Mixed-Gas Adsorption Dynamics of High-Concentration Components in a Particulate Bed

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The study of LeVan et al. (1988) concerning the dynamics of mixed-gas adsorption of components having high concentrations is extended to the case of multicomponent isotherms determined from either ideal or nonideal adsorbed solution theory. A discussion is given of the effect of isotherm properties on the dynamics of isothermal, mixed-gas adsorption when the adsorbate concentrations in the feed gas are large enough so that the interstitial fluid velocity varies significantly along the adsorption front.

Introduction

Many commercial separation processes that employ adsorption from the gas phase involve bulk separations, such as the recovery of oxygen from air. A complicating factor under these conditions is that the adsorbate concentrations in the feed gas are usually large enough so that the interstitial fluid velocity varies significantly along the adsorption front. Although there have been several numerical studies of gas-phase adsorption dynamics which include this effect (see, for example, the review by Yang, 1987), these studies tend to be laborious and generally do not provide insights into the underlying causes of the observed behavior. There is a need, therefore, to develop analytical solutions based on simplifying assumptions, in particular the assumption of local equilibrium, so that these solutions describe essential features of the adsorption process. In fact, the determination of the front behavior using local-equilibrium theory for the case of uniform initial conditions in the bed and constant feed composition (a Riemann's problem) is often all that is needed for the qualitative design and optimization of even relatively complex adsorption processes.

Recently, LeVan et al. (1988) developed a local-equilibrium theory for the dynamics of mixed-gas adsorption when the interstitial fluid velocity varies along the front. These authors also described a method for determining the adsorption front type. In general, a front can be self-sharpening (a front that forms a concentration discontinuity from a concentration profile which is initially continuous), proportionate pattern (a continuous concentration profile that broadens in proportion to the distance traveled), square-root broadening (a contact discontinuity), or a composite front. The purpose of this study is to extend the work of LeVan et al., who investigated nonlinear adsorption using multicomponent Langmuir isotherms, to the case of multicomponent isotherms predicted from either ideal or nonideal adsorbed solution theories. This study is motivated by the fact that, as was noted by LeVan et al., multicomponent Langmuir isotherms are not consistent with the Gibbs adsorption equation if the monolayer capacities for the individual components are unequal. These isotherms may therefore predict front types that disagree with predictions using thermodynamically consistent multicomponent isotherms based on the same single-gas Langmuir isotherms (Frey, 1990). Of special interest in this regard is the case of crossing single-gas isotherms—a type of behavior which tends to arise whenever the adsorbates differ significantly in size [see, for example, the case of CO_2/C_2H_4 adsorption on Type A zeolite (Persichini and Mersmann, 1991)]. This study considers only the case of monovariant adsorption where there are two adsorbates but no additional inert component.

Composition of Adsorbed Phase

To ensure that the front type determined from material-balance relations agrees with existence criteria from entropy relations, the adsorbed-phase composition will be determined using ideal-adsorbed-solution theory and its extension to nonideal mixtures using the Wilson equation (Valenzuela and Myers, 1989). For an ideal gas, the adsorbed-phase composition in equilibrium with a specified gas composition can be determined from the following relations:

$$P\, y_i = P_i^o(\Psi_i^o)\, x_i \gamma_i \tag{1}$$

$$\Psi_1^o(P_1^o) = \Psi_2^o(P_2^o) = \ldots \tag{2}$$

$$\sigma^e = \frac{1}{q_{\text{total}}} - \sum_i \frac{x_i}{q_i^o} \tag{3}$$

$$q_i = x_i\, q_{\text{total}} \tag{4}$$

$$RT \ln \gamma_i = \left[\frac{\partial(q_{\text{total}} g^e)}{\partial q_i}\right]_{T,\Psi,q_j} \tag{5}$$

$$\sum_{i=1}^{m} x_i - 1 = 0 \tag{6}$$

In the above equations P_i^o and q_i^o are the pressure and amount adsorbed of component i which yield the spreading pressure of the mixture. The spreading pressure is given by:

$$\Psi \equiv \frac{\Pi A}{RT} = \int_{\xi_0}^{\xi} \sum_i \frac{q_i}{P_i}\, dP_i \tag{7}$$

where ξ_0 and ξ denote the state where $P_i = q_i = 0$ and the state corresponding to the composition in question, respectively. According to the Wilson equation, the reciprocal excess amount adsorbed, σ^e, and the excess free energy, g^e, are given, respectively, by:

$$g^e = -RT(1 - e^{-C\Psi}) \sum_i x_i \ln \sum_j x_j \Lambda_{ij} \tag{8}$$

$$\sigma^e = -Ce^{-C\Psi} \sum_i x_i \ln \sum_j x_j \Lambda_{ij} \tag{9}$$

Consider the case where single-gas adsorption is characterized by Langmuir isotherms of the following form:

$$q_i = \frac{a_i C_i}{1 + b_i C_i} \tag{10}$$

Since $P_i = C_i RT$, Eq. 7 leads to the following relation for $P_i^o(\Psi_i^o)$:

$$P_i^o = \frac{RT}{b_i}\left(e^{\frac{b_i \Psi_i^o}{a_i}} - 1\right) \tag{11}$$

For specified values of gas pressure and gas-phase mole fractions, Eqs. 1-9 can be solved as follows:

Step 1. Substitute Eq. 11 into Eq. 1 to eliminate P_i^o.

Step 2. Solve the result from step 1 for x_i and substitute that result into Eq. 6 to yield an expression whose only unknowns are Ψ_i^o and γ_i.

Step 3. Initially assume $\gamma_i = 1$ and $\sigma^e = 0$.

Step 4. Determine Ψ_i^o by solving the single equation developed in step 2 using Newton's method.

Step 5. Determine progressively x_i, q_{total}, and q_i using in sequence Eqs. 1, 3 and 4.

Step 6. Determine new values for γ_i and σ^e from Eqs. 5, 8 and 9.

Step 7. Repeat steps 4-6 until converged values for γ_i and σ^e are obtained.

When single-gas adsorption is not characterized by Langmuir isotherms, analytical expressions for $P_i^o(\Psi_i^o)$ are often not possible. In this case, Eqs. 1-9 must be solved using the more general methods discussed by Valenzuela and Myers (1989) (see also Sircar and Myers, 1973).

Selectivity Contours for an Ideal Adsorbed Phase

The adsorption selectivity for an ideal adsorbed phase is given by:

$$\alpha_{ij} \equiv \frac{y_i x_j}{x_i y_j} = \frac{P_i^o}{P_j^o} \tag{12}$$

Since P_i^o and P_j^o are functions solely of the spreading pressure of the mixture, Ψ, it follows that each of the variables α_{ij}, P_i^o, and Ψ are functions of any of the other two variables [for example, $\Psi = \Psi(\alpha_{ij}, P_i^o)$]. As shown by Antia and Horváth (1991), this implies that Eq. 1 can be written for the two components i and j to yield:

$$C_i = \frac{P_j^o}{RT} + \frac{C_j}{\alpha_{ij}} \tag{13}$$

Equation 13 indicates that for an ideal adsorbed phase a constant selectivity contour in the $C_i - C_j$ plane is a straight line with a slope of $-1/\alpha_{ij}$ and an intercept of P_j^o/RT.

Local-Equilibrium Theory and Criteria for Front Types

When two adsorbates are present, when there are no inert components, and when the pressure is constant, the succession of gas-phase compositions on a front (termed here the composition path) is a contour of constant C_{total}. For this case, under local-equilibrium conditions the velocity of a specific concentration level, v_c, and the interstitial fluid velocity, v_{fluid}, for a continuous concentration profile can be determined by integrating the following two equations (LeVan et al., 1988):

$$v_c = \frac{\alpha\, v_{\text{fluid}} C_{\text{total}}}{(1-\alpha)[(C_{\text{total}} - C_1)dq_1/dC_1 - C_1 dq_2/dC_1] + \alpha\, C_{\text{total}}} \tag{14}$$

$$\frac{d \ln v_{\text{fluid}}}{dC_1} = \frac{(1-\alpha)(dq_1/dC_1 + dq_2/dC_1)}{(1-\alpha)[(C_{\text{total}} - C_1)dq_1/dC_1 - C_1 dq_2/dC_1] + \alpha\, C_{\text{total}}} \tag{15}$$

Similarly, for specified plateau compositions and for a specified upstream fluid velocity, the velocity of a discontinuous concentration change, $v_{\Delta C}$, and the corresponding downstream fluid velocity are given by:

$$v_{\Delta C} = \frac{\alpha\, v_{\text{fluid},u} C_{\text{total}}/(1-\alpha)}{\dfrac{(C_{\text{total}} - C_{1,d})(q_{1,u} - q_{1,d})}{(C_{1,u} - C_{1,d})} - \dfrac{C_{1,d}(q_{2,u} - q_{2,d})}{C_{1,u} - C_{1,d}} + \dfrac{\alpha\, C_{\text{total}}}{1-\alpha}} \tag{16}$$

$$\frac{v_{\text{fluid},d}}{v_{\text{fluid},u}} = \frac{[(q_{1,u} - q_{1,d})(C_{\text{total}} - C_{1,u}) + (q_{2,d} - q_{2,u})C_{1,u}] + \dfrac{\alpha}{1-\alpha} C_{\text{total}}(C_{1,u} - C_{1,d})}{[(q_{1,u} - q_{1,d})(C_{\text{total}} - C_{1,d}) + (q_{2,d} - q_{2,u})C_{1,d}] + \dfrac{\alpha}{1-\alpha} C_{\text{total}}(C_{1,u} - C_{1,d})} \tag{17}$$

Table 1.

	Case 1	Case 2	Case 3
Isotherm Type for Each Component	1: Langmuir 2: Langmuir	1: Langmuir 2: Langmuir	1: Langmuir 2: BET
Isotherm Parameters	$a_1 = 300$ $a_2 = 300$ $b_1 = 0.05$ $b_2 = 0.125$ $\alpha = 0.5$ $\rho_b = 0.5$	$a_1 = 150$ $a_2 = 300$ $b_1 = 0.0125$ $b_2 = 0.125$ $\alpha = 0.5$ $\rho_b = 0.5$	$a_1 = 37.5$ $a_2 = 60$ $b_1 = 0.025$ $b_2 = 0.1$ $C_{2,\mathrm{sat}} = 40$ $\alpha = 0.5$ $\rho_b = 0.5$
Wilson Equations Parameters	$\Lambda_{12} = 1.15$ $\Lambda_{21} = 1.6$ $C = 10^{-3}$	$\Lambda_{12} = 1.05$ $\Lambda_{21} = 1.1$ $C = 10^{-3}$	

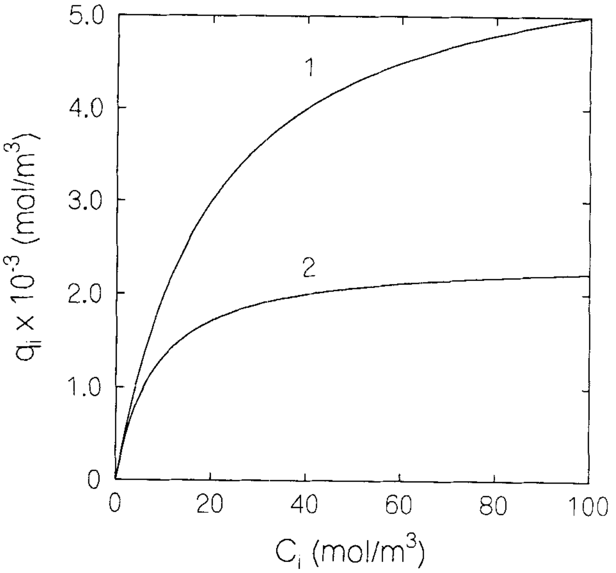

Figure 1. Adsorption isotherms for components 1 and 2 for case 1.

The front type that exists between two composition plateaus for a Riemann's problem can be determined from Eqs. 14 and 15 as follows. If the concentration velocity increases monotonically in the downstream direction between plateaus, then the front is proportionate-pattern in nature. If the concentration velocity decreases monotonically in the downstream direction, the front is self-sharpening and its velocity is given by Eq. 16. If the concentration velocity goes through a maximum, a composite front may occur, the nature of which can be determined through the requirement that the velocity of a self-sharpening section is equal to the concentration velocity at the point where self-sharpening and proportionate-pattern sections adjoin.

LeVan et al. (1988) showed that in a two-component system $d\ln(v_c)/d(C_1)$ is proportional to the second derivative of the function $f(C_1)$ where $f(C_1)$ is defined to be the quantity q_1 $(C_{\mathrm{total}} - C_1)$ $(1 - \alpha_{12})$. Therefore, the procedure just described can be implemented by conceptually wrapping a string anchored at the upstream plateau composition around the function $f(C_1)$ in the clockwise direction until it contacts the downstream plateau composition. Proportionate-pattern sections on the front correspond to locations where the string contacts the curve while self-sharpening sections correspond to the other locations. A contact discontinuity results if $f(C_1)$ is a straight line.

Equations 14-17 constitute a complete solution for a Riemann's problem. More generally, these equations yield the long time behavior of a front for any initial conditions and, through the use of wave interaction principles (Davis and LeVan, 1988), these equations can be used to construct solutions for arbitrary initial and boundary conditions.

Mixed-Gas Adsorption Dynamics of High-Concentration Components

Ideal adsorbed phase

This section examines two cases previously investigated by LeVan et al. (1988), in particular cases A and B of their example 7. These cases involve the determination of the front type between two composition plateaus, one corresponding to the feed composition and the other to the initial state of bed, when Langmuir isotherms apply to the individual components. In case 1 the two adsorbates have the same Henry's law constant but different maximum adsorption capacities while in case 2 the single-gas isotherms cross each other. For comparison purposes, a third case is also considered involving a single-gas isotherm with an inflection point. Physical parameters and isotherms for the three cases are displayed in Table 1 and Figures 1-3. Adsorption equilibrium was calculated from Eqs. 1-9 with $\gamma_i = 1$ and $\sigma^e = 0$. Variations in porosity caused by adsorption are not considered here, as they were in the work of LeVan et al., since these variations do not change the front type.

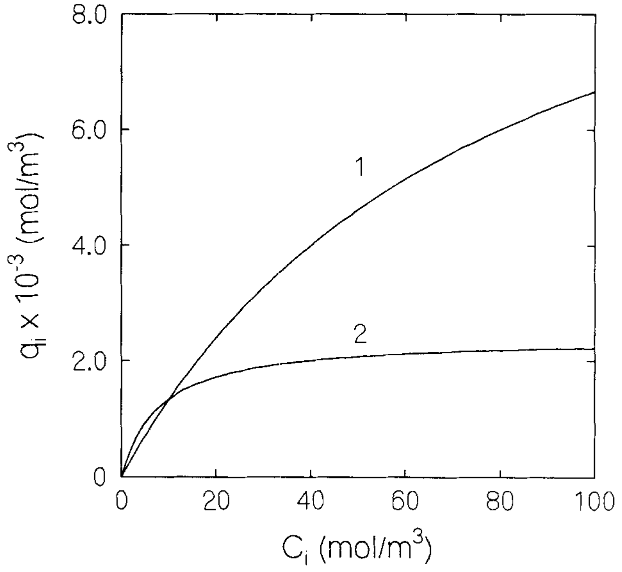

Figure 2. Adsorption isotherms for components 1 and 2 for case 2.

Adsorption selectivity contours and composition paths for

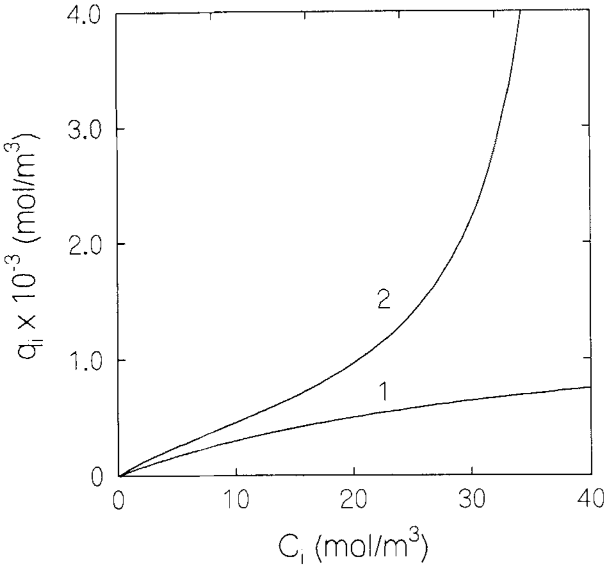

Figure 3. Adsorption isotherms for components 1 and 2 for case 3.

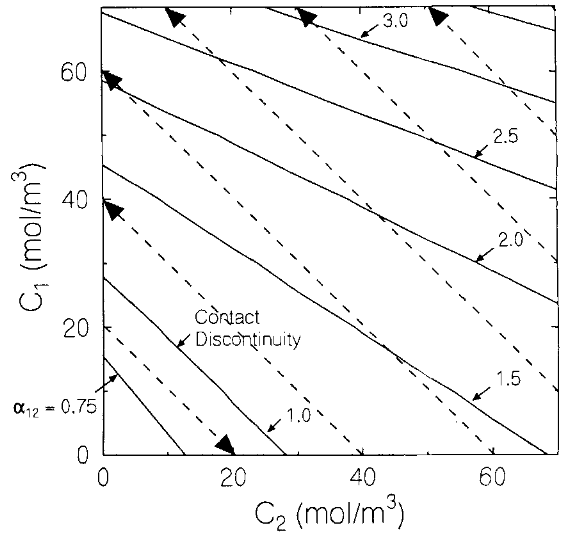

Figure 5. Selectivity contours (——) and directions in which concentration velocity determined from Eqs. 14 and 15 increases (– – →) for case 2 when adsorbed phase is ideal.

cases 1 and 2 for an ideal adsorbed phase are shown as dashed and solid lines, respectively, in Figures 4 and 5. The arrows on the composition paths denote the direction in which the concentration velocity increases on a proportionate-pattern front as calculated by Eqs. 14 and 15. Since there are no velocity maxima in either Figures 4 or 5, the fronts in these figures are all entirely self-sharpening or entirely proportionate pattern, that is, composite fronts are not possible.

Figure 5 shows the type of behavior which occurs when the single-gas isotherms cross each other. At high pressure the component with the higher maximum adsorption capacity (component 1) is selectively adsorbed and the front is self-sharpening if the concentration of that component decreases in the downstream direction. At low pressure the opposite behavior occurs. These high- and low-pressure regions are separated by a composition path corresponding to a contact discontinuity which is the line where $\alpha_{12} = 1$. Figure 4, which shows the behavior which occurs if the single-gas isotherms do not cross but are tangent at the origin, is similar to Figure 5 except that the low-pressure region is missing. Instead, a contact discontinuity exists in the limit $C_{\text{total}} \rightarrow 0$ and, at finite pressures, a self-sharpening front exists if the concentration of the component with the higher adsorption capacity (component 1) decreases in the downstream direction. For comparison, use of the multicomponent Langmuir isotherm [that is, $q_i = a_i C_i / (1 + \Sigma\, b_i C_i)$] leads to the conclusion that a contact discontinuity always exists for case 1 and that a self-sharpening front always exists for case 2 if component 1 increases in the downstream direction (LeVan et al., 1988).

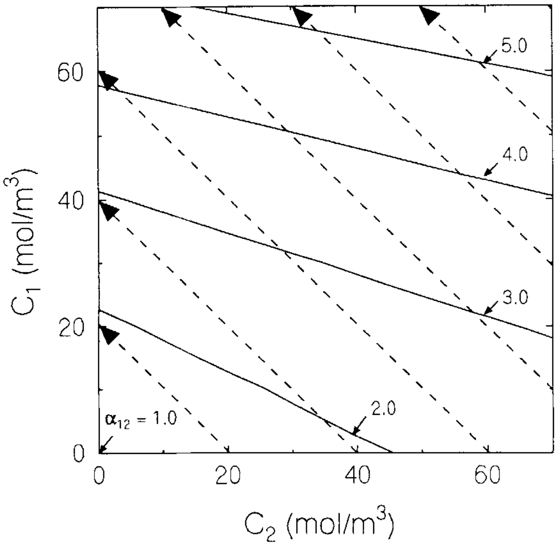

Figure 4. Selectivity contours (——) and directions in which concentration velocity determined from Eqs. 14 and 15 increases (– – →) for case 1 when the adsorbed phase is ideal.

Figures 4 and 5 indicate that for an ideal adsorbed phase, the magnitude of α_{12} in comparison to unity at any composition for the specified pressure can be used as a criterion to determine whether the front is self-sharpening or proportionate pattern. In addition, since composite fronts are not possible, the material-balance relations are "genuinely nonlinear" (Lax, 1955) and the sign of the entropy production rate assuming that a self-sharpening front exists (that is, the entropy admissibility criterion) also determines the front type. More specifically, if a self-sharpening front is assumed, the entropy produced by the front for any type of isotherm can be determined by enclosing the front in a control volume traveling at the front velocity and equating the temperature multiplied by the entropy production rate per unit cross section of column to the net flux of free energy per unit area into the control volume. When

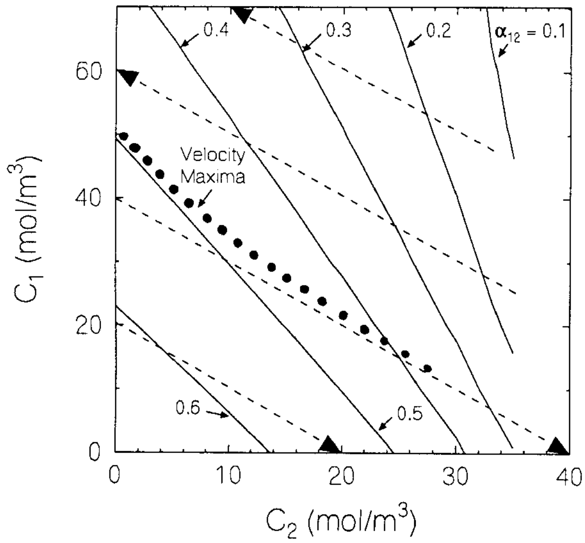

Figure 6. Selectivity contours (——) and directions in which concentration velocity determined from Eqs. 14 and 15 increases (– – →) for case 3 when adsorbed phase is ideal. Also shown is the locus of velocity maxima (. . . .).

the fluid velocity varies across the front, this procedure results in the following expression for the entropy production (see Eq. 35 of Frey, 1990):

$$\begin{aligned} T S_p = (1-\alpha)v_f\left(\sum_{i=1}^{m} q_{i,d}\mu_{i,d} - \sum_{i=1}^{m} q_{i,u}\mu_{i,u}\right) \\ -\alpha(v_{\text{fluid},d}-v_f)\sum_{i=1}^{m} C_{i,d}\mu_{i,d} \\ +\alpha(v_{\text{fluid},u}-v_f)\sum_{i=1}^{m} C_{i,u}\mu_{i,u} + [RT(1-\alpha)v_f(\Psi_u-\Psi_d)] \end{aligned} \quad (18)$$

where the conditions $S_p>0$, $S_p=0$, and $S_p<0$ correspond to self-sharpening, contact, and proportionate-pattern fronts, respectively. Note that if each composition plateau consists of a single gas, all terms on the right side of Eq. 18 cancel except the final term in square brackets and $T S_p$ becomes proportional to $\Psi_u - \Psi_d$.

These conclusions evidently apply not only whenever the single-gas isotherms are Langmuir isotherms, but also to any type of single-gas isotherm, including all cases where these isotherms cross, provided they do not have inflection points. A rigorous proof of this generalization will not be given here due to its complexity. However, this conjecture is supported by calculations similar to those described above for other types of single-gas isotherms and by the fact that Eq. 13 applies to any type of single-gas isotherm.

Figure 6 shows composition paths and contours of constant adsorption selectivity for case 3 of Table 1 where component 2 has a relatively low critical pressure and condenses on the adsorbent such that a BET isotherm of the following form applies:

$$q_2 = \frac{a_2 C_2}{(1 - C_2/C_{2,\text{sat}})(1 - C_2/C_{2,\text{sat}} + b_2 C_2)} \quad (19)$$

Component 1 is less strongly adsorbed than component 2 and has a much higher critical pressure so that a Langmuir isotherm applies in the pressure range of interest. As shown, even if the adsorbed phase is ideal, the composition paths may traverse a locus of velocity maxima unless C_{total} is below the gas-phase saturation concentration, that is, below the value of the parameter C_{sat} in the BET isotherm equation. Therefore, depending on the specific plateau compositions involved, composite fronts may exist when $C_{\text{total}} > C_{\text{sat}}$.

Nonideal adsorbed phase

The following relation is derived from the Gibbs adsorption equation and applies at constant temperature and pressure whether or not the adsorbed phase is ideal (Valenzuela and Myers, 1989):

$$\Psi_{x_1=1} - \Psi_{x_1=0} = \int_0^1 \frac{q_2(\alpha_{12}-1)}{y_2}\, dy_1 \quad (20)$$

The left side of Eq. 20 depends only on the single-gas isotherms and is zero at the pressure corresponding to a contact discontinuity in the thermodynamically ideal case since $\alpha_{12}=1$ under those conditions. Since the right side of Eq. 20 can be zero only if the integrand is zero for at least one point, it follows that the locus of selectivity reversals in the $C_1 - C_2$ plane when the adsorbed phase is nonideal must intersect that for the ideal case with the same single-gas isotherms.

Calculation results are shown in Figures 7 and 8 when negative deviations from ideality of the magnitude commonly observed in gas adsorption are introduced into cases 1 and 2. The calculated activity coefficients varied from 0.5 to 1.0 and from 0.9 to 1.0 in Figures 7 and 8, respectively. As shown in the figures, and in agreement with Eq. 20, one effect of nonideality is to cause selectivity reversals to occur over a finite pressure range which includes the pressure at which $\alpha_{12}=1$ in the ideal case. In addition, contact discontinuities in the ideal case change into regions where maxima occur in the concentration velocities.

The function $f(C_1)$ defined earlier is zero if either C_1 or C_2 are zero or if α_{12} is unity. Therefore, if each composition plateau consists of a single gas and the composition path intersects a locus of selectivity reversals, the function $f(C_1)$ must contain an inflection point and the corresponding front must be composite in nature. This situation is illustrated in Figure 9 which shows the axial profiles in composition and interstitial gas velocity under the conditions corresponding to Figure 8 when $C_{\text{total}}=20$ and when the initial condition in the bed and the feed composition (that is, the upstream and downstream composition plateaus) correspond to $C_{1,u}=20$ and $C_{1,d}=0$. In addition, since composition paths for composite fronts always contain a velocity maximum, the locus of velocity maxima must either coincide with the locus of selectivity reversals or more commonly, and as shown in Figures 7 and 8, it must intersect the locus of selectivity reversals such that it spans a pressure range greater than that spanned by the locus of selectivity reversals. Note that when the adsorbed phase is non-

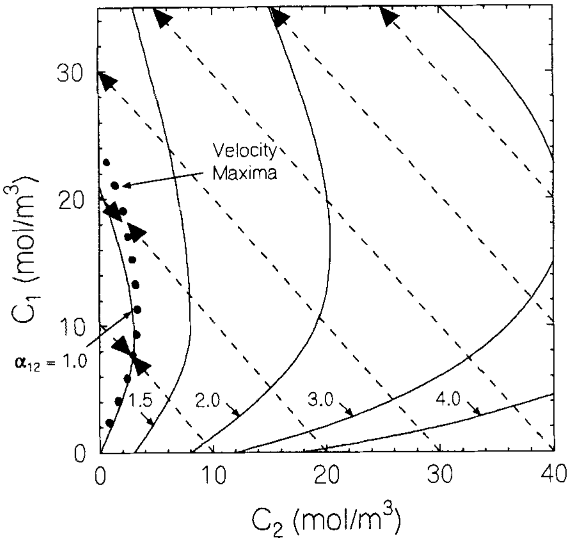

Figure 7. Selectivity contours (——) and directions in which concentration velocity determined from Eqs. 14 and 15 increases (– – →) for case 1 with negative deviations from ideality. Also shown is the locus of velocity maxima (. . . .).

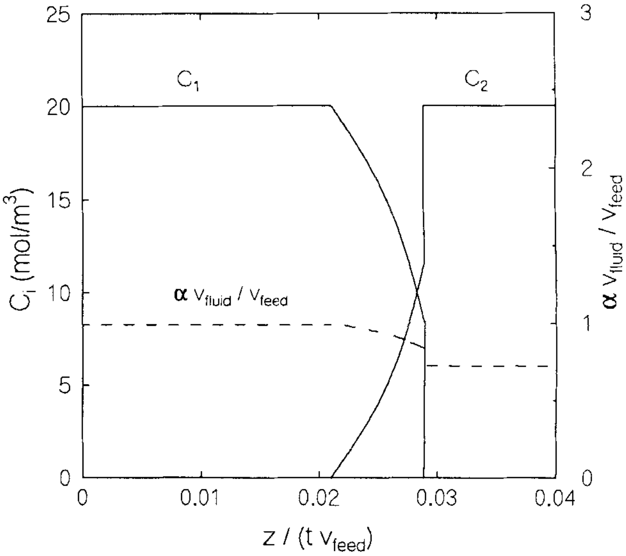

Figure 9. Concentrations of components 1 and 2 and interstitial fluid velocity plotted against dimensionless distance for case 2 with negative deviations from ideality.

Calculations correspond to Figure 8 with $C_{total} = 20$, $C_{1,u} = 20$, and $C_{1,d} = 0$.

ideal the magnitude of α_{12} along the path in comparison to unity may fail to identify the front type even when the composition path does not traverse a locus of selectivity reversals.

Implications for Pressure-Swing Adsorption

Figures 5 and 8 suggests that when pressure-swing adsorption is employed to separate a binary mixture, the use of an adsorbent which yields crossing single-gas isotherms for the two components may be advantageous since both the high-pressure feed step and the low-pressure purge step can be carried out with self-sharpening fronts propagating in the bed. For example, consider the case where Figure 5 applies and a simple pressure-swing adsorption process is employed which is comprised of the following four steps: (i) introduction of high-pressure feed gas to the bed; (ii) depressurization; (iii) low-pressure purging; and (iv) repressurization. In this case, a gas mixture of components 1 and 2 with $C_{total} > 28$ mol/m^3 can be fed to a bed which is saturated with component 2. Component 1 is therefore selectively adsorbed and a self-sharpening front propagates through the bed. After the bed is either partially or fully saturated with the feed gas, it can be depressurized to a state when $C_{total} < 28$ mol/m^3 so that component 2 becomes selectively adsorbed and the interstitial gas remaining in the bed becomes highly enriched in component 1. The bed can then be purged with a portion of the product gas from the feed step (pure component 2) so that a self-sharpening front again propagates through the bed. Finally, the bed can be repressurization with additional pure component 2. This process is likely to be more efficient than the usual situation where there is no selectivity reversal and the purge step is carried out with a proportionate-pattern front propagating in the bed (Bossy et al., 1992).

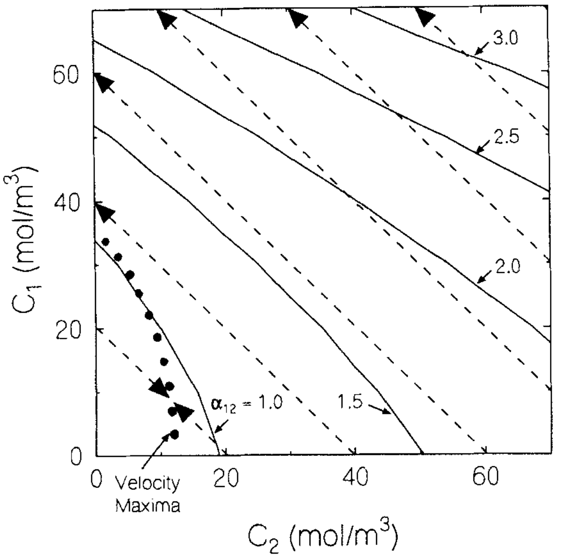

Figure 8. Selectivity contours (——) and directions in which concentration velocity determined from Eqs. 14 and 15 increases (– – →) for case 2 with negative deviations from ideality. Also shown is the locus of velocity maxima (. . . .)

Conclusions

If the adsorbed phase is ideal and the single-gas isotherms do not contain inflection points, then for mixed-gas adsorption with high-concentration components the material-balance relations are always genuinely nonlinear and none of the composition paths for proportionate-pattern fronts contain velocity maxima. Composite fronts are not possible under these conditions, even for crossing single-gas isotherms, and either the entropy admissibility criterion or the magnitude of α_{12} in comparison to unity for any composition at the column pressure determines the front type for specified plateau compositions. When the single-gas isotherms cross, two regions are present: (i) a high-pressure region where a self-sharpening front results if the concentration of the component with the higher maximum adsorption capacity decreases in the downstream direction and (ii) a low-pressure region of opposite behavior. A composition path corresponding to a contact discontinuity separates the high- and low-pressure regions. The presence of adsorbed-phase nonideality causes contact discontinuities present in the thermodynamically ideal case with the same single-gas isotherms to broaden into regions which are not genuinely nonlinear. In these regions the composition paths for proportionate-pattern fronts have a velocity maximum and, depending on the plateau compositions, composite fronts may exist.

Acknowledgment

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Notation

a_i = Langmuir or BET isotherm parameter
A = surface area per unit volume of particle, m^{-1}
b_i = Langmuir or BET isotherm parameter, $m^3 \cdot mol^{-1}$
C = Wilson equation parameter, $m^3 \cdot mol^{-1}$
C_i = concentration, $mol \cdot m^{-3}$
C_{sat} = saturation concentration in BET isotherm, $mol \cdot m^{-3}$
f = $q_1 (C_{total} - C_1)(1-\alpha_{12})$, $mol^2 \cdot m^{-6}$
g^e = excess free energy, $kg \cdot m^2 \cdot s^{-2} \cdot mol^{-1}$
P = total pressure, $kg \cdot s^{-2} \cdot m^{-1}$
P_i = partial pressure, $kg \cdot s^{-2} \cdot m^{-1}$
q_i = amount adsorbed per unit volume of particle, $mol \cdot m^{-3}$
R = gas constant, $kg \cdot m^2 \cdot s^{-2} \cdot mol^{-1} \cdot K^{-1}$
S_p = rate of entropy produced per cross-sectional area of column, $kg \cdot s^{-3} \cdot K$
t = time, s
T = temperature, K
v_c = velocity of a concentration level, $m \cdot s^{-1}$
v_{feed} = superficial velocity of feed gas, $m \cdot s^{-1}$
v_{fluid} = interstitial fluid velocity, $m \cdot s^{-1}$
$v_{\Delta C}$ = velocity of a discrete concentration change, $m \cdot s^{-1}$
x_i = mole fraction in adsorbed phase
y_i = mole fraction in gas phase
z = distance from front of bed, m

Greek letters

α = interstitial void fraction
α_{12} = adsorption selectivity of component 1 with respect to component 2 $[x_1 y_2/(x_2 y_1)]$
γ_i = activity coefficient in adsorbed phase
Λ_{ij} = Wilson equation parameters
μ_i = chemical potential, $kg \cdot m^2 \cdot s^{-2} \cdot mol^{-1}$
ξ = vector of gas-phase compositions
ξ_0 = vector of gas-phase compositions corresponding to $C_i = 0$
Π = spreading pressure, $kg \cdot s^{-2}$
σ^e = reciprocal excess amount adsorbed, $m^3 \cdot mol^{-1}$
Ψ = $\Pi A/(R T)$, $mol \cdot m^{-3}$

Subscript

a = average
d = downstream plateau
i, j = components i and j
m = number of components in system
total = total amount (sum for all components)
sat = saturation value in BET isotherm equation
u = upstream plateau

Superscript

o = pure component reference state

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