(0.892)*	0.0841†(0.667)*	0.48†(0.45)*	0.4†(0.44)*

† For c_o = 100 m mol/L.
* For c_o = 10 m mol/L.

TABLE 2. MASS TRANSFER PARAMETERS

Substance	D_l(cm^2/s)	D_s(cm^2/s)	k_l^*(cm/s)	k_s(s^{-1})
PNP	9×10^{-6}	2×10^{-8}	1.7×10^{-3}	6.89×10^{-5}
PCP	9×10^{-6}	2×10^{-8}	1.7×10^{-3}	6.89×10^{-5}
PA	9×10^{-6}	1.5×10^{-7}	1.7×10^{-3}	5.16×10^{-4}

$\rho_p = 0.59$ g/cm^3; $\rho_b = 0.39$ g/cm^3; $a_p = 6.6 \times 10^{-2}$ cm.
* Corresponding values estimated from the correlation suggested by Vermeulen et al. (1973).

$$\frac{3k_l}{a_p} = \frac{\frac{2.62}{1-0.4}(D_l u)^{0.5}}{(2a_p)^{1.5}}$$

are found to be approximately within 10% of the tabulated values.

1972 and Sircar and Myers, 1973) was proposed. The IAS method was found to give good agreement of isotherm data with activated carbon as adsorbents (Fritz, 1978). However the expression was considered too complex to be used in numerical calculations (DiGiano, 1978) and a simplified form was suggested (DiGiano et al., 1978).

In the present study, a numerical method for the solution of multicomponent adsorption, which permits the use of the IAS method for the estimation of the isotherm data, is proposed. The availability of this method makes it possible to carry out adsorption calculation involving an arbitrary large number of adsorbable species under fairly general conditions.

MULTICOMPONENT ADSORPTION ISOTHERM

The IAS (Ideal Adsorbed Solution) method defines the equilibrium relationship between the solution and adsorbed phases by a system of equations. The isotherm of the single species, in general, can be expressed as

$$q_i^o = f(c_i^o, T) \tag{1}$$

where the superscript, o, denotes the state of single species.

The concentration of the i-th species in the adsorbed phase, q_i, in equilibrium with a solution containing N-species with concentrations of $c_1, c_2, \ldots c_N$ is determined by the following set of equations:

$$c_i = c_i^o(\pi_i, T) z_i \tag{2}$$

$$q_i = q_T z_i \tag{3}$$

$$q_T = \frac{1}{\sum_{i=1}^{N} \frac{z_i}{q_i^o}} \tag{4}$$

$$\pi_i = \frac{RT}{\lambda} \int_o^{c_i^o} \frac{q_i^o}{c_i^0} dc_i^o \tag{5}$$

where λ is the area of the solution-solid interface and the spreading pressure, π is defined as the difference between the interfacial tension of the pure solvent-solid interface and that of the solution-solid interface at the same temperature; and

$$\sum_{i=1}^{N} z_i = 1 \tag{6}$$

Namely, for a liquid solution with concentrations $c_1, c_2, \ldots c_N$ for the various species, the adsorbed phase concentrations $q_1, q_2, \ldots q_N$ can be found from a trial and error procedure. The IAS method is formulated on the basis that at equilibrium, the spreading pressures for all the species are the same. A single value of π_i for $i = 1, 2, \ldots N$ will first be assumed. From the knowledge of the single species isotherm expressions (Eqs. 1 and 5), the values of c_i^o's can be calculated. The knowledge of the values c_i^o's and the known condition of the solution concentrations ($c_1, c_2, \ldots c_N$) can be used to calculate the values of z_i's from Eq. 2. The correctness of the assumed spreading pressure is checked against Eq. 6. Once the correct value of π_i is found, the values of the adsorbed phase concentrations can be found from Eqs. 1, 4 and 3; namely the values of q_i^o's are found from the corresponding values of c_i^o's, which together with the values of z_i's, yield the value of q_T. Once the value of q_T is known, the values of q_i's can be obtained from Eq. 3.

The difference in the manner in which the solution phase concentrations and the adsorbed phase concentrations are related obviously has its implications in the calculations of adsorption in fixed bed. Intuitively it is also reasonable to assume that for a given system in fixed bed operations, the accuracy of the breakthrough curve obtained and the computation effort required will be different when different isotherm expressions are used. The selection of a particular form of isotherm expression to be used in the calculation of multispecies adsorption therefore involves the adjudication of several conflicting factors. An examination of this problem is the main objective of the present work.

GOVERNING EQUATIONS

The governing equations of the fixed bed absorption with N adsorbable species can be written as

$$u\left(\frac{\partial c_i}{\partial z}\right) + \rho_b \left(\frac{\partial q_i}{\partial \theta}\right) = 0 \tag{7}$$

$$\frac{\partial q_i}{\partial \theta} = \frac{3k_{l_i}}{a_p \rho_p}(c_i - c_{s_i}) = k_{s_i}(q_{s_i} - q_i) \tag{8a}$$

or

$$q_{s_i} = \phi_i(c_i - c_{s_i}) + q_i, \quad \phi_i = \frac{3k_{l_i}}{a_p \rho_p k_{s_i}} \tag{8b}$$

$$q_{s_i} = f(c_{s1}, c_{s2}, \ldots c_{sN}) \tag{9}$$

$$i = 1, 2, \ldots N$$

These equations are written with assumptions such as plug flow, negligible axial dispersion, etc. which are commonly used in fixed bed processes. Equation 7 gives the material balance of the i-th species. The rate equation given by Eq. 8a makes the general assumption that mass transfer effects in both liquid and particle phases are important and Glueckauf's linear driving force assumption is used to describe the particle phase diffusion. The equilibrium relationship is assumed to be maintained at the particle-liquid interface.

Equations 7 and 8 are of the type of semi-linear hyperbolic equations. They can be solved by the third order algorithms developed by Vanier (1970), and subsequently applied successfully to a class of fixed bed processes (Vanier and Tien, 1970; Hsieh et al., 1977). In essence, the algorithms enable the calculation of the values of c_i and q_i at point (l, m) (Figure 1) from the values of c_i, q_i, c_{s_i}, q_{s_i} at the neighboring points (l − 1, m), (l − 1, m − 1) and (l, m − 1). Once the values of c_i and q_i at point (l, m) are determined, the corresponding values of c_{s_i} and q_{s_i} can be found from Eqs. 8a and 9. The specific functional form of the isotherm therefore determines the degree of complexity of this second step of computation. In the earlier study (Hsieh et al., 1977) the finding of the interphase concentrations was made in an iterative manner. Difficulty in convergence was experienced if the resistances to mass transfer in both phases were comparable.

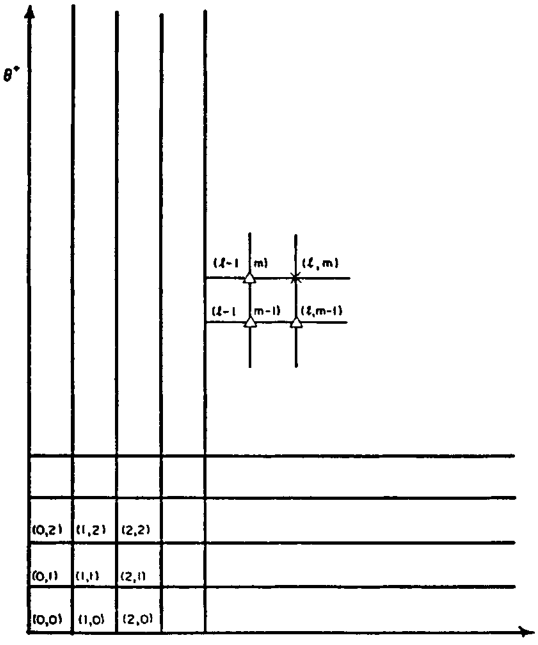

Figure 1. Computation grids for the numerical integration.

DEVELOPMENT OF COMPUTATION ALGORITHMS

The governing equations of fixed bed adsorption (Eqs. 7 and 8) can be written into dimensionless form as

$$\frac{\partial c_i^+}{\partial z^+} + \frac{\Lambda_i}{\Lambda_1}\frac{\partial q_i^+}{\partial \theta^+} = 0 \qquad (10)$$

$$\frac{\Lambda_i}{\Lambda_1}\frac{\partial q_i^+}{\partial \theta^+} = \frac{k_{l_i}}{k_{l_1}}(c_i^+ - c_{s_i}^+) = \Lambda_i \frac{a_p k_{s_i} \rho_p}{3 k_{l_1} \rho_b}(q_{si}^+ - q_i^+) \qquad (11)$$

where

$$\Lambda_i = \rho_b q_i^* / c_{i_o} \qquad (12a)$$

$$\theta^+ = \frac{\theta}{\Lambda_1}\frac{3}{a_p}\frac{\rho_b}{\rho_p} k_{l_1} \qquad (12b)$$

$$z^+ = \frac{z}{u}\frac{3}{a_p}\frac{\rho_b}{\rho_p} k_{l_1} \qquad (13)$$

and the dimensionless interphase concentrations $c_{s_i}^+$ and $q_{s_i}^+$ are related by the isotherm expression (Eq. 9).

As stated earlier the computation proceeds in two stages. Referring to Figure 1, assuming that all the dependent variables are known at points (l − 1, m), (l, m − 1) and (l − 1, m − 1), the values of c_i^+ and q_i^+ at point (l, m) can be calculated from the algorithms developed earlier (Vanier, 1970; Hsieh et al., 1977); namely,

(A) A first estimate of c_i^+ and q_i^+ is found to be

$$c_{il,m}^{+(1)} = c_{il-1,m}^+ + c_{il,m-1}^+ - c_{il-1,m-1}^+ + \Delta z^+[-P_{il-1,m} + P_{il-1,m-1}] \qquad (14a)$$

$$q_{il,m}^{+(1)} = q_{il-1,m}^+ + q_{il,m-1}^+ - q_{il-1,m-1}^+ + \frac{\Delta\theta^+ \Lambda_1}{\Lambda_i}[P_{il,m-1} - P_{il-1,m-1}] \qquad (14b)$$

where

$$P_i = \frac{k_{l_i}}{k_{l_1}}(c_i^+ - c_{s_i}^+)$$

(B) An iterative calculation is carried out as follows

$$c_{il,m}^{+(k)} = c_{il,m}^{+(1)} + \frac{\Delta z^+}{2}[-P_{il,m}^{(k-1)} - P_{il-1,,m-1} + P_{il,m-1} + P_{il-1,m}] \qquad (15a)$$

$$q_{il,m}^{+(k)} = q_{il,m}^{+(1)} + \frac{\Delta\theta^+}{2}\frac{\Lambda_1}{\Lambda_i}[P_{il,m}^{(k-1)} + P_{1l-1,m-1} - P_{il,m-1} - P_{il-1,m}] \qquad (15b)$$

where $P_i^{(k-1)}$ is the value of P_i evaluated with the $(k-1)$th iterative values of c_i^+ and q_i^+. The iteration stops when the desired degree of convergence is achieved.

Interspersed in the above-mentioned procedures is the need to calculate the values of $c_{s_i}^+$ and $q_{s_i}^+$ for every set of iterated values of $c_i^{+(k)}$ and $q_i^{+(k)}$ (as well as their final values). It was found more convenient to make this calculation with dimensional equations. Although there is no problem in converting the isotherm expression, i.e., Eq. 9 into dimensionless form, such transformation causes the presence of terms containing reference species concentration and therefore yields no particular advantages.

Since the interphase concentrations are assumed to be in equilibrium, q_{s_i} and c_{s_i} are related by the set of Eqs. 1 to 6. The calculation of q_{s_i} and c_{s_i}, once the values of c_i and q_i are known, can be proceeded as follows. First a general expression for the single species isotherm can be written as

$$q_i^o = (A_i)_k (c_i^o)^{1/(n_i)_k} \qquad \text{for } (c_i^o)_{k-1} \leq c_i^o < (c_i^o)_k \qquad (16)$$

namely the single species isotherm data can be approximated by the Freundlich expression in a piecewise basis as was done by Fritz and Schlunder (1981). The number of segments to be used, of course, depends on the data as well as the desired degree of association. The spreading pressure of the i-th species (Eq. 5) becomes

$$\Pi = \int_o^{c_i^o} \frac{q_i^o}{c_i^o} dc_i^o = (n_i)_k (A_i)_k (c_i^o)^{1/(n_i)_k} - (\delta_i)_k \quad (c_i^o)_{k-1} \leq c_i^o < (c_i^o)_k \qquad (17)$$

where

$$\Pi = \frac{\pi_i \lambda}{RT} \qquad (18)$$

$$(\delta_i)_k = (n_i)_k (A_i)_k [(c_i^o)_{k-1}]^{1/(n_i)_k} - \sum_{m=1}^{k-1} (n_i)_m (A_i)_m \{[(c_i^o)_m]^{1/(n_i)_m} - [(c_i^o)_{m-1}]^{1/(n_i)_m}\} \qquad (19)$$

Equations 3 and 4 can be combined to give

$$q_{s_i} = \left[\sum_{j=1}^{N} \frac{z_j}{q_{s_j}^o}\right]^{-1} z_i \qquad (20)$$

Equation 17 can be rearranged to yield

$$(n_i)_k (A_i)_k (c_i^o)^{1/(n_i)_k} = \Pi + (\delta_i)_k \qquad \text{for } (c_i^o)_{k-1} \leq c_i^o < (c_i^o)_k \qquad (21)$$

Combining Eqs. 16, 20 and 21, one has

$$q_{s_i} = \left[\sum_{j=1}^{N} \frac{(n_j)_k z_j}{\Pi + (\delta_j)_k}\right]^{-1} z_i \qquad (22)$$

Also substituting Eq. 21 into Eq. 2 yields

$$c_{s_i} = \left[\frac{\Pi + (\delta_i)_k}{(n_i)_k (A_i)_k}\right]^{(n_i)_k} z_i \qquad (23)$$

with c_{s_i} given by the above expression, Eq. 8b becomes

$$q_{s_i} = q_i + \phi_i c_i - \phi_i \left[\frac{\Pi + (\delta_i)_k}{(n_i)_k (A_i)_k}\right]^{(n_i)_k} z_i \qquad (24)$$

From Eqs. 22 and 24, the following expression of z_i is established, i.e.

$$z_i = \frac{q_i + \phi_i c_i}{\phi_i \left[\frac{\Pi + (\delta_i)_k}{(n_i)_k (A_i)_k}\right]^{(n_i)_k} + \left[\sum_{j=1}^{N} \frac{(n_j)_k z_j}{\Pi + (\delta_j)_k}\right]^{-1}} = \frac{q_i + \phi_i c_i}{\phi_i \left[\frac{\Pi + (\delta_i)_k}{(n_i)_k (A_i)_k}\right]^{(n_i)_k} + \left(\frac{\Pi}{S}\right)} \qquad (25)$$

where

$$S = \sum_{j=1}^{N} \frac{(n_j)_k z_j}{1 + (\delta_j)_k/\Pi} = \Pi \sum_{j=1}^{N} \frac{(n_j)_k z_j}{\Pi + (\delta_j)_k} \qquad (26)$$

By definition, $\Sigma_{i=1}^{N} z_i = 1$. From Eq. 25 one has

$$\sum_{i=1}^{N} \frac{q_i + \phi_i c_i}{\phi_i \left[\frac{\Pi + (\delta_i)_k}{(n_i)_k (A_i)_k}\right]^{(n_i)_k} + \frac{\Pi}{S}} - 1 = 0 \qquad (27)$$

Also from Eqs. 25 and 26, one has

$$\sum_{i=1}^{N} \left[\frac{(n_i)_k (q_i + \phi_i c_i)}{[\Pi + (\delta_i)_k]} \frac{1}{\phi_i \left[\frac{\Pi + (\delta_i)_k}{(n_i)_k (A_i)_k}\right]^{(n_i)_k} + \frac{\Pi}{S}}\right] - \frac{S}{\Pi} = 0 \qquad (28)$$

Equations 27 and 28 are two algebraic equations with two unknowns Π and S. Thus with values of c_i and q_i known and the parameters of the single species isotherms available, Π and S can be found from these two equations. Once Π and S are calculated, c_{s_i} and q_{s_i} can be calculated from Eqs. 25, 22 and 23. The calculation of Π and S can be made using the Newton's iterative method; namely

$$\Pi^{(k)} = \Pi^{(k-1)} + \Delta\Pi^{(k)} \qquad (29)$$

$$S^{(k)} = S^{(k-1)} + \Delta S^{(k)} \qquad (30)$$

where the superscript k denotes the k-th iterated value. The cor-

TABLE 3. CONDITIONS AND CPU TIME OF THE SAMPLE CALCULATIONS

		CPU Time (s) IBM 370/155								
Case	Substrate	Method I Langmuir Isotherm	Method II IAS Isotherm	Method III Simplified IAS Isotherm	Inlet Conc. c_o (m mol/L)	Superficial Velocity u(cm/s)	Column Length z	Δz	Time (h) θ	$\Delta\theta$
1	PNP	11	28	26	1.02	6.43×10^{-2}	10	0.25	80	0.5
2	PCP	12	28	26	1.0	6.12×10^{-2}	10	0.25	80	0.5
3	PA	11	26	25	10.5	6.12×10^{-2}	18	0.45	8	0.05
4	PNP	32	95	85	1.01	6.12×10^{-2}	10	0.25	80	0.5
	PCP				0.99					
5	PNP	34	88	77	1.02	6.12×10^{-2}	10	0.25*	80	0.5*
	PA				100.					
6	PCP	34	90	77	1.0	6.12×10^{-2}	10	0.25*	80	0.5*
	PA				100					
7	PNP	48	128	111	1.0	6.12×10^{-2}	10	0.25*	80	0.5*
	PCP				0.98					
	PA				100					

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* $\Delta z = 0.5$ cm and $\Delta\theta = 0.25$ h were used in Method I calculation.

rection terms $\Delta\Pi^{(k)}$ and $\Delta S^{(k)}$ are found from the simultaneous solution of the following equations

$$\left(\frac{\partial f}{\partial \Pi}\right)_{\Pi^{(k-1)}S^{(k-1)}} \Delta\Pi^{(k)} + \left(\frac{\partial f}{\partial S}\right)_{\Pi^{(k-1)}S^{(k-)}} \Delta S^{(k)} = -f(\Pi^{(k-1)}S^{(k-1)}) \quad (31)$$

$$\left(\frac{\partial g}{\partial \Pi}\right)_{\Pi^{(k-1)}S^{(k-1)}} \Delta\Pi^{(k)} + \left(\frac{\partial g}{\partial S}\right)_{\Pi^{(k-1)}S^{(k-1)}} \Delta S^{(k)} = -g(\Pi^{(k-1)}S^{(k-1)}) \quad (32)$$

The subscript terms denote the values at which the derivatives are evaluated. The functions f and g are

$$f(\Pi,S) = \sum_{i=1}^{N} \frac{q_i + \phi_i c_i}{\phi_i \left[\frac{\Pi + (\delta_i)_k}{(n_i)_k (A_i)_k}\right]^{(n_i)_k} + \frac{\Pi}{S}} - 1 \quad (33)$$

$$g(\Pi,S) = \sum_{i=1}^{N} \left\{ \frac{(n_i)_k (q_i + \phi_i c_i)}{[\Pi + (\delta_i)_k]} \frac{1}{\phi_i \left[\frac{\Pi + (\delta_i)_k}{(n_i)_k (A_i)_k}\right]^{(n_i)_k} + \frac{\Pi}{S}} \right] - \frac{S}{\Pi} \quad (34)$$

The above development can be simplified if the single species isotherms can be approximated by the Freundlich expression over the entire interested concentration ranges, i.e.

$$q_i^o = A_i (c_i^o)^{1/n_i} \quad (35)$$

The corresponding expressions become

$$q_{s_i} = \left[\sum_{j=1}^{N} z_j n_j\right]^{-1} \Pi z_i \quad (36)$$

$$c_{s_i} = \left[\frac{\Pi}{n_i A_i}\right]^{n_i} z_i \quad (37)$$

$$f(\Pi,S) = \sum_{i=1}^{N} \frac{q_i + \phi c_i}{\phi_i \left(\frac{\Pi}{n_i A_i}\right)^{n_i} + \frac{\Pi}{S}} - 1 \quad (38)$$

$$g(\Pi,S) = \sum_{i=1}^{N} \frac{(q_i + \phi_i c_i) n_i}{\phi_i \left(\frac{\Pi}{n_i A_i}\right)^{n_i} + \frac{\Pi}{S}} - S \quad (39)$$

The calculation procedure remains the same as stated before.

NUMERICAL RESULTS AND COMPARISONS

A number of sample calculations were made in order to test the accuracy of the algorithms developed and to determine the required CPU time. These samples calculations correspond to the experimental data of fixed bed carbon adsorption of aqueous solutions of p-nitrophenol (PNP), p-chlorophenol (PCP) and propionic acid (in various combination) reported by Merk (1978). These experiments were chosen because of the availability of the relevant equilibrium and mass transfer data (Merk, 1978) and the fact that carbon adsorption of organics from aqueous solutions represent a most significant example of multicomponent adsorption processes.

The conditions used in the sample predictions are listed in Table 3. Seven cases were included; namely, three cases of single species adsorption (solutions containing PNP, PCP and PA respectively), three cases of two species adsorption (solutions containing PNP and PCP, PCP and PA and PNP and PA) and one case of three species adsorption (solution containing PNP, PCP and PA). The single species adsorption isotherm data for these three substances (with carbon of the type B 10 II, Lurgi Frankfurt/Main) determined experimentally by Merk are shown in Figure 2. Merk suggested that these data can be fitted piecewise by the Freundlich expression with the values of the parameters given in Table 4. These data were also fitted by the Langmuir and the Freundlich expressions over the concentration range of 0.01 c_o to c_o where c_o is the influent concentration used by Merk in obtaining the breakthrough curve data. (See Table 1 for the parameter values.)

For each sample calculation, three predictions were made. For single species adsorption cases, breakthrough curves were predicted with the use of the Langmuir isotherm (Method I), the Freundlich isotherm in piecewise manner (Method II) and the Freundlich isotherm (Method III). For multispecies adsorption cases, breakthrough curves were predicted with the use of the Langmuir isotherm (Method I), the IAS method with the individual single species

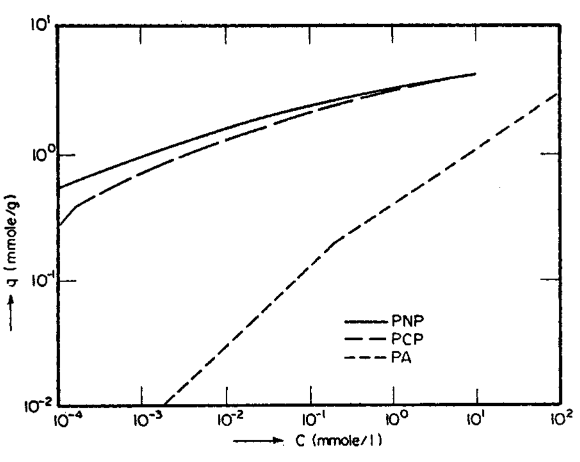

Figure 2. Adsorption isotherms.

TABLE 4. ADSORPTION ISOTHERMS FITTED PIECEWISE BY THE FREUNDLICH EXPRESSION

Substrate	Segment	Maximum Concentration $c_i^{\max}$(m mol/L)	A_i	$1/n_i$
PNP	1	8.2×10^{-5}	137	0.62
	2	8.15×10^{-4}	10.8	0.35
	3	1.05×10^{-2}	4.6	0.23
	4	0.141	3.5	0.17
	5	10	3.3	0.14
PCP	1	2.02×10^{-4}	52	0.57
	2	3.29×10^{-3}	6.2	0.32
	3	8.83×10^{-2}	3.5	0.22
	4	1	3.1	0.17
	5	100	3.1	0.14
PA	1	0.167	0.67	0.67
	2	2.34	0.46	0.46
	3	19	0.48	0.41
	4	1000	0.54	0.37

isotherms represented by the Freundlich expression piecewise (Method II) and the IAS method with the individual single species represented by the Freundlich expression (simplified IAS or Method III).

For predictions by Method 1, the algorithms developed earlier (Hsieh et al., 1977) were used with one modification in the calculation of the interphase concentrations. Details of the modification are given in the Appendix.

The mass transfer parameters used in the prediction were obtained in the following manner. The liquid phase mass transfer coefficient, k_e was estimated from the correlation (Shlunder, 1975):

$$k_l = \frac{[1 + 1.5(1 - \epsilon)]D_l}{2a_p} \left[2 + \sqrt{0.664 N_{Sc}^{1.5} N_{\mathrm{Re}} + \left[\frac{0.037 N_{\mathrm{Re}}^{0.5} N_{Sc}}{1 + 2.44(N_{Sc}^{2/3} - 1) N_{\mathrm{Re}}^{-0.1}}\right]^2}\right] \tag{40}$$

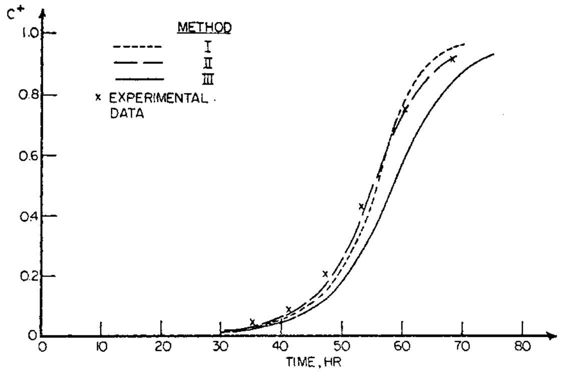

Figure 3. Effluent concentration profiles: PNP.

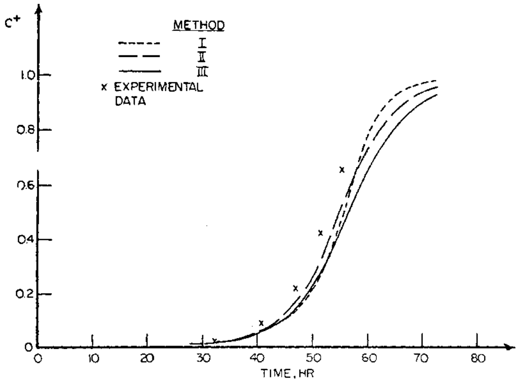

Figure 4. Effluent concentration profiles: PCP.

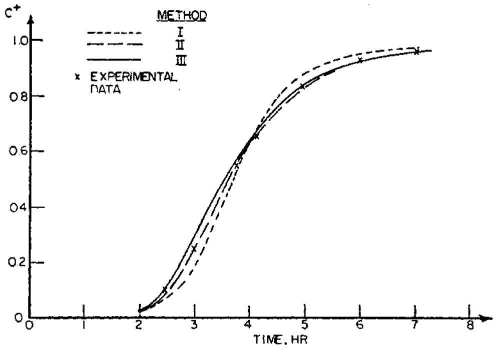

Figure 5. Effluent concentration profiles: PA.

and the particle phase transfer coefficient, k_s, estimated according to

$$k_s = \frac{15D_s}{a_p^2} \tag{41}$$

The values of the transfer coefficients are listed in Table 2.

The predicted breakthrough curves for the single species adsorption cases and their comparisons with experiments are shown in Figures 3–5. The predictions from Methods II and III were essentially the same and their agreement with experiments was slightly better than that of Method I. Generally speaking, all three methods gave satisfactory prediction, especially in view of the fact that the concentration levels involved in these experiments were extremely low.

The two species adsorption calculations, as shown in Figures 6–8 however, reveal different trends. The IAS method (Method II) is found to consistently give better results than the Langmuir method (Method I) and the simplified IAS method (Method III). The prediction of the overshoot portion of the breakthrough from the Langmuir expression was found to deviate significantly from the

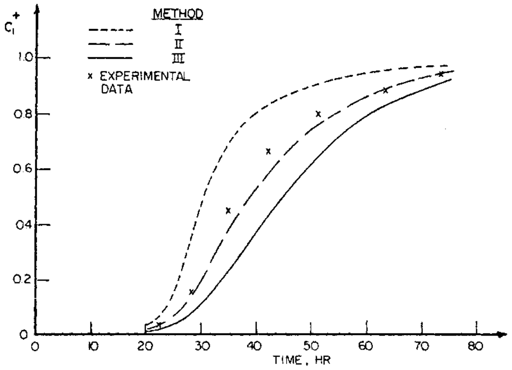

Figure 6(a). Effluent concentration profiles: PNP(1)-PCP(2) mixture.

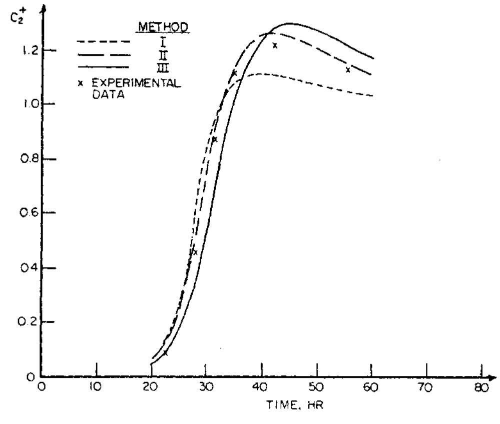

Figure 6(b). Effluent concentration profiles: PNP(1)-PCP(2) mixture.

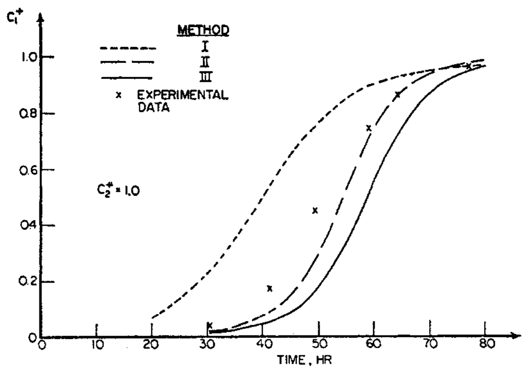

Figure 7. Effluent concentration profiles: PNP(1)-PA(2) mixture.

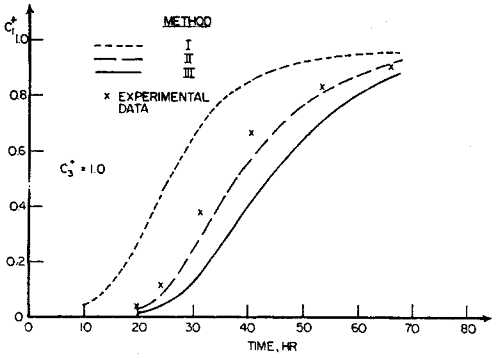

Figure 9(a). Effluent concentration profiles: PNP(1)-PCP(2)-PA(3) mixture.

experimental data (Figure 6b). The same trend was also found true for the three species adsorption calculations. This comparison is shown in Figures 9a and 9b. The breakthrough curves for propionic acid are not shown in these figures. Its relatively low adsorption affinity (Figure 2) means that in contrast to the other two species, propionic acid was only slightly adsorbed. Its effluent concentration remained essentially the same as its influent concentration.

A number of inferences can be made from the results of these calculations and their comparisons with experiment. In comparing the results obtained from the IAS and the simplified IAS methods, the IAS method gives more accurate prediction than the simplified IAS method yet the CPU time requirement in either case is entirely comparable (Table 3). The fact that the solutions of Eqs. 33 and 34 appear to be more complicated than those of Eqs. 38 and 39 apparently have only modest effect on CPU time. The major consideration in this situation is the accurate representation of the single species adsorption isotherm. A piecewise representation of the isotherm is justified as long as it approximates experimental data with sufficient accuracy.

When the Langmuir isotherm was employed in the calculation, depending upon the concentration level, it was often found necessary to use a smaller time increment, $\Delta\theta$, as compared with that used in the IAS case. This is due to the fact that a small error in q_{s_i} may lead to a rather large error in c_{s_i} as a consequence of the asymptotic behavior of the Langmuir expression. Thus, in the case studies considered in this work, the $\Delta\theta$ used in Method I (Langmuir expression) was half of the value of those used in Methods II and III. This limitation does not apply when the IAS method is used.

The comparison between the predictions lead to the clear conclusion that Method II yields the best results in the calculation of breakthrough curves in fixed bed multispecies adsorption. Whether these results extend to systems beyond those considered in this work remains unanswered at this point. The relatively poor results obtained when the Langmuir isotherm was used was derived from the fact that the Langmuir isotherm is inappropriate to activated carbon. The Langmuir isotherm is formulated on the premise of surface homogeneity while the carbon surface is far from homogeneous. Thus, for one class of important adsorption problems (granular activated carbon adsorption), the use of the IAS expression is definitely preferred. The implicit form of the IAS method in expressing multicomponent adsorption isotherms, does not increase the CPU time requirement in a prohibitive way.

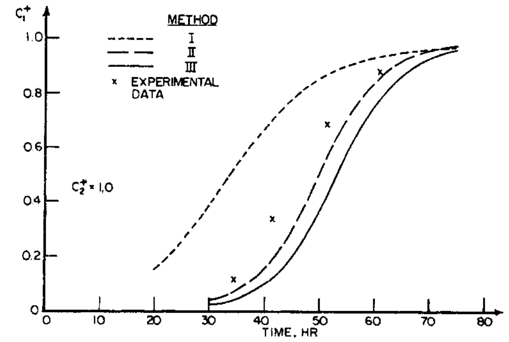

Figure 8. Effluent concentration profiles: PCP(1)-PA(2)-mixture.

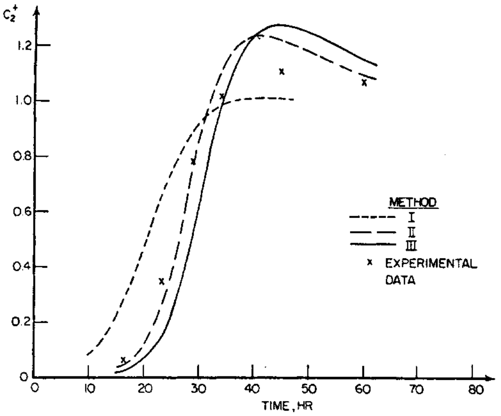

Figure 9(b). Effluent concentration profiles: PNP(1)-PCP(2)-PA(3) mixture.

The algorithms developed in this work are based on the assumption of negligible axial dispersion and the use of the Glueckauf linear driving force expression for intraparticle diffusion. However, the conclusion that the use of the IAS method in estimating the equilibrium relationship does not increase the CPU time prohibitively holds true in general. As stated before, the numerical calculation of fixed bed adsorption consists of two steps; the calculation of both phase concentrations followed by the calculation of the interphase concentrations. The use of a different form of rate expression and/or the inclusion of axial dispersion only complicates the first step of calculation. Thus, on a relative basis, the increase in CPU time due to the use of the IAS method, when the exact intraparticle diffusion equation is used, is less than in the present case.

EXTENSIONS TO BATCH ADSORPTION CALCULATION

Although the methods developed in this work are aimed at fixed bed processes, they can readily extend to batch calculation. Consider a fixed quantity of adsorbent (M) being brought in contact with a certain value of liquid solution containing N adsorbable species. The governing equations are

$$V\frac{dc_i}{dt} + M\cdot\frac{dq_i}{dt} = 0 \tag{42}$$

$$\frac{dq_i}{dt} = \frac{3k_i}{a_p\cdot\rho_p}(c_i - c_{s_i}) = k_{s_i}(q_{s_i} - q) \tag{43}$$

$$q_{s_i} = q(c_{s1}, c_{s2}, \ldots c_{sN}) \tag{44}$$

$$c = c_{io}, \quad t \le 0, \quad q_i = q_{s_i} = 0 \tag{45}$$

The numerical calculation of the above set of equations can be carried out in two steps. In the first step, values of c_i and q_i at $t = j(\Delta t)$ can be found from values of c_i, q_i, c_{s_i} and q_{s_i} at the previous time increment. The second step involve the calculation of c_{s_i} and q_{s_i} from the values of c_i and q_i; at the same time. The first step can be taken care of with the use of a number of algorithms (e.g., Runge-Kutta method or Moulten-Adams predictor corrector method). The problems encountered in the second step, of course, are identical to that of the fixed bed case. Thus, Eqs. 29–34 (IAS Isotherm case) can be applied directly.

ACKNOWLEDGMENT

This study was performed under Grant No. 79-08893, National Science Foundation.

NOTATION

A = constant in Freundlich isotherm
a_p = particle radius
c_i = concentration of solute in liquid phase
D_l = liquid phase diffusion coefficient
D_s = solid phase diffusion coefficient
k_l = liquid phase mass transfer coefficient
k_s = solid phase mass transfer coefficient
l = index of distance from column inlet
M = amount of adsorbent in batch adsorption
m = index of time elapsed
N = number of adsorbable species
n = constant in Freundlich isotherm
P_i = defined as $[(k_{li})/(k_{l1})](c_i^+ - c_{s_i}^+)$
q = ideal concentration of solute in solid phase
R = gas low constant
N_{Re} = Reynolds number
S = defined in Eq. 26
N_{Sc} = Schmidt number
T = absolute temperature
t = time
u = superficial velocity of liquid
v = volumn of liquid in batch adsorption
z = distance from column inlet
z_i = mole fraction

Greek Letters

λ = surface area of adsorbent
δ = defined in Eq. 19
ϵ = void fraction of fixed bed
θ = time elapsed, defined as $t - z\epsilon/u$
Λ = partition coefficient, defined as $(\rho_b q^*)/c_o$
Π = defined as $\pi\lambda/\mathrm{RT}$
π = spreading pressure
ρ_b = bulk density of column
ρ_p = particle density
ϕ_i = defined as $(3k_{li})/(a_p \rho_p k_{s_i})$

Superscripts

k = iteration
o = single-solute
$+$ = dimensionless
$*$ = equilibrium

Subscripts

i = component
j = component
k = number of segments for the Freundlich isotherm
m = index of concentration segment
s = interphase
T = total
o = inlet

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APPENDIX: CALCULATION OF INTERPHASE CONCENTRATIONS WITH LANGMUIR ISOTHERM

If the Langmuir isotherm expression is used to describe the equilibrium relationship, Eq. 9 is given as

$$q_{s_i} = \frac{a_i c_{s_i}}{1 + \sum_{j=1}^{N} b_{ij} c_{s_j}} \qquad \text{(A1)}$$

where a_i and b_i are the Langmuir adsorption parameters for the single i-th species. Eq. A1 can be rewritten as

$$q_{s_i} = \frac{a_i c_{s_i}}{D} \qquad \text{(A2)}$$

and

$$D = 1 + \sum_{j=1}^{N} b_j c_{s_j} \qquad \text{(A3)}$$

Substituting Eq. A2 into Eq. 8b, one has

$$c_{s_i} \frac{a_i}{D} = \phi_i (c_i - c_{s_i}) + q_i \qquad \text{(A4)}$$

Upon rearrangement, the above equation becomes

$$c_{s_i} = \frac{c_i + \dfrac{q_i}{\phi_i}}{1 + \dfrac{a_i}{\phi_i D}} \qquad \text{(A5)}$$

Substituting Eq. A5 into Eq. A3, one has

$$D = 1 + \sum_{j=1}^{N} b_j \frac{c_j + \dfrac{q_j}{\phi_j}}{1 + \dfrac{a_j}{\phi_j D}} \qquad \text{(A6)}$$

or

$$1 - D + \sum_{j=1}^{N} b_j \frac{c_j + \dfrac{q_j}{\phi_j}}{D + \dfrac{a_j}{\phi_j}} = 0 \qquad \text{(A7)}$$

Thus, at point (l, m), with c_i and q_i known, the value of D can be obtained from Eq. A7. Once D is known, one can calculate c_{s_i} from Eq. A5 and q_{s_i} from Eq. A2.

Manuscript received November 14, 1980; revision received August 5, and accepted August 24, 1981.

Nitrogen Pollutant Formation in a Pulverized Coal Combustor: Effect of Secondary Stream Swirl

Concentrations of NO, NH_3, and HCN, together with coal particle burnout and gas composition, were measured during combustion of a bituminous coal. Control of incoming secondary gas swirl level and overall stoichiometric ratio led to significant reductions in nitrogen oxide pollutant concentration. In-situ measurements showed that coal particles were confined near the reactor center during rapid particle reaction. This took place in a locally fuel-rich environment, producing near-quantitative conversion of fuel-nitrogen to NH_3 and HCN, with some NO. Subsequent gas phase reactions of these nitrogen species were identified as important in establishing the ultimate NO concentration.

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SCOPE

It has been shown (e.g., Pershing et al., 1975; Rees et al., 1980) that control of nitrogen oxide can be achieved through control of the pulverized coal mixing and combustion processes. It has also been shown (Pershing and Wendt, 1979) that oxidation of the nitrogen in the coal is the major source of the oxides of nitrogen, and that NO can be controlled through staging (Chen et al., 1980; Wendt, 1980). However, work is continuing to understand the NO formation and to further reduce NO levels. The objective of this work was to investigate the extent and causes of NO formation in the presence of secondary inlet air swirl level. Experiments were conducted in a cylindrical, laboratory pulverized coal combustor (13.7 kg coal/h) with samples being withdrawn 145 cm aft of the fuel-inlet port. Pulverized coal and air were injected through a cylindrical primary port while the secondary air stream was injected in a swirling fashion surrounding the primary stream. Measurements were made on gas composition (Ar, CO, CO_2, CH_4, H_2, N_2, O_2), elemental particulate composition (ash, C, H, N), and pollutant concentration (NO, NH_3, HCN). Effects of secondary stream swirl, stoichiometric ratio, primary stream velocity and solids loading level, coal particle size, and secondary stream preheat temperature were tested on coal burnout and N-pollutant level.

Experiments were also conducted at three swirl levels with gas-particulate samples obtained at various axial and radial positions. Resultant data provided NO concentration maps for interpreting the test results.

N. S. Harding, Jr., is currently with Conoco, Inc., Library, PA.

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