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Adiabatic Adsorption Column: Pressure Reduction to Subatmospheric Levels

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Abstract

An adiabatic equilibrium model to simulate the pressure reduction of an adsorption column from ambient pressure to subatmospheric pressure is presented. The column is initially saturated with a binary mixture of gases. The partial differential equations (PDEs) describing the mass and heat balances for the pressure reduction of the bulk binary gas mixture are reduced to simple ordinary differential equations (ODEs) by assuming no axial variation of gas-phase mole fraction, temperature, pressure, and solid-phase capacity. These ODEs describe the unique relationships between gas-phase mole fraction and column pressure, and column temperature and column pressure, as functions of equilibrium isotherm parameters and other constants. The ODEs are solved by first principles to generate gas-phase mole fraction, column temperature, solid-phase loading, and desorbed gas quantity as a function of column pressure. The simplified ODEs can be solved in approximately two seconds CPU time of an IBM 370/165, which is only a fraction of that required to solve the corresponding PDEs on a computer. Pressure reduction of a column initially saturated with a mixture of CO_2/N_2 on BPL carbon is used to illustrate the mathematical model. The simulation results for the subatmospheric pressure reduction step are compared against the results from the superatmospheric pressure reduction step where the pressure is reduced to ambient level.

INTRODUCTION

An adiabatic equilibrium model for the pressure reduction of an adsorption column, initially saturated with a bulk binary gas mixture, was recently published (*1*). This study extends the previously published model to subatmospheric pressure levels.

MATHEMATICAL MODEL

The mass and heat balance equations for the pressure reduction of an adiabatic adsorption column, initially saturated with a bulk binary gas mixture at ambient pressure, are described as follows:

Mass balance for component 1 ($i = 1$):

$$\epsilon\frac{\partial}{\partial t}(y\rho_g)\Big|_x = -\frac{\partial}{\partial x}(Qy)\Big|_t - \rho_s\frac{\partial n_1}{\partial t}\Big|_x \tag{1}$$

Overall mass balance:

$$\epsilon\frac{\partial}{\partial t}(\rho_g)\Big|_x = -\frac{\partial}{\partial x}(Q)\Big|_t - \rho_s\Sigma\frac{\partial n_i}{\partial t}\Big|_x, \qquad i = 1, 2 \tag{2}$$

Overall heat balance:

$$\frac{\partial}{\partial t}[(\epsilon\rho_g C_g + \rho_s C_s)\theta]\Big|_x = -C_g\frac{\partial}{\partial x}(Q\theta)\Big|_t + \rho_s\Sigma q_i\frac{\partial n_i}{\partial t}\Big|_x \tag{3}$$

The solid-phase capacity of component i is a function of P, y, and θ:

$$n_i = n_i(P,y,\theta)$$

and the total solid phase capacity is the sum of the individual component capacity:

$$n = \Sigma n_i$$

The assumption of local equilibrium at all times in the column gives

$$\frac{\partial n_i}{\partial t} = n_{iP}\frac{dP}{dt} + n_{iy}\frac{dy}{dt} + n_{i\theta}\frac{d\theta}{dt} \tag{4}$$

$$\frac{\partial n}{\partial t} = n_P\frac{dP}{dt} + n_y\frac{dy}{dt} + n_\theta\frac{d\theta}{dt} \tag{5}$$

where

$$n_{iP} = \frac{\partial n_i}{\partial P}\Big|_{y,\theta}$$

$$n_{iy} = \frac{\partial n_i}{\partial y}\Big|_{P,\theta}$$

$$n_{i\theta} = \frac{\partial n_i}{\partial \theta}\Big|_{y,P}$$

and

$$n_P = \Sigma n_{ip}$$

$$n_y = \Sigma n_{iy}$$

$$n_\theta = \Sigma n_{i\theta}$$

Equations (1)–(3) assume that the axial mass or heat transport in the bulk gas and the adsorbed phases are negligible. It is further assumed that ϵ, C_g, C_s, ρ_s, and q_i are independent of temperature, and θ, y, and P are functions of time only. The heat capacity of adsorbed phase is neglected and θ, y, and P are assumed constant along the entire column length at any time. As previously outlined (*1*), Eqs. (1)–(5) can be solved to give

$$\frac{dy}{dP} = \frac{X_1X_2 + EX_3 + X_8X_4}{X_5X_2 - FX_3 - X_8X_6 - X_7} \tag{6}$$

and

$$\frac{d\theta}{dP} = \frac{dy}{dP}\left(\frac{F + n_yX_8}{X_2 - n_\theta X_8}\right) + \frac{E + n_PX_8}{X_2 - n_\theta X_8} \tag{7}$$

where

$$A = \frac{\epsilon}{\rho_s RT} \tag{8}$$

$$B = q_1n_{1\theta} + q_2n_{2\theta} \tag{9}$$

$$E = q_1n_{1P} + q_2n_{2P} \tag{10}$$

$$F = q_1n_{1y} + q_2n_{2y} \tag{11}$$

$$X_1 = yn_P - n_{1P} \tag{12}$$

$$X_2 = C_s + APC_g - B \tag{13}$$

$$X_3 = yn_\theta - n_{1\theta} \tag{14}$$

$$X_4 = n_{2\theta}n_{1P} - n_{1\theta}n_{2P} \tag{15}$$

$$X_5 = AP + n_{1y} - yn_y \tag{16}$$

$$X_6 = n_{2\theta}n_{1y} - n_{1\theta}n_{2y} \tag{17}$$

$$X_7 = AP\theta C_g n_\theta \tag{18}$$

and

$$X_8 = \theta C_g \tag{19}$$

Substitution of Eqs. (4) and (5) into Eq. (2), and integration over the entire column length, gives the specific gas quantity desorbed as a function of time:

$$Q_d(t) = -\int_0^t \frac{dP}{dt}\left\{(A + n_P) + n_y\frac{dy}{dP} + \left(n_\theta - \frac{AP}{(T_0 + \theta)}\right)\frac{d\theta}{dP}\right\}dt \tag{20}$$

or, the total quantity of desorbed gas as a function of column pressure:

$$D(P) = -LA_*\rho_s\int_{P_s}^{P}\left\{(A + n_P) + n_y\frac{dy}{dP} + \left(n_\theta - \frac{AP}{(T_0 + \theta)}\right)\frac{d\theta}{dP}\right\}dP \tag{21}$$

EQUILIBRIUM ISOTHERM

Equilibrium isotherms are needed to calculate n_{iP}, n_{iy}, and $n_{i\theta}$. While any equilibrium model with an explicit form may be used, the Langmuir model is used for mathematical simplicity to demonstrate the applicability of the present model:

$$n_1 = \frac{mb_1Py}{1 + b_1Py + b_2P(1 - y)}$$

and

$$n_2 = \frac{mb_2P(1 - y)}{1 + b_1Py + b_2P(1 - y)}$$

where

$$b_i = \hat{b}_i \exp\left\{\frac{q_i}{R(T_s + \theta)}\right\}$$

Therefore,

$$n_{1P} = \frac{mb_1 y}{Z} \tag{22}$$

$$n_{2P} = \frac{mb_2(1 - y)}{Z} \tag{23}$$

$$n_{1y} = \frac{mb_1 P(1 + b_2 P)}{Z} \tag{24}$$

$$n_{2y} = -\frac{mb_2 P(1 + b_1 P)}{Z} \tag{25}$$

$$n_{1\theta} = \frac{mb_1 Py}{ZR(T_s + \theta)^2}[Pb_2(1 - y)(q_2 - q_1) - q_1] \tag{26}$$

$$n_{2\theta} = \frac{mb_2 P(1 - y)}{ZR(T_s + \theta)^2}[Pb_1 y(q_1 - q_2) - q_2] \tag{27}$$

where

$$Z = [1 + b_1 Py + b_2 P(1 - y)]^2 \tag{28}$$

METHOD OF SOLUTION

Equations (6) and (7) show that the local equilibrium theory reduces the partial differential mass and heat balance equations into a set of ordinary differential equations relating y and θ to the equilibrium parameters and other constants. The independent parameter in these equations is column pressure (P) rather than distance (x) or time (t).

Equations (6) and (7) can, therefore, be solved for y and θ as a function of P. The total quantity of desorbed gas (D) is calculated as a function of column pressure from Eq. (21). However, for design purposes the pressure reduction step variables (y, θ, and D) should be related with time to calculate the duration of this step and size the machinery required to carry out this step. This can be done by either of the following approaches.

a. If column pressure as a function of time is empirically known:

$$P = f_1(t) \tag{29}$$

Then, since y, θ, and D are known functions of column pressure, Eq. (29) reduces y, θ, and D as functions of time, t.

b. If the flow characteristic of the machinery at the column exit is empirically known:

$$FL = f_2(P) \tag{30}$$

Then, the combination of Eqs. (21) and (30) gives time as a function of column pressure:

$$t = \frac{D(P)}{f_2(P)} = f_3(P) \tag{31}$$

Again, since y, θ, and D are known functions of column pressure, Eq. (31) gives y, θ, and D as functions of time, t.

In the present study, the second approach is chosen since Eq. (30) is generally available from manufacturer's technical information. The following equations is used:

$$FL = \rho_g(\text{ACFM}) \tag{32}$$

where the gas density (ρ_g) is calculated at column pressure and temperature and ACFM is a known constant.

PARAMETRIC STUDY

The above described local equilibrium theory and the method of solution were used to evaluate the effect of final column pressure (P_f) and initial gas composition (y_s) on the adiabatic pressure reduction step for subatmospheric pressure levels. Pressure increments of 0.005 atm were used to solve the ordinary differential Eqs. (6), (7), and (21) by the numerical technique of finite differences. Pressure increments of 0.005 atm were found to be sufficiently accurate after comparing pressure reduction profiles for pressure increments of 0.1, 0.01, 0.005, and 0.002 atm. A typical computation time on an IBM 370/165 computer was approximately two seconds.

TABLE 1
Adsorbent Properties and Other Constants

Column length, L = 100 cm
Inside column diameter, i.d. = 2 cm
Volumetric flow rate, ACFM = 0.05 ft^3/min
Initial column pressure, P_s = 1 atm
Initial column temperature, T_s = 300 K

Gas-phase heat capacity, C_g = 8.86 (CO_2) 6.96 (N_2) cal/(mol·K)

Adsorbent: BPL carbon

Solid-phase heat capacity, C_s = 0.22 cal/(g·K)
Bulk density, ρ_s = 0.484 g/cm^3
Void volume, ϵ = 0.763

BPL-activated carbon was used as the adsorbents. CO_2 was taken as component 1 and N_2 was considered as component 2. All the runs were carried out at an initial column temperature of 300 K and an initial column pressure of 1 atm. Other constants used in the calculations are listed in Table 1.

The pure component adsorption equilibrium of both the gases was described by the Langmuir isotherm, and the binary equilibrium was described by the mixed Langmuir equations (*2*). Table 2 summarizes the parameters of the equilibrium isotherms.

EFFECT OF FINAL COLUMN PRESSURE

The effect of final column pressure (P_f) on the pressure reduction step was calculated for P_f = 0.1, 0.2, 0.4, 0.6, and 0.8 atm. CO_2/N_2 on BPL carbon with $y_s = 0.5$ and $P_s = 1.0$ atm was used as the example. Table 3 shows that, as expected, the final column temperature (T_f) decreases and the final concentration of the effluent gas (y_f) increases with decreasing

TABLE 2
Langmuir Parameters for the Pure Adsorbate

	Adsorbent: BPL activated carbon		
Adsorbates	m	b	q
CO_2	3.65×10^{-3}	2.8×10^{-4}	4900
N_2	3.65×10^{-3}	13.5×10^{-4}	2500

TABLE 3
Summary of Results

System	P_f (atm)	y_s	T_f (K)	y_f	$\bar{y}_D$	Q_d (mmol/g)
CO_2 (1) + N_2 (2) on BPL carbon	0.8	0.50	298.8	0.570	0.537	0.082
	0.6	0.50	297.2	0.664	0.577	0.182
	0.4	0.50	294.8	0.810	0.645	0.318
	0.2	0.50	289.5	0.980	0.767	0.580
	0.1	0.50	283.7	0.9998	0.841	0.853
	0.2	0.20	295.3	0.636	0.349	0.352
	0.2	0.80	283.7	0.999	0.941	0.815

final column pressure. Figure 1 plots the concentration of the effluent gas (y) and the specific desorbed gas quantity (Q_d) against the column pressure (P). As previously observed (*1*), the desorbed gas quantity and the slope of this curve ($\Delta Q_d/\Delta P$) increase as the column pressure decreases. Also, as previously observed, the concentration of the effluent gas increases as

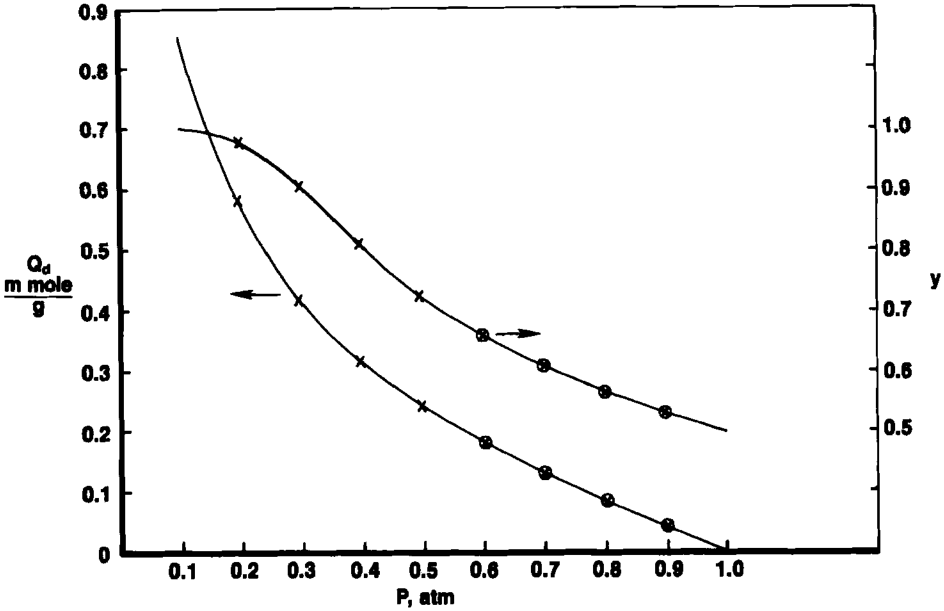

FIG. 1. Variation in the desorbed gas quantity and desorbed gas concentration during the pressure reduction step from ambient pressure to subatmospheric level: CO_2/N_2 on BPL carbon. P_s = 1 atm; (——) P_f = 0.1 atm, (×) P_f = 0.2 atm, and (○) P_f = 0.6 atm.

the column pressure decreases. However, in contrast to the case where the pressure is reduced from superatmospheric to ambient pressure (Fig. 2), the shape of the concentration profile, especially at higher concentrations of the effluent gas, is remarkably different. The concentration profile for the subatmospheric pressure reduction step approaches 1 in an asymptotic manner, whereas, for superatmospheric pressure reduction step, the effluent gas concentration never approaches 1.

Figure 3 plots the average concentration of the desorbed gas ($\bar{y}_D$) against the ratio of the maximum and minimum pressures (P_{max}/P_{min}) for the subatmospheric and superatmospheric pressure reduction steps. It is observed

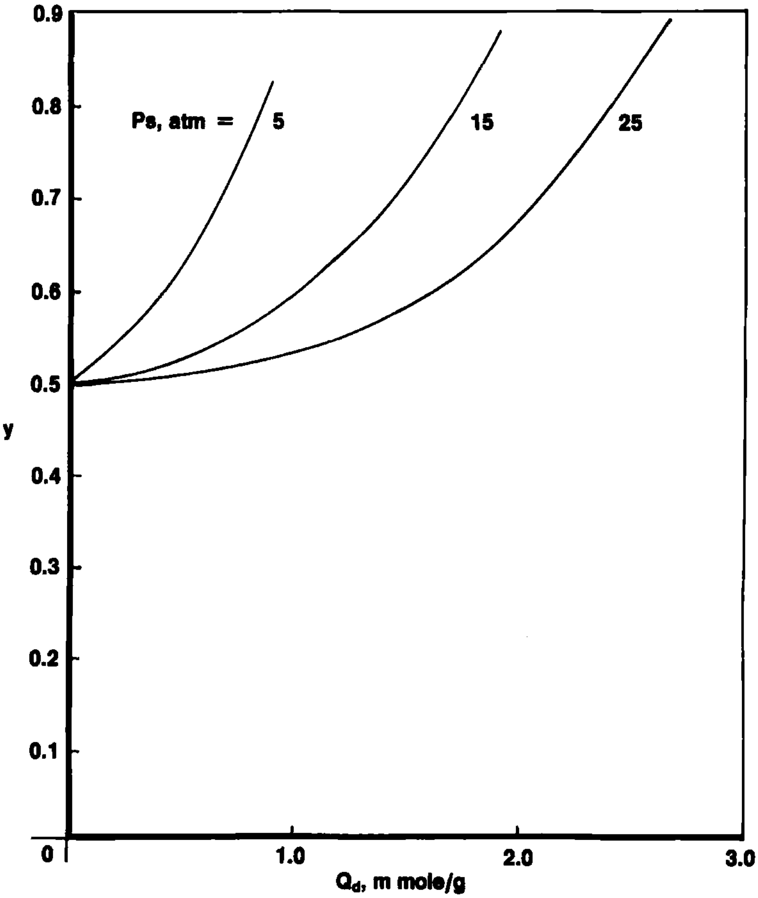

FIG. 2. Variation in the desorbed gas concentration during the pressure reduction step from super ambient pressure to ambient pressure level: CO_2/N_2 on BPL carbon, P_f = 1 atm.

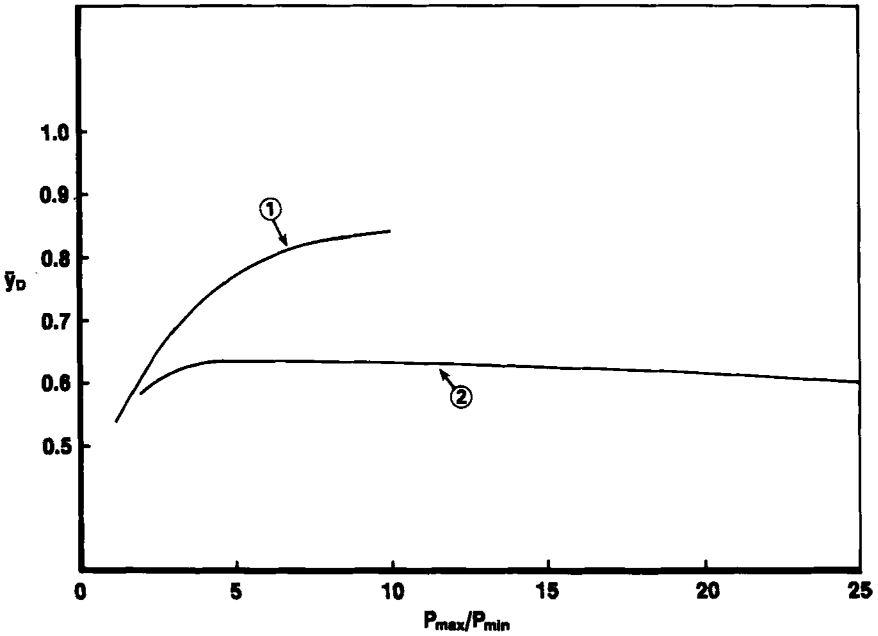

FIG. 3. Variation in the average concentration of the strongly adsorbed species in the desorbed gas with the ratio of maximum and minimum pressure during the pressure reduction step: CO_2/N_2 on BPL carbon. Curve 1: Pressure reduction from ambient pressure ($P_{max} = P_s = 1$ atm) to subatmospheric levels. Curve 2: Pressure reduction from superatmospheric levels to ambient pressure ($P_{min} = P_f = 1$ atm).

that $\bar{y}_D$ for the subatmospheric pressure reduction step is always higher than for the superatmospheric pressure reduction step. For the present case, the superatmospheric pressure reduction step has a maximum around $\bar{y}_D = 0.64$ whereas the subatmospheric pressure reduction step shows an increasing trend with P_{max}/P_{min}. This implies that pressure has to be reduced to subatmospheric levels to obtain high purity of the more strongly adsorbed species in the desorbed gas.

EFFECT OF INITIAL GAS COMPOSITION

The effect of initial gas composition on the subatmospheric pressure reduction step was calculated for $y_s = 0.2$, 0.5, and 0.8. A mixture of CO_2 and N_2 on BPL carbon with $P_f = 0.2$ atm was used as the example. Figure 4 plots the column temperature (T) against the column pressure (P).

Column temperature for the highest initial gas-phase composition is lowest since, at any given pressure, the desorbed gas quantity is higher for the higher initial gas composition run. This, in turn, results in higher tem-

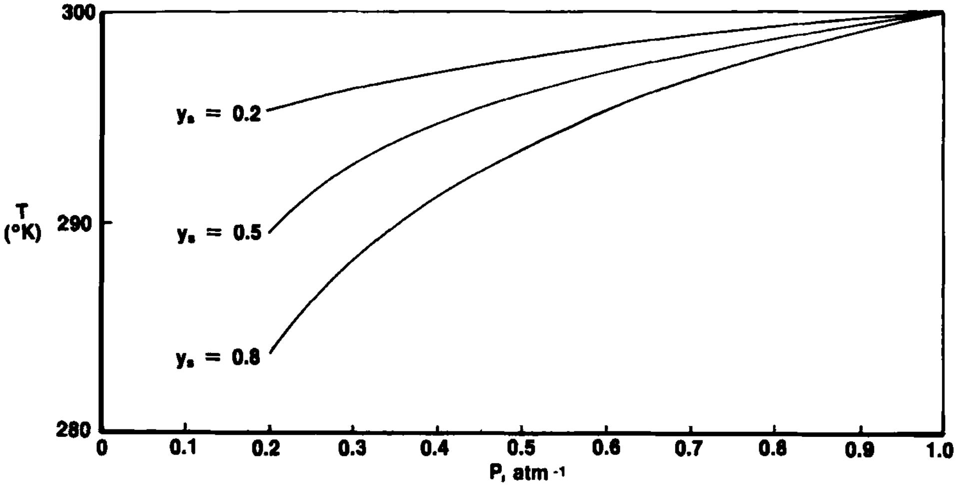

FIG. 4. Effect on initial gas composition on variation in the column temperature with column pressure during the pressure reduction step: CO_2/N_2 on BPL carbon. P_s = 1 atm, P_f = 0.2 atm.

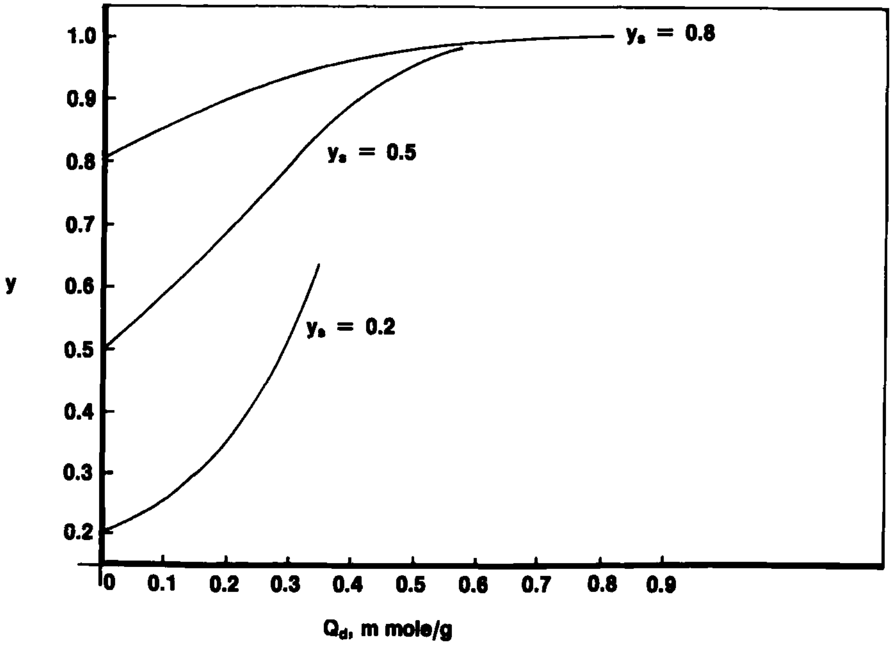

FIG. 5. Effect of initial gas composition on variation in the desorbed gas concentration with the desorbed gas quantity during the subatmospheric pressure reduction step: CO_2/N_2 on BPL carbon. P_s = 1 atm, P_f = 0.2 atm.

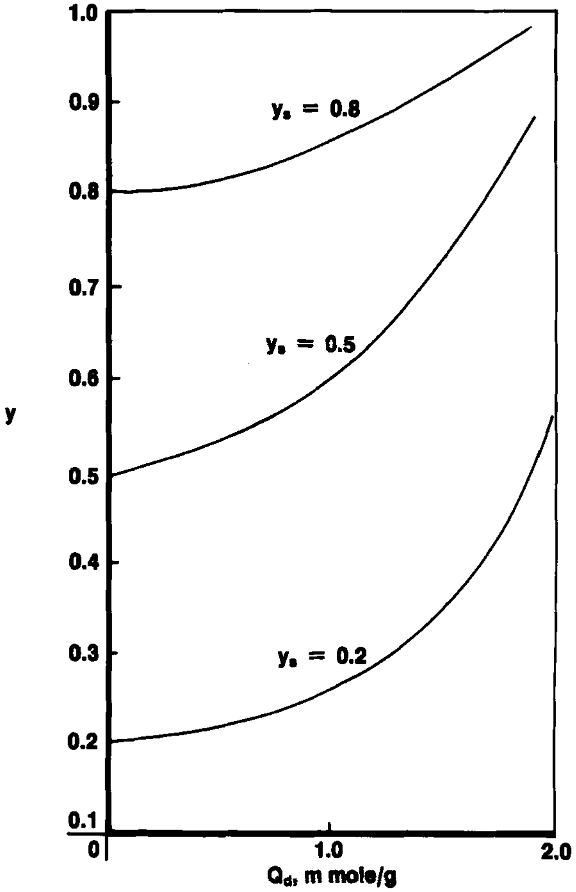

FIG. 6. Effect of initial gas composition on variation in the desorbed gas concentration with the desorbed gas quantity during the superatmospheric pressure reduction step: CO_2/N_2 on BPL carbon. P_s = 15 atm, P_f = 1.0 atm.

perature drop due to heat of desorption and therefore lower column temperature at any given pressure.

Figure 5 plots the composition of the desorbed gas against the quantity of the desorbed gas for various initial gas-phase compositions. As expected, the gas-phase concentration rises as the pressure reduction step proceeds (i.e., Q_d increases). However, in contrast to the superatmospheric pressure reduction step (Fig. 6), the shape of the subatmospheric pressure reduction step profile is quite different, especially at high initial gas-phase composition. In general, the purity of the desorbed gas during the subatmospheric

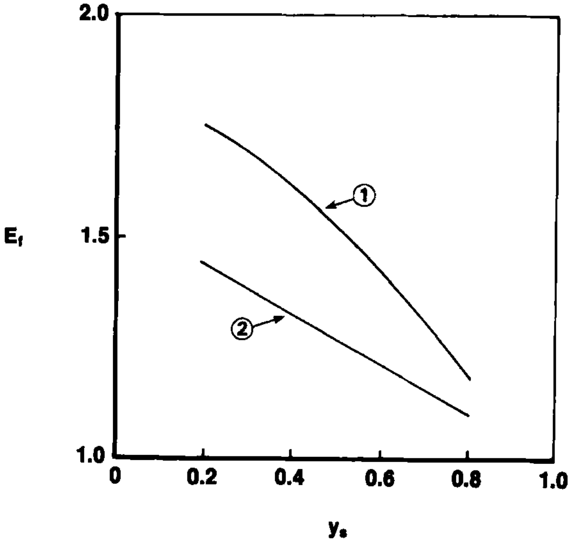

FIG. 7. Variation of the desorbed gas enrichment factor ($E_f = \bar{y}_D/y_s$) with the initial gas composition: CO_2/N_2 on BPL carbon, $P_{max}/P_{min} = 5$. Curve 1: Subatmospheric pressure reduction step. Curve 2: Superatmospheric pressure reduction step.

pressure reduction step is higher than the purity of the desorbed gas during the superatmospheric pressure reduction step. This is further illustrated in Fig. 7, which shows that the enrichment factor ($E_f = \bar{y}_D/y$) for a subatmospheric pressure reduction step is always higher than for a superatmospheric pressure reduction step.

CONCLUSIONS

The adiabatic equilibrium model for the blowdown of an adsorption column from superatmospheric pressure to ambient pressure levels was successfully extended to pressure reduction step from ambient pressure level to subatmospheric pressure levels. The desorbed gas concentration profiles for the subatmospheric pressure reduction step are significantly different than for the superatmospheric pressure reduction step. The subatmospheric pressure reduction step results in a higher average concentration of the desorbed gas and a higher enrichment factor than for the superatmospheric pressure reduction step.

Acknowledgment

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NOMENCLATURE

A	defined by Eq. (8)
A_*	area of column cross-section (cm^2)
ACFM	constant volumetric flow rate of the machinery at column exit (ft^3/min)
B	defined by Eq. (9)
b	Langmuir constant (atm^{-1})
$\hat{b}$	Langmuir constant at infinite T (atm^{-1})
C_g	gas-phase heat capacity (cal/mol·K)
C_s	adsorbent heat capacity (cal/g·K)
D	total desorbed gas quantity (mol)
Q_d	specific desorbed gas quantity (mol/g)
E	defined by Eq. (10)
E_f	enrichment factor
F	defined by Eq. (11)
FL	flow rate at column exit (mol/s)
L	length of the column (cm)
m	monolayer capacity in Langmuir model (mol/g)
n	solid phase capacity (mol/g)
P	pressure (atm)
Q	gas flow rate ($mol/cm^2 \cdot s$)
q	isosteric heat of adsorption (cal/mol)
R	gas constant
T	temperature (K)
t	time (s)
X_1–X_7	defined by Eqs. (12)–(19)
x	distance variable (cm)
y	gas-phase mole fraction of the strongly adsorbed species (i = 1)
$\bar{y}_D$	average concentration of the strongly adsorbed species in the desorbed gas
Z	defined by Eq. (28)
ϵ	adsorbent column void fraction (dimensionless)
θ	$T - T_s$ (K)
ρ_g	gas-phase density (mol/cm^3)
ρ_s	adsorbent density (g/cm^3)

Superscripts and Subscripts

1	more strongly adsorbed species
i	component i ($i = 1, 2$)
s	conditions at the start of the pressure reduction step
f	conditions at the end of the pressure reduction step

REFERENCES

1. R. Kumar, "Adsorption Column Blowdown: Adiabatic Equilibrium Model for Bulk Binary Gas Mixtures," *Ind. Eng. Chem., Res.*, *28*, 1677 (1989).
2. S. Sircar and R. Kumar, *Ind. Eng. Chem., Prod. Res. Dev.*, *22*, 271 (1983).

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