

Solute Condensation in Adsorption Beds During Thermal Regeneration

This theoretical study shows that a liquid phase can be developed in and passed through a fixed-bed adsorber during thermal regeneration. The liquid results from passing hot gas from the inlet end of the bed, where the adsorbate is desorbed, towards the cool outlet end, where condensation of the solute occurs. The stage model of an adsorption bed is applied to two examples, the regeneration of an activated carbon bed with adsorbed benzene using hot nitrogen and the regeneration of a 4A molecular sieve bed with adsorbed water using hot methane.

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SCOPE

Displacement of adsorbed compounds from a fixed-bed adsorber often results from the passage of a hot gas into the column. This process, called thermal regeneration, finds wide application in solvent recovery, dehydration, and liquid treating operations. Following the heating step, the bed is cooled and is then ready for reuse.

This work considers theoretically the thermal regeneration of an adiabatic adsorption column with the development of a liquid phase in the bed. The objectives of this paper are, first, to show that the liquid condensate phase can be formed during thermal regeneration and, second, to present a simple yet versatile model that can be used to predict regeneration behavior for various systems and operating conditions. Thorough treatment will lead to improved methods for the design of adsorption systems and to a better fundamental understanding of coupled heat and mass transfer in adsorptive media.

The phenomenon of solute condensation has not been investigated previously although a basis for it has been described by Basmadjian et al. (1975). In their study of thermal regeneration of 5A molecular sieve with adsorbed carbon dioxide using nitrogen, a plateau of re-adsorbed carbon dioxide was predicted for which the adsorbed-phase concentration exceeded the initial loading. Basmadjian et al. referred to this phenomenon as roll-up.

Several methods are available that can be applied to this problem. Many recent theoretical analyses of adiabatic pro-

cesses in fixed-bed adsorbers have been based on the method of characteristics (Amundson et al., 1965; Rhee et al., 1970; Pan and Basmadjian, 1971; Banks, 1972; Basmadjian et al., 1975). The theory neglects heat and mass transfer resistances and effects of dispersion and channeling and is used to obtain exact solutions to coupled material and energy balances. A related approach is taken in this paper. Following investigators in various fields including chromatography (Martin and Synge, 1941; van Deemter et al., 1956), reaction engineering (Deans and Lapidus, 1960), and fixed-bed adsorption (Chen et al., 1972; Rodrigues and Beira, 1979; Ikeda, 1979), the packed bed is modeled as a number of stages, plates, mixing cells, or tanks in series. Our model is obtained by discretizing in the axial direction the partial differential equations for conservation of mass and energy in a fixed bed to obtain ordinary differential equations for each stage. As in the method of characteristics approach, the effects of heat and mass transfer resistances are neglected. Since the model used here is based on finite differences, as the number of stages is increased the results for concentration and temperature profiles in the bed approach those given by the method of characteristics.

Two systems are examined: the passage of hot nitrogen into a fixed bed of activated carbon with adsorbed benzene, and the passage of hot methane into a fixed-bed of 4A molecular sieve with adsorbed water. Phase equilibria are described by favorable isotherms and standard vapor pressure equations.

CONCLUSIONS AND SIGNIFICANCE

As shown here, in situations of practical importance, a liquid phase can be developed in a fixed-bed adsorber during thermal regeneration. The liquid results from the passage of hot regeneration gas from the inlet end of the bed, where the adsorbate is stripped from the adsorbent to create a concentrated vapor, towards the cooler outlet end. As this rich vapor is cooled by heat transfer to the adsorbent, condensation of the solute occurs. In other words, roll-up occurs giving solid-phase concentrations that are greater than the adsorptive capacity of the adsorbent. As regeneration proceeds, the zone of saturated vapor and liquid is transferred through the bed by evaporation and condensation

until it is passed from the column as saturated vapor.

A model has been presented to treat the thermal regeneration of adiabatic adsorption columns with solute condensation. It is both flexible and easy to program on a digital computer. The model can be used with nonuniform initial loadings and transient feed temperatures and concentrations.

The formation of the liquid phase has important implications for the design and operation of adsorption systems. Since regeneration is expensive and complete regeneration is impractical, it is worthwhile to be able to estimate accurately the extent of regeneration, gas requirements, optimal feed temperatures and pressures, duties of condensers used to recover solvents from the hot effluent vapors, and a variety of other variables. The methods developed in this study can be applied to determine these quantities for many systems.

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THEORY

The stage model for thermal regeneration with condensation is obtained here from the differential equations for conservation of mass and energy in an adsorption bed. Following a brief discussion on the method of implementation, the model is applied to the two systems.

Material and Energy Balances

The differential equations for conservation of mass and energy within an adiabatic adsorption bed, neglecting mass and heat transfer resistances, dispersion, and channeling, are

$$\rho_b \frac{\partial q}{\partial t} + \epsilon \frac{\partial c}{\partial t} + \epsilon \frac{\partial(v c)}{\partial z} = 0 \quad (1)$$

$$\rho_b \frac{\partial h_s}{\partial t} + \epsilon \frac{\partial(\rho_f h_f)}{\partial t} + \epsilon \frac{\partial(v \rho_f h_f)}{\partial z} = 0 \quad (2)$$

where

$$h_f = c_f(T - T_{ref}) \quad (3)$$

$$h_s = (c_s + c_a q)(T - T_{ref}) - \int_0^q \lambda dq \quad (4)$$

This set of equations can be applied in the following way to thermal regeneration with condensation. In writing Eqs. 1 and 2, the liquid phase is treated as stationary. The solid-phase concentration q then represents the total amount of solute present as both adsorbate and condensate. (The assumption of a stationary liquid phase is appropriate if the fraction of the void space in the packing that fills with condensate is small. For this case, the liquid is passed through the bed by a vaporization-condensation mechanism rather than by bulk flow). The latent heat λ , a positive quantity, is either the isosteric heat of desorption or the heat of vaporization of liquid, depending on the value of q .

Equations 1 and 2 can be simplified and written in terms of dimensionless independent variables. In adsorptive operations involving gases at low and moderate pressures, the rates of accumulation of mass and energy in the gas phase are generally small compared to values for the stationary phase. The second terms in Eqs. 1 and 2, therefore, can be discarded. This point will be examined later in the paper. The following dimensionless variables can be defined

$$v^* = \frac{v}{v_0} \quad \zeta = \frac{z}{L} \quad \tau = \frac{\epsilon v_0 t}{L} \quad (5,6,7)$$

The dimensionless time τ is equal to the number of bed volumes of hot regeneration gas that have been passed into the bed, based on an open column. Equations 1 and 2 become

$$\rho_b \frac{\partial q}{\partial \tau} + \frac{\partial(v^* c)}{\partial \zeta} = 0 \quad (8)$$

$$\rho_b \frac{\partial h_s}{\partial \tau} + \frac{\partial(v^* \rho_f h_f)}{\partial \zeta} = 0 \quad (9)$$

In evaluating solutions, parameters appearing in Eqs. 3, 4, 8, and 9 can be treated as functions of temperature and composition. However, to simplify the analysis the following approximations are made. The heat capacities c_f and c_s are treated as constants with mean values used. The heat capacity c_a is set equal to the heat capacity of the solute as liquid, also taken as a constant. The vapor phase is assumed to be ideal for the calculation of densities and vapor pressures. Also, the effect of composition on the gas-phase density and velocity is neglected, giving

$$v^* = \frac{T}{T_0} \quad \rho_f = \rho_{f0} \frac{T_0}{T} \quad (10,11)$$

Now, ρ_{f0} , the density of the hot inlet gas, is the only pressure dependent parameter in the analysis.

The stage model is depicted in Figure 1. Each stage is considered to be well mixed with the effluent concentration and temperature of stage i constituting the feed concentration and temperature of stage $i + 1$. The appropriate equations for stage i are obtained by

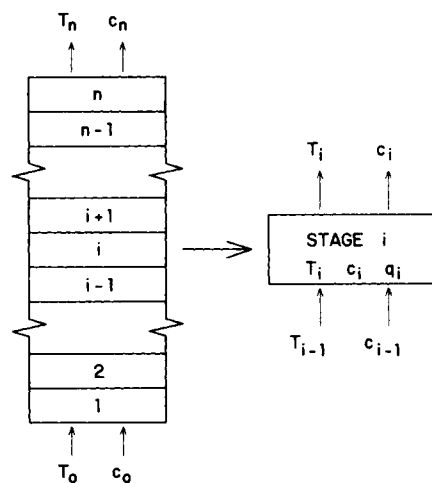


Figure 1. Stage model of fixed-bed absorber.

writing the spatial derivatives in Eqs. 8 and 9 in finite difference form using backward differences. This gives, after minor rearrangement,

$$\frac{dq_i}{d\tau} = \frac{1}{\rho_b \Delta \zeta} [(v^* c)_{i-1} - (v^* c)_i] \quad (12)$$

$$\frac{dT_i}{d\tau} = \frac{1}{\rho_b(c_s + c_a q_i)} \left\{ \frac{\rho_{f0} c_f}{\Delta \zeta} (T_{i-1} - T_i) - \rho_b [c_a (T_i - T_{ref}) - \lambda_i] \frac{dq_i}{d\tau} \right\} \quad (13)$$

Method of Solution

Phase equilibria relations must be available for the adsorbate, giving c as a function of T and q for values of q less than q_{sat} , and for the condensate, giving c as a function of only T for values of q greater than q_{sat} . It is also necessary to know q_{sat} or to be able to calculate it from the adsorbed-phase relation.

The procedure for integrating Eqs. 12 and 13 over one time step is straightforward, given the existing values of T_i and q_i for the stage and T_{i-1} and c_{i-1} for the feed to the stage. A comparison is made between q_i and q_{sat} to determine if stage i contains condensate. The appropriate relation is then used to determine c_i . For example, if q_i is less than q_{sat} , then c_i is determined from an adsorption isotherm correlation and λ_i in Eq. 13 is λ_d , the heat of desorption. Alternatively, if q_i is greater than q_{sat} , then c_i is calculated from a vapor-liquid phase equilibria relation and λ_i is λ_v , the heat of vaporization of liquid. Then, the right sides of Eqs. 12 and 13 can be evaluated and the new values of T_i and q_i determined.

The actual integration process can be carried out using many standard numerical techniques for solving coupled ordinary differential equations. We used a fourth-order Runge-Kutta method. All results in this paper were obtained using fifty stages.

RESULTS

Of the two systems examined here, one has been studied previously but the authors did not consider conditions for which solute condensation would occur; the other finds wide application in industry. First, the regeneration of a fixed bed of activated carbon with adsorbed benzene using hot nitrogen is analyzed. This was the system selected by Rhee et al. (1970) for their detailed analysis of an adiabatic adsorption column. Their isotherm correlation is used here to describe adsorbed-phase equilibria. Second, the regeneration using hot methane of a fixed bed of 4A molecular sieve with adsorbed water is considered. Thermodynamic properties for the adsorbed phase are taken from data sheets supplied by the LINDE Div. of Union Carbide Corp. and the Davison Chemical

TABLE 1. SYSTEM PARAMETERS

	Benzene on Activated Carbon	Water on 4A Molecular Sieve
ρ_b (kg/m ³)	480	650
c_f (kJ/kg ^o K)	1.06	2.70
c_s (kJ/kg ^o K)	1.05	0.96
c_a (kJ/mol ^o K)	0.140	0.0754
λ_v (kJ/mol)	33.9	45.0
T_{ref} (°K)	298	273

Div. of W. R. Grace and Co. Some of the parameters used to describe the two systems are given in Table 1.

Benzene on Activated Carbon

In addition to the parameters listed in Table 1, phase equilibria relations and a heat of desorption are needed to characterize each system completely. Following Rhee et al. (1970), the Langmuir isotherm measured by James and Phillips (1954) is used for benzene adsorbed on activated carbon. This isotherm is of the form

$$q = \frac{QKc}{1 + Kc} \quad (14)$$

with

$$Q = 4.4 \text{ mol/kg}$$

Rhee et al. give

$$K = K_0 \sqrt{T} \exp(\lambda_d/RT) \quad (15)$$

$$K_0 = 3.88 \times 10^{-8} \text{ m}^3/\text{mol}^\circ\text{K}^{1/2}$$

$$\lambda_d = 43.5 \text{ kJ/mol}$$

Note that the heat of desorption for the Langmuir isotherm is independent of the surface coverage. When liquid benzene is present its vapor pressure is determined here using Antoine's equation

$$\log_{10} p = A - \frac{B}{C + T} \quad \begin{array}{l} p \text{ in MPa} \\ T \text{ in } ^\circ\text{K} \end{array} \quad (16)$$

with

$$A = 3.0305 \quad B = 1211 \quad C = -52.2$$

For this system, q_{sat} is calculated by inserting the saturated vapor concentration, obtained from Eq. 16, into Eq. 14.

Prior to considering the effects of pressure, inlet gas temperature, and initial bed loading on the quantity of condensate formed, the general dynamic behavior of the regeneration process is illustrated by treatment of a base case. For the heating of an activated carbon bed with adsorbed benzene using nitrogen, let the base case total pressure be 1.0 MPa. At $\tau = 0$, let the bed have a uniform temperature and loading given by

$$T_i = 298^\circ\text{K} \quad q_i = 4.12 \text{ mol/kg} \quad i = 1 \text{ to } 50$$

and for $\tau > 0$, let the feed to the first stage be

$$T_0 = 403^\circ\text{K} \quad c_0 = 0$$

This initial loading of the adsorbent is the adsorbed-phase concentration in equilibrium with gas ten percent saturated with solute at the initial temperature; that is, $\phi = 0.1$, where ϕ is the initial fractional saturation of the vapor phase in the bed. Because the isotherm is favorable, the initial value of q is large, 94% of q_{sat} .

The solution to Eqs. 12 and 13 for this base case is shown in Figures 2 and 3. Temperature and concentration profiles in the bed at $\tau = 20$ are plotted in Figure 2. The temperature decreases from the feed temperature at the inlet to the initial temperature at the outlet. The gas-phase and solid-phase concentrations of benzene pass from zero at the inlet, through maximums, to the initial concentrations at the outlet. The bed contains liquid benzene between $\zeta = 0.28$ and $\zeta = 0.82$. The maximum value of q , 6.8 percent greater than q_{sat} , occurs at $\zeta = 0.30$. (This is not the maximum value

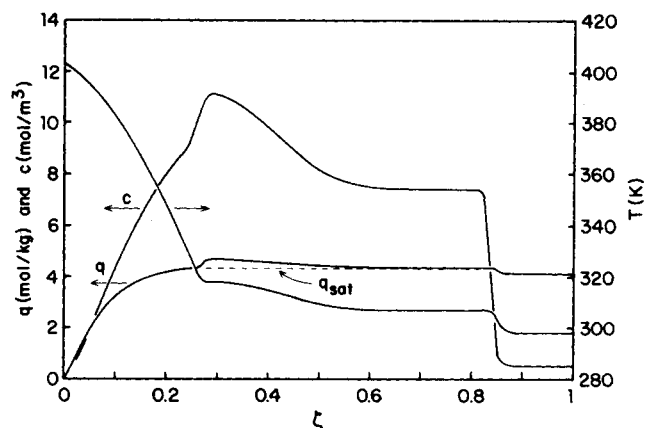


Figure 2. Bed profiles for benzene on activated carbon at $\tau = 20$.

which occurs during the entire regeneration process. The maximum value of q reached in any stage is slightly greater than that reached in previous stages. For this base case, q reaches a maximum, 8.3% greater than q_{sat} , in the last stage at about $\tau = 100$). In Figure 2, the average value of q is still approximately equal to the initial loading since the amount of material in the gas phase is small compared to that in the solid phase and only a small quantity of solute has left the bed. Thus, solute molecules that originally were part of the adsorbed phase near the inlet of the bed have been transferred to the middle of the bed where they are part of the adsorbed and liquid phases.

Breakthrough curves for this system are shown in Figure 3. Effluent temperature and concentration begin to change at $\tau = 23$, when the waves on the right side of Figure 2 reach the end of the bed. From $\tau = 24$ to $\tau = 100$ the effluent vapor is saturated with benzene. Thereafter, the concentration decreases and the temperature increases toward the feed value.

The effects of pressure, inlet gas temperature, and initial bed loading on the maximum amount of condensate formed in the bed are shown in Figure 4. In making these comparisons the initial temperature of the bed and the concentration of benzene in the feed were maintained at 298°K and zero, respectively. The maximum solid-phase concentration which occurs in the bed during regeneration divided by the capacity of the adsorbed phase is plotted versus the temperature of the hot regeneration gas for initial bed loadings corresponding to $\phi = 0.1$ and $\phi = 1.0$ at pressures of 0.5 MPa and 1.0 MPa. Note that for $\phi = 1.0$ the initial adsorbed phase loading is q_{sat} . The general trends shown in Figure 4 indicate that an increase in pressure, inlet temperature, or initial loading increases the amount of condensate formed. It is also possible to prevent condensate from forming by decreasing these variables below certain limits. For example, if the base case pressure had been 0.5 MPa or if the base case inlet gas temperature had been 375°K, then no condensate would have been formed.

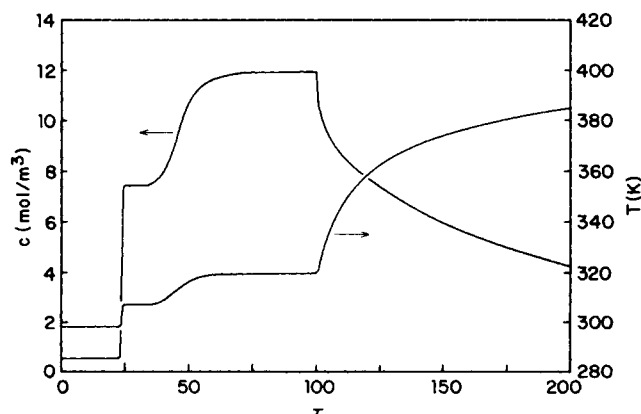


Figure 3. Breakthrough curves for benzene on activated carbon.

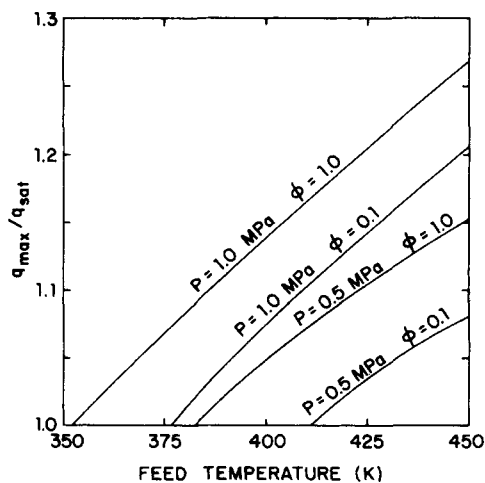


Figure 4. Effect of regeneration conditions on maximum solid-phase concentration of benzene.

Water on 4A Molecular Sieve

Typical inlet gas temperatures for the thermal regeneration of hydrated 4A molecular sieve range from roughly 500 to 600°K. The phase equilibria relation for the adsorbate must be valid, therefore, over a wide range of temperatures. One empirical fit for this system is available (Jury and Horng, 1973) but it was obtained using data taken only at temperatures of up to 367°K.

It was necessary, therefore, to develop a correlation for the adsorbed phase. Nine adsorption isotherms, corresponding to temperatures from 273 to 588°K, for hydrated 4A molecular sieve have been provided by the LINDE Div. of Union Carbide Corp. (Data Sheet F-43-1) with the partial pressure of water vapor, on a logarithmic scale, varied over ten decades. The isotherms have an abrupt change in slope at about $q = 2.5$ mol/kg which Morris (1968) has interpreted as indicating coverage of the most energetic sites.

The often smooth behavior of adsorption isosteres, plotted as $\log_{10} p$ versus $1/T$, suggests that Eq. 16 might be used as the basis of the adsorbed-phase equilibria relation with the coefficients A , B , and C depending on q . At complete saturation the coefficients should become equal to the accepted values for the vapor pressure of liquid. Several points were taken from each of the LINDE isotherms and used to develop such a correlation. With $\theta = q/q_{\text{sat}}$ and $q_{\text{sat}} = 12.8$ mol/kg, we obtained

$$\begin{aligned}
 A &= 4.092 && \text{all } \theta \\
 B &= \theta^{-0.372} (2176 - 67.4 \theta - 8700 \theta^2) \\
 C &= -273 + \theta^{-0.329} (200.3 - 81 \theta - 163 \theta^2) && \left. \begin{array}{l} \\ \\ \end{array} \right\} \theta \leq 0.196 \\
 B &= 3845 - 2542 \theta + 103 \theta^2 + 262 \theta^3 \\
 C &= 50 - 37 \theta - 347 \theta^2 + 289 \theta^3 && \left. \begin{array}{l} \\ \\ \end{array} \right\} 0.196 \leq \theta \leq 1 \\
 B &= 1668 \\
 C &= -45 && \left. \begin{array}{l} \\ \\ \end{array} \right\} \theta \geq 1
 \end{aligned}$$

The system is specified completely now except for the heat of desorption, which can be expected to depend on the adsorbed-phase concentration of water. Morris (1968) calculated the isosteric heat of desorption directly from the LINDE isotherms and found anomalous behavior which he attributed to experimental error at low loadings. Therefore, we took an alternative approach. Davison Chemical, in their adsorption literature, has supplied a plot of isosteric heat of desorption versus loading for water on 4A molecular sieve. We linearized this function over three segments obtaining

$$\begin{aligned}
 \lambda_d &= 75.3 - 120 \theta && \theta \leq 0.15 \\
 \lambda_d &= 57.3 && 0.15 \leq \theta \leq 0.8
 \end{aligned}$$

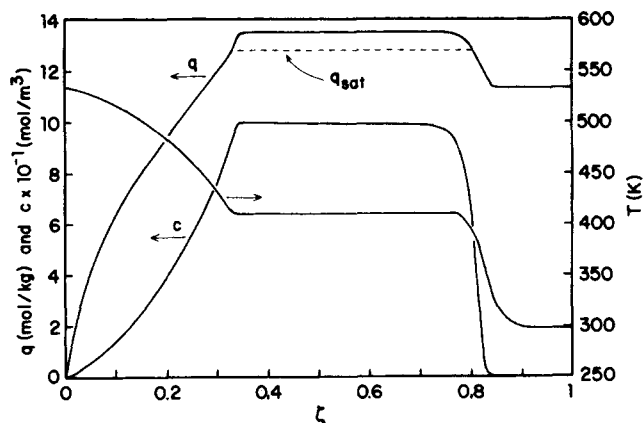


Figure 5. Bed profiles for water on 4A molecular sieve at $\tau = 15$.

$$\lambda_d = 106.5 - 61.5 \theta \quad 0.8 \leq \theta \leq 1$$

where λ_d has units of kJ/mol. At $\theta = 1$, λ_d is equal to λ_v .

As a base case for thermal regeneration of a fixed bed of 4A molecular sieve with adsorbed water using hot methane, we chose conditions typical of those found in cryogenic natural gasoline plants. A total pressure of 4.0 MPa was used. We let the initial condition of the bed be

$$T_i = 298^\circ\text{K} \quad q_i = 11.35 \text{ mol/kg} \quad i = 1 \text{ to } 50$$

and let the feed to the first stage be

$$T_0 = 533^\circ\text{K} \quad c_0 = 0$$

As with the base case for benzene adsorbed on activated carbon, this initial condition corresponds to $\phi = 0.1$, a ten percent initial saturation of the vapor phase in the bed. The initial value of q is 89% of q_{sat} .

The solution to Eqs. 12 and 13 for this base case is shown in Figures 5 and 6. After fifteen bed volumes of hot methane have been passed into the column, the part of the bed containing condensate extends from $\zeta = 0.34$ to $\zeta = 0.80$. The condensate is spread fairly uniformly over this region with the average value of q being about 5.5% greater than q_{sat} . In the concentration breakthrough curve shown in Figure 6 the effluent water concentration begins to rise at $\tau = 17$ from the very low initial value. From $\tau = 19$ to $\tau = 54$ saturated water vapor at 410°K leaves the bed.

The effect of regeneration conditions for water adsorbed on 4A molecular sieve is shown in Figure 7 with the initial temperature of the bed held constant at 298°K and the feed containing no water. The behavior of this system is similar to that shown in Figure 4 for benzene adsorbed on activated carbon. An increase in initial loading, regeneration pressure, or feed temperature increases the

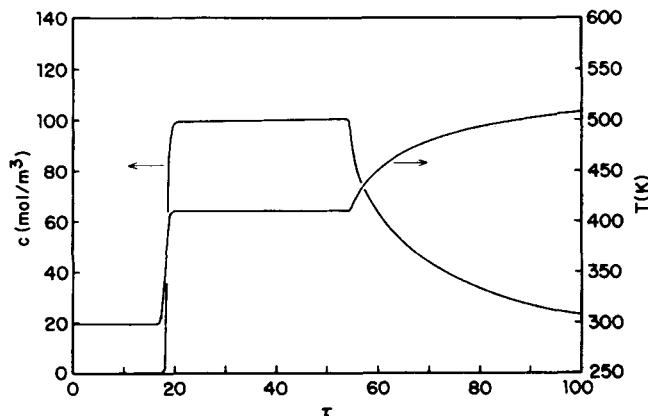


Figure 6. Breakthrough curves for water on 4A molecular sieve.

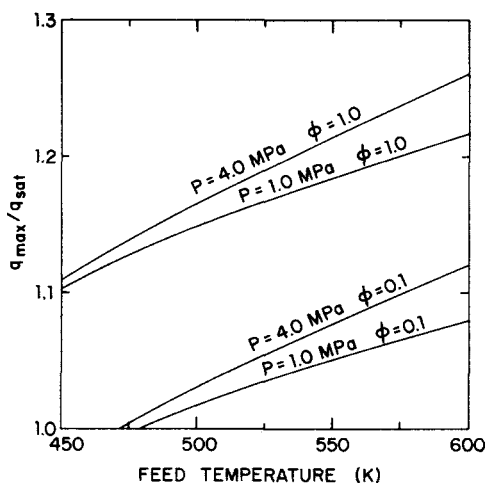


Figure 7. Effect of regeneration conditions on maximum solid-phase concentration of water.

maximum amount of condensate contained in any unit volume of bed at any time.

DISCUSSION

It has been shown in this paper that a liquid phase can be formed in an adsorption bed during thermal regeneration at moderate pressures. The examples considered involve strongly adsorbed components with high initial loadings of the adsorbents. Because the isotherms are favorable, however, the high initial loadings can be obtained with only a moderate initial fractional saturation of the vapor phase in the bed. Even for $\phi = 0.1$ the development of the liquid phase was predicted for both systems.

The stage model has been extended here to treat adsorber regeneration with condensation. Our approach has been to view the bed as a continuum rather than a series of discrete void spaces between particles, each of which is a mixing cell (Deans and Lapidus, 1960; Ikeda, 1979). Our equations were obtained by a finite difference approximation of the coupled material and energy balances for an adiabatic adsorption column with dispersion neglected. As $\Delta\zeta$, appearing in Eqs. 12 and 13, is allowed to approach zero, our approximate solution should approach the exact solution to Eqs. 8 and 9.

In writing Eqs. 8 and 9 we have assumed that the rates of accumulation of mass and energy in the vapor phase are small compared to the values for the solid phase. We have checked this assumption by solving the coupled material and energy balances with the vapor phase accumulation terms retained. For this case, the evaluation of the discretized equations is more difficult. (Our approach involved calculating the partial derivatives $\partial c/\partial q$ at constant T and $\partial c/\partial T$ at constant q at each integration step.) The two different methods gave results for temperature and concentration profiles that agreed typically to three significant figures. Based on this comparison, the additional computations required to include the fluid-phase accumulation terms are unnecessary. The assumption should be used with caution, of course, especially when concentrations and volumetric heat capacities for the fluid phase are not small compared to those for the solid phase.

The bed profiles and breakthrough curves for the two systems considered here have distinctly different shapes. For regeneration of activated carbon, two plateaus of temperature and concentration appear in the breakthrough curves, shown in Figure 3, as saturated vapor leaves the bed. In contrast, the breakthrough curves shown in Figure 6 for regeneration of molecular sieve indicate single plateaus for saturated effluent. These differences result from the parameters and correlations used to describe the two systems, notably the adsorption equilibria relations. The Langmuir isotherm, taken from James and Phillips (1954) and Rhee et al. (1970) for

benzene on activated carbon, and our correlation using Antoine's equation of the LINDE data for water on 4A molecular sieve are quite different approaches to the characterization of phase equilibria. Our correlation gives a smooth transition from vapor-adsorbate equilibria to vapor-liquid equilibria while the Langmuir isotherm does not. Furthermore, the Langmuir isotherm may not be realistic near saturation, where it predicts a solid-phase concentration q_{sat} that is less than the monolayer capacity Q .

It has been shown in Figures 4 and 7 that the initial loading of the bed, the regeneration pressure, and the feed temperature have a marked effect on the maximum quantity of condensate contained in a unit volume of bed. The dependence on initial loading is explained easily. From Figures 2 and 5, the initial solid-phase concentration is the plateau on which roll-up occurs. An increase in the height of this plateau leads to an increase in the maximum solid-phase concentration reached during regeneration, regardless of whether or not the liquid phase is formed. The effects of regeneration pressure and feed temperature can be explained in terms of the rate at which energy is passed into the bed to desorb the adsorbate relative to the rate at which solute is swept from the bed in the effluent. An increase in regeneration pressure or feed temperature increases the enthalpy of a unit volume of feed. This results in an increase in the quantity of adsorbate which is stripped from the adsorbent near the bed inlet prior to breakthrough. Thus, the degree of roll-up of the solid-phase concentration near the bed outlet is enhanced and the quantity of condensate formed is increased.

For the systems considered in this paper, it appears from Figures 4 and 7 that for realistic regeneration conditions the maximum amount of condensate that can be formed is roughly twenty to thirty percent of q_{sat} . It is likely that this quantity of liquid can be contained within the macropores of a bidisperse adsorbent or within the binder of a molecular sieve. The condensate has been assumed here to be part of the stationary phase. For the amounts of liquid formed in the systems considered, this appears to be a reasonable assumption. If situations are encountered in which a large quantity of condensate develops and fills a significant fraction of the void spaces in the packing, it may be necessary to apportion the liquid between the gas and solid phases or to treat it as a third phase. Such situations can be expected to occur during the regeneration of a bed used to dry a supersaturated vapor or a vapor containing a fine mist. For this case, regeneration would begin with an adsorbent in which all available adsorption sites are filled and the macropores contain liquid or the binder is wet.

Since condensation of solute in fixed-bed adsorbents during thermal regeneration has not been recognized previously, it is not possible to say with any degree of certainty what adverse effects it may have on the performance of an adsorption system. However, if a significant amount of condensate were to collect in a bed during thermal regeneration by upflow and it was not distributed uniformly over the cross section of the packing, severe channeling could result.

Unfortunately, there are no published experimental investigations to compare with the theoretical results of this work. In a related study, Chi (1978) measured the progress of the thermal wave down a bed of hydrated 4A molecular sieve during regeneration using heated air. His initial loading, however, is lower than those used here and corresponds to equilibrium with gas only about 0.1% saturated with water. For this low loading, condensation does not occur during thermal regeneration.

ACKNOWLEDGMENT

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NOTATION

A, B, C = parameters appearing in Eq. 16
 c = gas-phase concentration of solute (mol/m^3)

c_a = heat capacity of adsorbate and condensate (kJ/mol °K)
 c_f = heat capacity of gas phase (kJ/kg °K)
 c_s = heat capacity of adsorbent (kJ/kg °K)
 h_f = enthalpy of gas phase (kJ/kg)
 h_s = enthalpy of solid phase (kJ/kg)
 K = Langmuir isotherm parameter, Eq. 15
 K_0 = constant appearing in Eq. 15
 L = bed length (m)
 p = partial pressure of solute (MPa)
 P = total pressure (MPa)
 q = solid-phase concentration (mol/kg)
 q_{\max} = maximum solid-phase concentration (mol/kg)
 q_{sat} = adsorbed-phase concentration in equilibrium with saturated vapor (mol/kg)
 Q = Langmuir monolayer capacity (mol/kg)
 R = gas constant
 t = time
 T = temperature (°K)
 T_0 = temperature of hot inlet gas (°K)
 T_{ref} = reference temperature (°K)
 v = interstitial velocity (m/s)
 v_0 = interstitial velocity of hot inlet gas (m/s)
 v^* = dimensionless velocity, Eq. 5

Greek Letters

ϵ = void fraction of packing
 ζ = dimensionless axial coordinate, Eq. 6
 θ = fractional saturation of adsorbed phase
 λ = latent heat (kJ/mol)
 λ_d = isosteric heat of desorption (kJ/mol)
 λ_v = heat of vaporization of liquid (kJ/mol)
 ρ_b = bulk density of packing (kg/m³)
 ρ_f = density of gas phase (kg/m³)
 ρ_{fo} = density of hot inlet gas (kg/m³)
 τ = dimensionless time, Eq. 7
 ϕ = initial fractional saturation of vapor phase in bed

Subscript

i = stage index

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Mixing and Fluid Dispersion of Viscous Liquids

A model based on extension and secondary motions of striations in a deforming flow is used to predict details of the mixing and dispersion of viscous liquids. Generally, extension of intermaterial area and interfacial surface occurs in stagnation regions, and breakup ensues when the striated flow has left such a region or has time to form unmixing regions of smaller scale in the stretching flow. Complex criteria for the types of mixing anticipated are based on differences in viscosity, differences in density, striation scale, rate of stretch, and, for various degrees of immiscibility, interfacial tension.

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SCOPE

Mixing and fluid dispersion of viscous liquids have been studied in terms of specific and limiting cases with results based on complex fluid mechanical analysis. Experimental observations have been even more narrow in scope and, in the case of immiscible fluids, have been obscured by coalescence. In the

present paper, a basic stretching flow is used to distort a "discontinuous phase" as though it were part of the continuous flow. At various times during this imagined distortion stresses on the boundary of the discontinuous phase are evaluated for realizability, for direction of movement of the boundary, and for rate