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NOTE

Analytical Scaling of Thermal Swing Adsorption

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With many applications of fixed-bed gas–solid adsorption systems, it is not surprising to find a considerable amount of work reported in the literature, presented in conferences, and summarized in a number of textbooks. Reviews of different adsorption systems are available from Ruthven (*5*), Wankat (*9*), Yang (*11*), and Suzuki (*7*). The oldest adsorption process for gas purification employs thermal swing adsorption (TSA) cycles. Strongly adsorbed species are desorbed by raising the temperature of the adsorbent and sweeping the strongly adsorbed species out of the void space with a purge gas which is frequently the direct heating medium.

Scaling methods can be used to rapidly design adsorption systems and to study the intensification of these systems. For complicated mathematical models without simple analytical solutions, one can obtain the scaling rules by dimensionless analysis (*2*, *4*). For simple models (constant pattern in this case), analytical solutions can be obtained. This makes it possible to find the scaling rules directly from the solution. In this paper we concentrate on finding TSA scaling rules based on solutions of the adiabatic constant pattern model developed by Sircar and Kumar (*6*). This approach was previously used by Wankat (*8*) and Wankat and Koo (*10*) for isothermal adsorption and chromatography.

FILM MASS TRANSFER CONTROL

Sircar and Kumar (*6*) used the constant pattern model for adsorption of bulk binary gas mixtures in an adiabatic column. By assuming the formation of constant pattern mass and heat transfer fronts (zones) in the column, Sircar and Kumar reduced the partial differential equations describing the mass and energy balances to a set of algebraic and ordinary differential equations and solved the problem analytically. The results can describe the experimental data satisfactorily for most practical design purposes.

Consider an adiabatic adsorption process in the column. A feed gas consists of one adsorbing species (Component 1) and one nonadsorbing species (Component 2, $n_2 = 0$). The column is initially saturated with pure Component 2 ($y_2^s = 0$) at p^0 and T_0. The following assumptions are made: 1) the gas flow in the column is essentially plug flow; 2) C_{ps}, ϵ, and ρ_s are independent of y_i, n_i, and T; 3) the column is adiabatic and isobaric; 4) there is an instantaneous thermal equilibrium between the gas/solid phase; and 5) the heat capacity of the adsorbent is much greater than the combined heat capacities of the gas and the adsorbed phases. Here y is the mole fraction and n is the amount adsorbed.

Based on the assumptions listed above, Sircar and Kumar (6) developed the following equations for a gas film driving force model:

$$\left.\frac{\partial n_i}{\partial t}\right|_x = k_{mi}(y_i - \bar{y}_i) \tag{1}$$

$$\sum y_i = 1, \qquad \sum \bar{y}_i = 1 \tag{2}$$

where $\bar{y}$ is the gas-phase mole fraction in equilibrium with n, p, and T while y is the gas-phase mole fraction. The following two equations can be derived from the constant pattern mass and energy balance equations:

$$\frac{n_1(1 - y_1)}{y_1} = \frac{n_1^0(1 - y_1^0)}{y_1^0} \tag{3}$$

and

$$u_{MTZ} = \frac{Q^0 y_1^0}{\epsilon y_1^0 \rho_f + \rho_s n_1^0} \tag{4}$$

where superscript 0 indicates the initial feed condition and Q is the gas flow rate. Langmuir adsorption equilibria are also used:

$$n_1^0 = \frac{m b_1 y_1^0}{1 + b_1 y_1^0}, \qquad n_1 = \frac{m b_1 \bar{y}_1}{1 + b_1 \bar{y}_1}, \qquad \bar{n}_1 = \frac{m b_1 y_1}{1 + b_1 y_1} \tag{5}$$

where $\bar{n}$ is the equilibrium amount adsorbed at p, T, and y. Equations (3)–(5) are used to integrate Eq. (1) for Component 1 to obtain the following analytical equations for the time difference $(t_2 - t_1)$ in the breakthrough curve corresponding to two arbitrary composition levels ϕ_1 and ϕ_2 (*6*):

$$k_{m1}(t_2 - t_1)\frac{(1 + b_1)y_1^0}{b_1 n_1^0} = \frac{m}{n_1^0}\ln\left(\frac{\phi_2(1 - \phi_1)}{\phi_1(1 - \phi_2)}\right) + \ln\frac{1 - \phi_2}{1 - \phi_1} - \frac{my_1^0}{n_1^0}\ln\frac{\phi_2}{\phi_1} + y_1^0(\phi_2 - \phi_1) \quad (6)$$

and the length of mass transfer zone (L_{MTZ}) can be calculated as

$$L_{MTZ} = u_{MTZ}(t_2 - t_1) \quad (7)$$

Usually, t_2 corresponds to 95% $(c_{FD} - c_{INIT})$ and t_1 corresponds to 5% $(c_{FD} - c_{INIT})$. In the meantime, we have the usual pressure drop equation for laminar flow in a fixed bed (*1*):

$$\Delta p = \frac{\mu u L}{K d_p^2} \quad \text{where } K = \frac{\epsilon^3}{(1 - \epsilon)^2}\frac{d_p^2}{150} \quad (8)$$

and we also have the following definition for Q^0:

$$Q^0 = \frac{4N^0}{\pi D^2} = \frac{p^0 u^0}{R_g T} \quad (9)$$

We want to scale the fractional bed use and to keep it constant in the old and the new designs. The fractional bed use will be constant in both designs if (*8*)

$$\left(\frac{L_{MTZ}}{L}\right)_{new} = \left(\frac{L_{MTZ}}{L}\right)_{old} \quad (10)$$

We choose the same composition levels ϕ_2 and ϕ_1 in the old and the new designs since the concentration profile will be kept the same with respect to its dimensionless distance along the column. The same Langmuir isotherms can be used since the temperature profile, the gas, and the adsorbent do not change. The feed composition is kept the same in the old and new designs. Therefore, all terms regarding the concentrations and the constants in the Langmuir equation will be the same in the old and the new systems.

Combining Eqs. (4), (6), and (7), the following equation can be obtained for scaling:

$$\frac{L_{MTZ}}{L} \propto \frac{Q^0}{\mathrm{Lk}_{m1}} \tag{10a}$$

By defining $R_X = X_{new}/X_{old}$, we introduce the scaling factors to the above relationship and obtain

$$R_{(L_{MTZ}/L)} = \frac{R_{L_{MTZ}}}{R_L} = \frac{R_{Q^0}}{R_L R_{k_{m1}}} \tag{11}$$

From Eq. (9) we have

$$R_{Q^0} = R_{u^0} \tag{11a}$$

where $R_{u^0} = R_u$. By assuming that the gas phase is ideal, and combining the correlation of Petrovic and Thodos (*3*) for film diffusion, we obtain the following expression for the gas-phase film mass transfer coefficient (*6*):

$$k_{m1} = \frac{A_1(Q^0)^{1-\beta)}(T^0)^{0.5\beta}}{d_p^{(1+\beta)}} \tag{11b}$$

which yields

$$R_{k_{m1}} = \frac{R_{Q^0})^{1-\beta}}{R_{d_p}^{1+\beta}} = \frac{R_u^{1-\beta}}{R_{d_p}^{1+\beta}} \tag{11c}$$

From Eqs. (11), (11a), and (11c) we obtain

$$R_u^{\beta} R_{d_p}^{1+\beta} = R_L \tag{12}$$

and by scaling the pressure drop we obtain the following:

$$R_u R_L = R_{d_p}^2 \tag{13}$$

Therefore, the scaling results for the adiabatic constant pattern model in laminar flow with gas film control are

$$R_L = R_{d_p}^{(1+3\beta)/(1+\beta)}, \qquad R_u = R_{d_p}^{(1-\beta)/(1+\beta)} \tag{14}$$

Consequently, we have the following for $t_{ad} = L/u$ and D:

$$R_{t_{ad}} = \frac{R_L}{R_u} = R_{d_p}^{4\beta/(1+\beta)}, \qquad R_D = (R_{N^0})^{0.5} R_{d_p}^{(\beta-1)/(2+2\beta)} \tag{15}$$

Using the numerical value $\beta = 0.359$ (*3*), we have

$$R_L = R_{d_p}^{1.528}, \qquad R_u = R_{d_p}^{0.472}, \qquad R_{t_{ad}} = R_{d_p}^{1.057}, \qquad R_D = (R_{N^0})^{0.5} R_{d_p}^{-0.236} \tag{16}$$

Therefore, the scaling rules are identical to those obtained by dimensionless analysis as given by Rota and Wankat (*4*) for PSA and Chen and Wankat (*2*) for TSA.

SOLID DIFFUSION CONTROL

For the solid diffusion (internal diffusion) model, the analytical solution obtained by Sircar and Kumar (*6*) can also be used to develop the scaling rules. When solid diffusion controls, Eq. (6) becomes (*6*)

$$k_{s1}(t_2 - t_1)\frac{1 + b_1}{b_1} = \frac{m}{n_1^0} \ln\left(\frac{\phi_2(1 - \phi_1)}{\phi_1(1 - \phi_2)}\right) + \ln\frac{\phi_1}{\phi_2} + \frac{(1 + b_1)}{b_1} \ln\frac{1 - \phi_2 y_1^0}{1 - \phi_1 y_1^0} \tag{17}$$

By combining Eq. (4), (7), and (17), the following equation can be used for scaling:

$$\frac{L_{MTZ}}{L} \propto \frac{Q^0}{Lk_{s1}} \tag{18}$$

where k_{si} is given by (*6*)

$$k_{s1} = \frac{A_2 D_p^0 \exp(-E_1/R_g T)}{d_p^2} \tag{19}$$

Combining Eqs. (18) and (19) and introducing the scaling factors, one can obtain

$$R_{L_{MTZ}/L} = \frac{R_u R_{d_p}^2}{R_L} \tag{20}$$

By making the above equation equal to 1 and combining with Eq. (13), the scaling rules for the adiabatic constant pattern model in laminar flow with solid diffusion control are

$$R_u = 1, \qquad R_L = R_{d_p}^2 \tag{21}$$

Consequently, we have the following for $t_{ad} = L/u$ and D:

$$R_{t_{ad}} = R_L, \qquad R_D = (R_{N^0})^{0.5} \tag{22}$$

The same scaling rules were obtained by dimensionless analysis for the internal diffusion mechanism by Rota and Wankat (*4*) for PSA and Chen and Wankat (*2*) for TSA.

TURBULENT FLOW

So far, we have shown the scaling rules for the film transfer and solid diffusion models under laminar flow conditions. For turbulent flow, the scaling rules can also be obtained. Considering the gas film driving model, we have Eq. (12) and the following pressure drop equation (*1*):

$$\Delta p = \frac{1.75\rho(1 - \epsilon)}{\epsilon^3} \frac{u^2 L}{d_p} \tag{23}$$

Introducing the scaling factors to Eq. (23), one can obtain

$$R_{d_p} = R_L R_u^2 \tag{24}$$

Therefore, Eqs. (12) and (24) give

$$R_u = R_{d_p}^{-\beta/(2+\beta)}, \qquad R_L = R_{d_p}^{(2+3\beta)/(2+\beta)} \tag{25}$$

and

$$R_{t_{ad}} = R_{d_p}^{(2+4\beta)/(2+\beta)}, \qquad R_D = (R_{N^0})^{0.5} R_{d_p}^{\beta/(4+2\beta)} \tag{26}$$

Similarly, the scaling rules for the solid diffusion model with turbulent flow are

$$R_u = R_{d_p}^{-1/3}, \qquad R_L = R_{d_p}^{5/3}, \qquad R_{t_{ad}} = R_{d_p}^2, \qquad R_D = (R_{N^0})^{0.5} R_{d_p}^{1/6} \tag{27}$$

The results obtained in Eqs. (25) to (27) agree with the results obtained by Wankat (*8*) for isothermal systems using a different analysis procedure.

DISCUSSION

Once the particle size and the throughput are chosen, other operating and design parameters in the new system can be obtained based on the original design. Then, the numerical values can be used in the above calculations to find the appropriate parameter values. For example, for solid diffusion control with laminar flow and $R_{N^0} = 1$, $R_{d_p} = 0.5$, one obtains $R_D = 1$, $R_L = 0.25$, and $R_{t_{ad}} = 0.25$. The column is shorter, cycles faster, and requires less absorbent.

The scaling rules obtained here are derived from the equations related only to the fixed-bed section. Overall scaling rules should include extra-column effects. Theoretical analyses for extra-column effects have been given by Rota and Wankat (*4*) and Chen and Wankat (*2*). To prevent excessive energy use in TSA when decreasing the cycle time, one must use internal insulation. Other extra-column effects and practical limitations of this procedure are discussed by Rota and Wankat (*4*) and Chen and Wankat (*2*).

NOTATION

A_1	constant in Eq. (11b)
A_2	constant in Eq. (19)
b_1	constant in Langmuir equation
c	mole concentration (mol/m^3)
C_p	heat capacity [J/kg·K (solid) and J/mol·K (gas)]
C_{ps}	adsorbent heat capacity (J/mol·K)
d_p	particle diameter (m)
D	column diameter (m)
D_p	pore diffusivity (m^2/s)
E_1	activation energy for diffusion (J/mol)
k_m	film mass transfer coefficient (mol/kg·s)
k_s	solid diffusion mass transfer coefficient (1/s)
K	constant in Eq. (12)
L	column length (m)
m	Langmuir constant (mol/kg)
n	amount adsorbed (mol/kg)
$\bar{n}$	amount adsorbed in equilibrium with y (mol/kg)
N	total feed rate (mol/s)
p	pressure (atm)
Q^0	gas flow rate (mol/m^2·s)
R	scaling operator, $R_X = X_{new}/X_{old}$
R_g	ideal gas constant (atm·m^3/mol·K)
t	time (s)

T	temperature (K)
u	interstitial velocity (m/s)
x	column coordinate (m)
y	mole fraction
$\bar{y}$	mole fraction in equilibrium with n

Greek Letters

β	constant in film transfer correlation
Δp	pressure drop across the bed (atm)
ϵ	fractional void space available for flow
μ	viscosity (kg/m·s)
ϕ	gas composition
ρ	density [mol/m^3 (gas) or kg/m^3 (solid)]
ρ_s	adsorbent density (kg/m^3)

Subscripts

ad	adsorption
f	fluid
FD	feed
i	ith component
$INIT$	initial state
MTZ	mass transfer zone
new	new design
old	old design

Superscripts

0	feed condition
s	saturating condition

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