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Effects of desorbent flowrate on simulated moving bed process

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Abstract−This article presents the effects of the desorbent flowrate (or m_1) on simulated moving bed (SMB) process performance at constant m_2, m_3 and m_4, where the m-values (m_j) are defined as the net flowrate ratios of the zone, j, to the solid flowrate. A complete m-plane analysis of SMB systems (ComPASS) has been developed that illustrates how the desorbent flowrate is determined within the complete m-plane (i.e., fluid-solid flowrate ratio plane) to enhance the SMB process performance. The effects of desorbent flowrate are presented numerically for linear/equilibrium and nonlinear/nonequilibrium SMB processes. The results of the studies using ComPASS show that for linear/equilibrium SMB process, it is desirable to determine the minimum desorbent flowrate (m_1) within the complete separation region. For the nonlinear/nonequilibrium SMB process, the desorbent flowrate can be determined at the minimum value which maximizes the raffinate purity.

Key words: Simulated Moving Bed (SMB) Chromatography, Desorbent Consumption, Triangle Theory, Process Simulation and Optimization, Complete m-Plane Analysis of SMB Systems (ComPASS)

INTRODUCTION

Simulated Moving Bed (SMB) processes have emerged as a promising technology for the separation of not only conventional compounds (e.g., petro-chemicals and sugar), but also pharmaceutical (e.g., chiral compounds), and bio-chemical (e.g., amino acids, peptides and proteins) compounds [1,2]. SMB chromatography has an inherent advantage of a high driving force, resulting in less solvent consumption, smaller apparatus scale, lower investment costs and higher yields. However, in order to take full advantage of this principle, a large number of operational parameters (e.g., flowrates, switching time, column dimension and configuration) need to be adjusted properly [3]. Model-based simulation and optimization are of practical importance in searching optimum operation conditions, because an experimental evaluation of such conditions is very time-consuming and costly.

In SMB applications, throughput (or productivity) and desorbent consumption are two key factors that control process cost. Practically, the operating conditions are selected to reach maximum productivity with lowest desorbent consumption [4,5]. To achieve this purpose, a multi-level optimization procedure (MLOP) was proposed for optimization of four-zone nonlinear SMB chromatography [2]. The MLOP systematically approaches from initialization to optimization and from simple models (e.g., linear isotherms) to complex models (e.g., nonlinear and nonequilibrium adsorption models).

In this study, Triangle theory [4] is extended to a complete m-plane analysis taking into account various process performance indexes (e.g., productivity, yield, desorbent consumption and dilution) for optimization of SMB operating conditions. This article aims to show the effects of m_1 (or desorbent flowrate) at a constant m_2, m_3 and m_4 for linear/equilibrium and nonlinear/nonequilibrium SMB processes.

The remainder of the paper is organized as follows. Section 2 describes the theoretical background on ComPASS (complete m-plane analysis of SMB systems). The numerical studies carried out on linear/equilibrium and nonlinear/nonequilibrium SMB processes are illustrated in section 3 to show the effects of m_1 on SMB process performance. Section 4 concludes this work.

COMPASS (COMPLETE M-PLANE ANALYSIS OF SMB SYSTEMS)

When the column dimensions and the configuration are fixed for a target mixture in the four-zone SMB, operating variables such as flowrates (desorbent (Q_{des}), extract (Q_{ext}), feed (Q_{feed}) and raffinate (Q_{raf})) and the cycle time (τ) should be properly adjusted to obtain desirable process performance (e.g., productivity, desorbent consumption (or dilution), purity and yield). Flowrates at the four zones such as zone I (desorbent-extract), zone II (extract-feed), zone III (feed-raffinate) and zone IV (raffinate-desorbent) are expressed as:

$$Q_1=Q_{des}+Q_4 \tag{1a}$$
$$Q_2=Q_1-Q_{ext} \tag{1b}$$
$$Q_3=Q_2+Q_{feed} \tag{1c}$$
$$Q_4=Q_3-Q_{raf} \tag{1d}$$

The operation principle of SMB systems can be described by an equivalent true moving bed (TMB) configuration where the solid particle moves in the opposite direction of the fluid flow [4]. The TMB system with the equilibrium adsorption is well analyzed by Triangle theory for linear and Langmuir adsorption isotherms [4].

The net flowrate ratios (m_j) of each zone to the solid flowrate are defined as:

$$m_j=\frac{Q_j^{TMB}}{Q_s} \tag{2}$$

where, $Q_s=(V_c(1-\varepsilon))/\tau$ is the solid flowrate defined as the net solid

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volume divided by the cycle time (τ). ε is the overall bed voidage including the interstitial bed voidage (ε_b) and intraparticle porosity (ε_p), i.e., $\varepsilon=\varepsilon_b+\varepsilon_p(1-\varepsilon_b)$. The equivalence between the TMB flowrate (Q_j^{TMB}) and the SMB flowrate (Q_j^{SMB}) is:

$$Q_j^{SMB}=Q_j^{TMB}+Q_s\frac{\varepsilon}{1-\varepsilon} \tag{3}$$

Substituting Eq. (3) for Eq. (2),

$$m_j=\frac{Q_j^{SMB}-Q_s\dfrac{\varepsilon}{1-\varepsilon}}{Q_s}=\frac{Q_j^{SMB}\tau-V_c\varepsilon}{V_c(1-\varepsilon)}$$

Then, the fluid flowrate ratio (m_j) is rearranged as follows:

$$m_j=\frac{Q_j^{SMB}}{Q_s}-\phi \tag{4}$$

where the phase ratio $\phi=\varepsilon/(1-\varepsilon)$ can be assumed to be constant. Eq. (1) is expressed in terms of m_j as follows:

$$\begin{aligned} m_1&=m_4+m_D\\ m_2&=m_1-m_E\\ m_3&=m_2+m_F\\ m_4&=m_3-m_R \end{aligned} \tag{5}$$

where $m_D=Q_{des}/Q_s$, $m_E=Q_{ext}/Q_s$, $m_F=Q_{feed}/Q_s$ and $m_R=Q_{raf}/Q_s$. Therefore, the four physical operating variables (Q_{des}, Q_{ext}, Q_{feed} and Q_{raf}) are transformed into the dimensionless flowrate ratios (m_j, j=1, 2, 3 and 4).

According to Triangle theory [4], a triangle-shaped complete separation region exists within m_2-m_3 plane for a linear TMB system with equilibrium adsorption (see Fig. 1). Here, to obtain complete separation of components A (more adsorptive) and B (less adsorptive), the following constraints should be satisfied.

$$\begin{aligned} &K_A\le m_1<\infty\\ &K_B\le m_2\le K_A\\ &K_B\le m_3\le K_A \end{aligned}$$

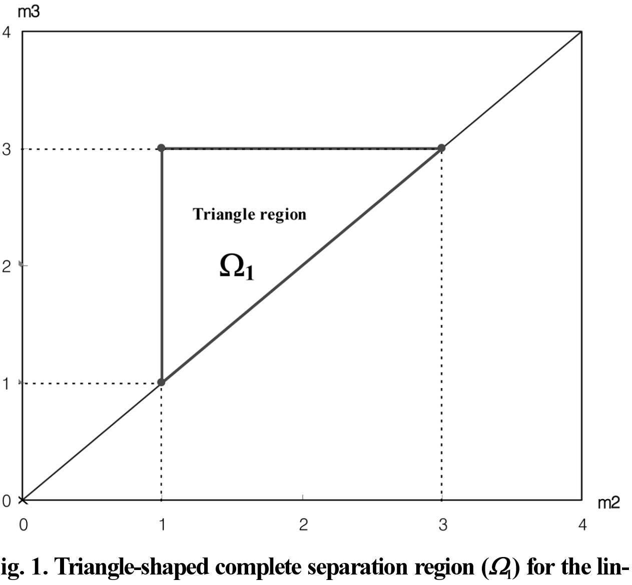

Fig. 1. Triangle-shaped complete separation region (Ω_1) for the linear TMB system with equilibrium adsorption (K_A=3 and K_B=1).

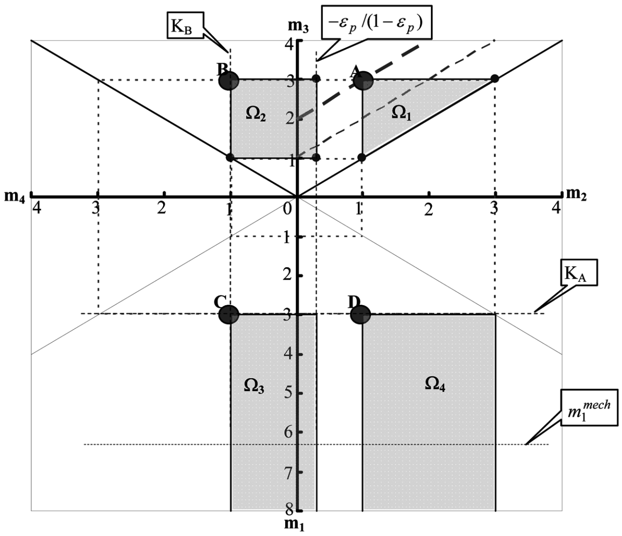

Fig. 2. Complete separation regions within complete m-planes for the linear TMB system with equilibrium adsorption (K_A= 3 and K_B=1).

$$-\frac{\varepsilon_p}{1-\varepsilon_p}<m_4\le K_B \tag{6}$$

where K_A is the linear isotherm constant of the more adsorptive component A and K_B is that of the less adsorptive component B. The complete separation region (Ω_1) for K_A=3 and K_B=1 is shown in Fig. 1. The four diagonal lines are drawn to represent the following four inequalities implying the positive-flowrate in each zone.

$$\begin{aligned} &m_1>m_2\\ &m_3>m_2\\ &m_3>m_4\\ &m_1>m_4 \end{aligned} \tag{7}$$

Combining the inequality conditions (Eq. (6) and Eq. (7)), three feasible regions for complete separation are created within other three m-spaces as shown in Fig. 2. The four regions (Ω_i, i=1, 2, 3 and 4) depict the boundary of the flowrate ratio (m_j) for obtaining 100% pure components in extract and raffinate.

A closed rectangular region in the m_3–m_4 plane, and an open rectangular region in the m_4-m_1 plane and the m_1-m_2 plane are observed, as shown in Fig. 2. It is evident from Fig. 2 that for a linear and equilibrium TMB system, m_2, m_3, and m_4 have a restricted range, while m_1 is open to the infinite. The focus of this study is to examine whether there is a desirable m_1 value to enhance process performance by means of a complete m-plane analysis of SMB systems (ComPASS) based on Triangle theory.

1. Process Performance for Linear/Equilibrium SMB System

Productivity (Pr: kg/hr/m^3-resin) can be defined as:

$$\Pr=\frac{Q_{ext}\overline{C}_{A,E}+Q_{raf}\overline{C}_{B,R}}{(1-\varepsilon_b)N_cV_c} \tag{8}$$

where N_c is the number of columns, V_c is the volume of single column, $\overline{C}_{A,E}$ and $\overline{C}_{B,R}$ and are the average concentrations of A and B in extract and raffinate, respectively, during the cycle time. In the complete separation region, the following mass balance is fulfilled in the TMB steady state:

$$Q_{feed}C_{A,F}=Q_{ext}\overline{C}_{A,E}$$
$$Q_{feed}C_{B,F}=Q_{raf}\overline{C}_{B,R} \tag{9}$$

Replacing Eq. (8) by Eq. (9), the equation for productivity becomes:

$$\mathrm{Pr}=\frac{Q_{feed}(C_{A,F}+C_{B,F})}{(1-\varepsilon_b)N_cV_c} \tag{10}$$

Eq. (10) states that for a fixed column configuration and constant feed concentration, productivity is a function of Q_{feed}. To maximize the productivity is to maximize the feed flowrate in the complete separation region. Using Eq. (5) and the definition of m_F, Eq. (10) can be rewritten in terms of the fluid flowrate ratios as follows:

$$\mathrm{Pr}=\eta_1 m_F Q_s \equiv \eta_1(m_3-m_2)Q_s \tag{11}$$

where $\eta_1=(C_{A,F}+C_{B,F})/(1-\varepsilon_b)N_cV_c$. It is clear from Eq. (11) that the cycle time (τ) should be decreased (or Q_s increased) and the value of (m_3-m_2) should be increased to maximize productivity. The latter is obtained from the linear programming (LP) within the m_2-m_3 plane as follows:

$$\mathrm{Max}(m_3-m_2)$$
$$\text{s.t. } m_2\in\Omega_1,\ m_3\in\Omega_1 \tag{12}$$

The point A, which is shown in Fig. 2, is a unique optimum point resulting from Eq. (12) at a given cycle time (τ).

Desorbent consumption (DC) is defined as:

$$\mathrm{DC}=\frac{Q_{des}}{Q_{feed}}\equiv\frac{m_D}{m_F}\equiv\frac{m_1-m_4}{m_3-m_2} \tag{13}$$

The dilution of the extract solution for more retained component A is defined as:

$$\mathrm{Dilution}_E=\frac{C_{A,F}-\overline{C}_{A,E}}{C_{A,F}} \tag{14a}$$

and the raffinate dilution for less retained component B is defined as:

$$\mathrm{Dilution}_R=\frac{C_{B,F}-\overline{C}_{B,R}}{C_{B,F}} \tag{14b}$$

Substituting Eq. (9) for Eq. (14), the dilution can be expressed by the flowrates or m-values:

$$\mathrm{Dilution}_E=1-\frac{Q_{feed}}{Q_{ext}}=1-\frac{m_3-m_2}{m_1-m_2}$$
$$\mathrm{Dilution}_R=1-\frac{Q_{feed}}{Q_{raf}}=1-\frac{m_3-m_2}{m_3-m_4} \tag{15}$$

When m_2 and m_3 are fixed at a maximum productivity (point A in Fig. 2), the extract dilution is proportional to m_1 and the raffinate dilution is inversely proportional to m_4. Higher dilution results in more dilute solution of the product, and it is desirable to minimize the dilution. Therefore, minimum m_1 and maximum m_4 are considered as an optimum operating condition. It is worth noting that minimizing desorbent consumption Eq. (13) is equivalent to minimizing dilution Eq. (15). The points B, C and D in Fig. 2 satisfy a maximum productivity and a minimum dilution (or desorbent consumption) in m_4-m_3, m_4-m_1 and m_2-m_1 planes, respectively.

The yield is determined by the ratio of the product mass-flowrate to the feed mass-flowrate:

$$\mathrm{Yield}_E=\frac{\overline{C}_{A,E}\cdot Q_{ext}}{C_{A,F}\cdot Q_{feed}}$$
$$\mathrm{Yield}_R=\frac{\overline{C}_{A,R}\cdot Q_{raf}}{C_{A,F}\cdot Q_{feed}} \tag{16}$$

Combining Eq. (9) and Eq. (16), the yields should be unity for the linear/equilibrium TMB system:

$$\mathrm{Yield}_E=1$$
$$\mathrm{Yield}_R=1 \tag{17}$$

However, the yield will be less than unity in the linear/equilibrium SMB operation because of periodic switching of flowrates (see Fig. 4).

Since the maximum pressure drop (ΔP) of columns is mechanically given for an SMB unit, the maximum flowrate (Q_{max}) of the column is fixed according to ΔP, which is normally the flowrate of zone I (Q_1) in the four-zone SMB unit. The relationship between the pressure drop and the flowrate in the packed-column is obtained from the Ergun equation [6]:

$$F_{LS}=\frac{\Delta P}{L_c}=A\left(\frac{1-\varepsilon_b}{\varepsilon_b}\right)^2\frac{\mu_L v_L}{d_p^2}+B\left(\frac{1-\varepsilon_b}{\varepsilon_b}\right)\frac{\rho_L v_L^2}{d_p} \tag{18}$$

where, F_{LS} [Pa/m] is the pressure drop per unit column length, μ_L [kg/m/s] is the liquid viscosity, ρ_L is the liquid density, v_L [m/s] is the liquid interstitial velocity and d_p [m] is the particle diameter. The Ergun coefficients, A and B, of the fluid are taken to 180 and 1.75, respectively [7] and the second term of the right hand side in Eq. (18) is negligible for a normal SMB unit. Thus, the flowrate ratio of Q_1 to Q_s (m_1) is mechanically limited within an allowable pressure drop as follows:

$$m_1^{mech}=\frac{Q_1}{Q_s}=\frac{v_L\cdot\varepsilon_b\cdot S}{S\cdot L_c\cdot(1-\varepsilon_b)/\tau}-\phi$$
$$=\frac{1}{180}\cdot\left(\frac{\varepsilon_b}{1-\varepsilon_b}\right)^3\left(\frac{d_p}{L_c}\right)^2\cdot\frac{\tau\cdot\Delta P}{\mu_L}-\phi \tag{19}$$

Eq. (6) is then modified for the linear/equilibrium TMB system as.

$$K_A\le m_1<m_1^{mech}$$
$$K_B\le m_2\le K_A$$
$$K_B\le m_3\le K_A$$
$$-\frac{\varepsilon_p}{1-\varepsilon_p}<m_4\le K_B \tag{20}$$

An expected mechanical m_1 value (m_1^{mech}) is also shown in Fig. 2. The above analysis with Eq. (20) and Fig. 2 is called ComPASS (complete m-plane analysis of SMB systems) for the linear and equilibrium case.

2. Process Performance for Nonlinear/Nonequilibrium SMB System

The process performance of the nonlinear and nonequilibrium SMB system is examined at a given m_2, m_3 and m_4 in terms of productivity and desorbent consumption, as yield and dilution correspond to productivity and desorbent consumption, respectively.

Eq. (8) can be expressed as a function of flowrate ratios (m_i)

$$\mathrm{Pr}=\frac{Q_s}{(1-\varepsilon_b)N_cV_c}\cdot((m_1-m_2)\cdot\overline{C}_{A,E}+(m_3-m_4)\cdot\overline{C}_{B,R}) \tag{21}$$

The mass balance in the SMB system is derived as follows:

$$
\begin{aligned}
&Q_{feed}C_{A,F}=Q_{ext}\overline{C}_{A,E}+Q_{ref}\overline{C}_{A,R}\\
&Q_{feed}C_{B,F}=Q_{ext}\overline{C}_{B,E}+Q_{ref}\overline{C}_{B,R}
\end{aligned}
\tag{22}
$$

Combining Eq. (21) and Eq. (22), the productivity is obtained as:

$$
\mathrm{Pr}=\frac{1}{(1-\varepsilon_b)N_cV_c}\cdot(Q_{feed}C_{A,F}-Q_{ref}\overline{C}_{A,R}+(m_3-m_4)\cdot Q_s\cdot\overline{C}_{B,R}) \tag{23}
$$

The productivity increases with decreasing $\overline{C}_{A,R}$ and with increasing $\overline{C}_{B,R}$ for constant m_2, m_3, and m_4 values. The effect of m_1 on the mean concentrations of raffinate ($\overline{C}_{A,R}$ and $\overline{C}_{B,R}$) is nonlinear in nature due to nonlinear adsorption isotherms and nonequilibrium adsorption kinetics, and the productivity in this case is not examined analytically. To reduce the desorbent consumption, m_1 that is greater than m_4 and less than m_1^{mech} should be small as given by Eq. (13) and Eq (20). As a result of the two criteria (productivity and desorbent consumption), it is desirable to have a minimum value for m_1 that maximizes the raffinate purity, $\mathrm{Purity}_R=\overline{C}_{B,R}/(\overline{C}_{A,R}+\overline{C}_{B,R})$. That is,

$$
\begin{aligned}
&\min_{m_1} m_1,\\
&\text{s.t. } m_4\le m_1\le m_1^{mech}\\
&\max_{m_1} \mathrm{Purity}_R=\frac{C_{B,R}}{\overline{C}_{A,R}+\overline{C}_{B,R}}
\end{aligned}
\tag{24}
$$

Eq. (24) is used to determine a desirable m_1 for a nonlinear/nonequilibrium SMB system discussed in section 2.

NUMERICAL STUDIES

The process performance is examined by changing m_1 at constant m_2, m_3 and m_4 for the linear/equilibrium and nonlinear/non-

Table 1. Parameters used for 4-zone SMB process simulation

Parameters		Linear/equilibrium SMB	Nonlinear/nonequilibrium SMB
Design para.	Column configuration	2-2-2-2	2-2-2-2
	Column length (L_c)	30 cm	10.5 cm
	Overall bed voidage (ε)	0.5	0.4
	Column diameter (d_c)	1.5962 cm	2.6 cm
	Phase ratio (ϕ)	1	0.6667
Opera. para.	Feed concentration (C_{feed})	0.5/0.5 g/ml	2.9/2.9 g/*l*
	Feed flowrate (Q_{feed})	3 ml/min	5.46 ml/min
	Desorbent flowrate (Q_{des})	3-60 ml/min	18.3-234.4 ml/min
	Extract flowrate (Q_{ext})	3-60 ml/min	15.5-231.6 ml/min
	Raffinate flowrate (Q_{raf})	3 ml/min	8.27 ml/min
	Recycle flowrate (Q_{rec})	3 ml/min	29.76 ml/min
	Cycle time (τ)	20 min	3.25 min
	No. shifting	16 (2 rounds)	44 (5.5 rounds)
Model para.	Adsorption isotherms	$K_A=3$, $K_B=1$	$n_A^*=\frac{3.73C_A}{1+0.0466C_A+0.0336C_B}+\frac{0.3C_A}{1+3C_A+C_B}$ $n_B^*=\frac{2.69C_B}{1+0.0466C_A+0.0336C_B}+\frac{0.1C_B}{1+3C_A+C_B}$
	Axial dispersion (D_{ax})	-	$0.00525\times v_L$
	Adsorption rate (k)	-	$k_A=6.0\ \mathrm{min}^{-1}$, $k_B=6.0\ \mathrm{min}^{-1}$
Comput. para.	No. grid	31	31
	Spatial stepsize (Δx)	1 cm	0.35 cm
	No. time steps	1,000-2,500	300
	Temporal stepsize (Δt)	0.02-0.0083 min	0.01 min
	max. CFL*	0.25-0.5	0.25-0.5
ComPASS para.	m_1	3-42	4-25
	m_2	1	2.4980
	m_3	3	3.0285
	m_4	1	2.2249
	Q_s	1.5 ml/min	10.29 ml/min
	m_1^{mech}	42	30
	Purity_R^{spec}	1.0	97.3
Analytic TMB solution	$\max\overline{C}_{A,E}$	0.5	-
	$\max\overline{C}_{B,R}$	0.5	-
	Productivity	$0.375\frac{g}{hr\cdot cm^3}$	-

$$*\text{max. CFL}=v_{L,max}\frac{\Delta t}{\Delta z}$$

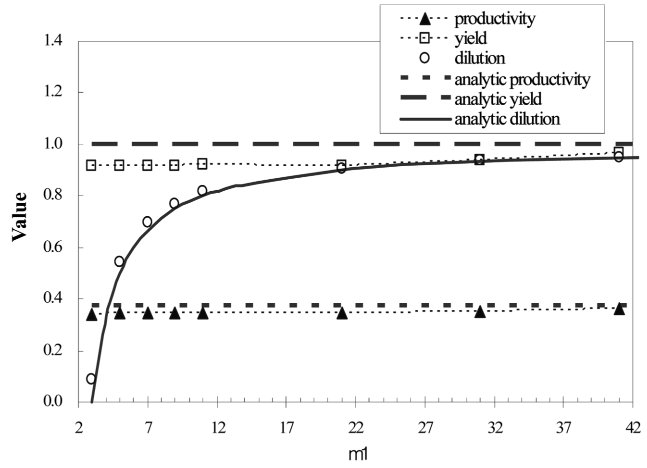

Fig. 3. Linear/equilibrium SMB process performance with m_1 at constant m_2, m_3, and m_4.

equilibrium SMB processes. Table 1 shows design, operation, model and simulation parameters for the two SMB processes. FAST-Chrom/SMB [8] including the conservation element and solution element (CE/SE) method [9,10] is used to solve the SMB model [2,11,12] in this study.

1. Linear/Equilibrium SMB process

The flowrates of the linear/equilibrium SMB process are initialized by ComPASS as proposed in section 2. The results of the SMB model simulation are given in Fig. 3. The analytic solution obtained from the TMB operation is also shown in Fig. 3 for comparison. The analytic dilution of extract (Dilution$_E$) is obtained by using Eq. (15) for fixed m_2 and m_3. The analytic productivity (P_r=0.375(g/hr·cm^3), see Table 1) and yield (Yield$_E$=Yield$_R$=1) are constant and obtained by using Eq. (11) and Eq. (17), respectively. In the SMB system, the two performance values are, however, deteriorated (P_r ≅0.35(g/hr·cm^3), Yield$_E$≅0.92) because of the periodical dynamics of the concentration profile.

As mentioned earlier, a lower dilution which means a lower desorbent consumption is preferred and m_1 should be determined at the smallest value, m_1=3. Therefore, ComPASS derived from Triangle theory is useful to identify the operating conditions of the linear/equilibrium SMB systems.

In Fig. 4, the fluid concentration distribution of components A and B is shown over eight columns at three different times within one cycle. Since m_2, m_3 and m_4 are fixed, the two concentration profiles of component B (thin lines with square points) are the same at m_1=7 and 31. When m_1 is large, the concentration profile of component A (circles) moves ahead of that of the small m_1 value for every moment within the cycle time.

2. Nonlinear/Nonequilibrium Binaphthol SMB Process

For separation of binaphthol enantiomers, the chiral stationary phase used is 3,5-dinitrobenzoyl phenylglycine bonded to silica gel, and the desorbent used is a mixture of 72/28 (v/v) heptane/isopropanol. Since the solubility limit of each enantiomer in this desorbent is 3 g/*l*, the feed composition is determined under the solubility limitation [11].

The operating conditions of the binaphthol SMB process were optimized by a multilevel optimization procedure (MLOP) proposed by Lim [2], and the simulation parameters used are reported in Table 1. The desorbent flowrate (Q_{des}) varies from 28.3 to 234.4 ml/min, corresponding to from m_1=4 to 25, respectively. An analytic TMB solution is not available in this nonlinear case.

Fig. 5 shows the process performance in terms of productivity, raffinate purity, yield and dilution. It is evident from Fig. 5 that the yield obtained from the process simulation has a good agreement with the analytic dilution. It is observed that the raffinate purity shows a maximum near m_1=5 and the productivity and yield remain constant over m_1=4.5. From Eq. (24), the optimum m_1 should be about 4.5 or Q_{des}=23.4. This value agrees well with the MLOP results (Q_{des}= 22.9) of Lim [2]. It is noted that productivity, yield and purity vary with m_1 in the nonlinear/nonequilibrium SMB case but remain constant in the linear/equilibrium SMB case.

The concentration profiles at three different times during one cycle are shown in Fig. 6. As m_2, m_3 and m_4 are fixed, those of the zones III and IV change little. When m_1 is large (m_1=25), the concentration of A ($C_{A,E}$) in extract becomes low.

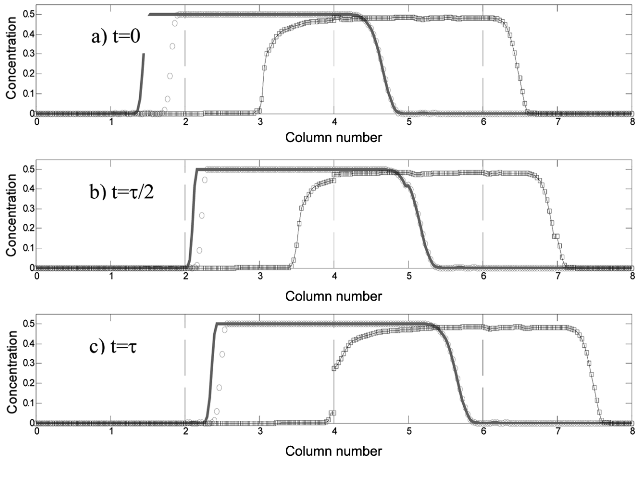

Fig. 4. Effect of m_1 at constant m_2, m_3 and m_4 in a linear and equilibrium SMB unit (solid line: m_1=7, circles: m_1=31).

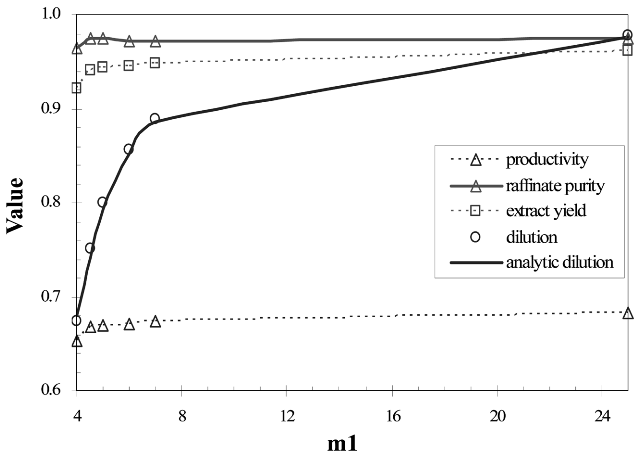

Fig. 5. Nonlinear/nonequilibrium SMB process performance with m_1 at constant m_2, m_3, and m_4.

CONCLUSION

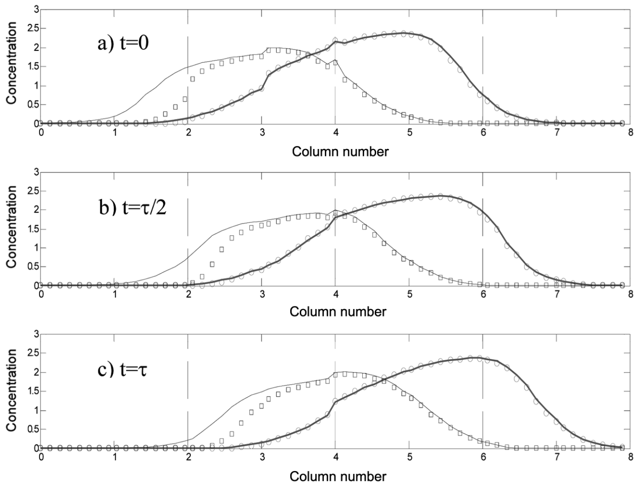

Fig. 6. Effect of m_1 at constant m_2, m_3 and m_4 in a nonlinear and nonequilibrium SMB unit (solid line: m_1=4.5, squares: m_1=25).

Triangle theory developed for linear/equilibrium TMB operation is extended to complete m-plane analysis of SMB systems (ComPASS) for identification of optimum operating conditions. The effects of the desorbent flowrate (m_1) at constant m_2, m_3 and m_4 values are examined on the process performance such as productivity, yield, desorbent consumption and dilution.

ComPASS well explains the effects of m_1 for the linear/equilibrium SMB systems. In the case of nonlinear/non equilibrium SMB systems, an optimum desorbent flowrate is determined at minimum m_1 value which maximizes the raffinate purity.

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NOMENCLATURE

A : slow-moving component
B : fast-moving component
CE/SE : conservation element/solution element
C_{feed} : feed composition [g/l on liquid volume basis]
C_i : concentration in fluid phase [g/l on liquid volume basis]
$\overline{C}_i$: average liquid concentration over the switching time [g/l on liquid volume basis]
D_{ax} : axial dispersion coefficient [m^2/min]
k : overall adsorption rate coefficient [1/min]
K_i : equilibrium constant
L_c : column length [m]
LDF : linear driving force
N_c : number of columns
Q_1 : flowrate in the zone I [ml/min]
Q_2 : flowrate in the zone II [ml/min]
Q_3 : flowrate in the zone III [ml/min]
Q_4 : flowrate in the zone IV [ml/min]
Q_{des} : desorbent flowrate [ml/min]
Q_{ext} : extract flowrate [ml/min]
Q_{feed} : feed flowrate [ml/min]
Q_{raf} : raffinate flowrate [ml/min]
Q_{rec} : recycle flowrate [ml/min]
S : cross-section area of column [cm^2]
SMB : simulated moving bed
t : time [min]
TMB : true moving bed
V_c : solid volume of one column [cm^3]
v_L : interstitial fluid velocity [cm/min]

Greek Letters

ε : overall bed voidage [$=\varepsilon_b+\varepsilon_p(1-\varepsilon_b)$]
ε_b : interstitial bed voidage
ε_p : intraparticle porosity
ϕ : phase ratio [$=\varepsilon/(1-\varepsilon)$]
ν : CFL number [$=v_L(\Delta t/\Delta z)$]
τ : cycle time or shifting time [min]
Δp : pressure drop in columns [=Pa]
Δt : uniform time step size [=min]
Δz : uniform spatial step size [=cm]

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