Improved Performance of Simulated Moving Bed Process Using Column-Modified Feed

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A "FeedCol" strategy was developed to improve separation performance in simulated moving bed (SMB) processes. In the FeedCol operation, a short chromatographic column was simply added to the SMB unit and feed was supplied by a pulse input through the column to the SMB process. Because the feed was made in the shape of partially separated chromatographic peaks through the column, the purities in the raffinate and extract products were improved efficiently in the SMB process. All the performance parameters for a binary mixture with low selectivity (α = 1.1) were better for the FeedCol operation than for the conventional SMB operation (2-2-2-2). Because the feed injection through the feed column was synchronized with the SMB process during the switching period, two new operating variables were introduced: injection length and injection time. Their effects on the suggested strategy were evaluated in terms of performance parameters through a detailed simulation study. © 2010 American Institute of Chemical Engineers *AIChE J,* 57: 2036–2053, 2011
Keywords: FeedCol, SMB, chromatography, injection length, injection time

Introduction

Simulated moving bed (SMB) chromatography is a continuous and effective separation process that allows for the purification of valuable products and has therefore received significant attention in many areas of industry. The pharmaceutical industry in particular requires efficient processes such as SMB to separate racemates for the commercialization of chiral drugs as pure enantiomers.

Due to tightened regulations by health and regulatory authorities, it is now necessary to produce higher purity enantiomers than were previously required. In addition, there is pressure on fine chemical industries to develop energy-saving processes for the production of higher purity products due to market demands. Hence, many studies of SMB have focused on the possibility of further improving the separation performance of SMB systems to satisfy these requirements.

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Recently, three new operation strategies for SMB have been suggested. One strategy is the direct manipulation of adsorption equilibria by a supercritical fluid,[1,2] a solvent gradient,[3,4] or a temperature gradient.[5,6] The second strategy is to combine a conventional SMB unit with an additional separation step. Lim et al.,[7] for example, reported that one or two pure enantiomers were obtained from a racemic mixture by combining a conventional SMB process with a crystallization step. In this application, SMB was used to generate partially enriched fractions from which pure products were obtained by crystallization. Also, the SMB process combining two SMB units was introduced to purify *p*-xylene[8] and a combination of a conventional SMB operation with a chromatographic operation in one SMB unit was suggested for the treatment of ternary mixtures.[9-12] Also, one system with both two SMB units and batch unit was designed to separate a multi-component.[13]

The third strategy is the periodic modulation of certain operation parameters during switching periods in the SMB process. An example of this strategy is the VariCol process[14-16] proposed by Novasep. This strategy is based on a nonsynchronous shift in the inlet and outlet ports in a multicolumn system, in contrast to the SMB operation in which the shift is synchronous. Hence, the Varicol process has various SMB configurations during the switching periods. Another example is the PowerFeed process.[17,18] The inlet, outlet, and internal flow-rates change in time during the switching period in the PowerFeed operation, but they are kept constant in the conventional SMB process. The ModiCon process[19,20] uses cyclic modulation of the feed concentration during the switching period to improve the performance of the conventional SMB. Also, the OSS strategy,[21] based on the concept of dynamic collection fronts in the equivalent true moving bed (TMB) model, leads to extract and raffinate the enrichment by increasing their purities in real SMB units.

Recently, our group suggested a partial-discard (PD) strategy[22] that discards a small fraction of the product during the switching periods to obtain high product purity. Because this strategy can be applied to both the raffinate and the extract, product purity can be controlled easily by discarding product fractions. More recently, a fractionation and feed-back approach was proposed.[23] Several fractions of the product are discarded during switching periods from the fractionation of the product peak, but the discarded portion is fed back into the SMB unit in an alternating manner, with the original feed through a separated buffer vessel.

Major impurities from both product ports (extract and raffinate) in an SMB process lean to the initial or last portion of product during a switching period. However, the generation of high purity products from conventional SMB processes generally leads to a decrease in other performance parameters, such as recovery, eluent consumption, and/or productivity. Therefore, a novel SMB operating strategy to produce a high-purity product and to minimize the decrease in other performance parameters is required.

In this study, we suggest a new strategy, the FeedCol operation, to improve the performance of the SMB processes. (FeedCol is an abbreviation of ‘‘feed pretreated by a column’’ or ‘‘feed modified by a column.") In the FeedCol operation, a short chromatographic column with the same selectivity as that of the SMB columns is added to the SMB unit, and the feed is supplied to the column by a pulse input. Therefore, the FeedCol is a hybrid system combined by the SMB separation and chromatographic separation. Because the feed with the partially separated chromatographic peaks is supplied to the SMB process during a switching period, the impurities in the raffinate and extract products can be removed more efficiently than in the conventional SMB process. In this study, the principle and performance results of the FeedCol strategy were evaluated using two new operating variables for pulse input feed: injection length and injection time. The performance of the FeedCol operation was compared with that of the conventional operation (2-2-2-2) under a low-selectivity condition ($\alpha = 1.1$) in terms of four performance parameters: purity, recovery, productivity, and eluent consumption. The new SMB strategy provides a valuable engineering solution to more efficiently separate products with low selectivity, such as enantiomers,[24] using SMB chromatography.

The Principle of the FeedCol Strategy

A schematic of the conventional SMB operation (2-2-2-2) is presented in Figure 1a. Feed is supplied continuously to

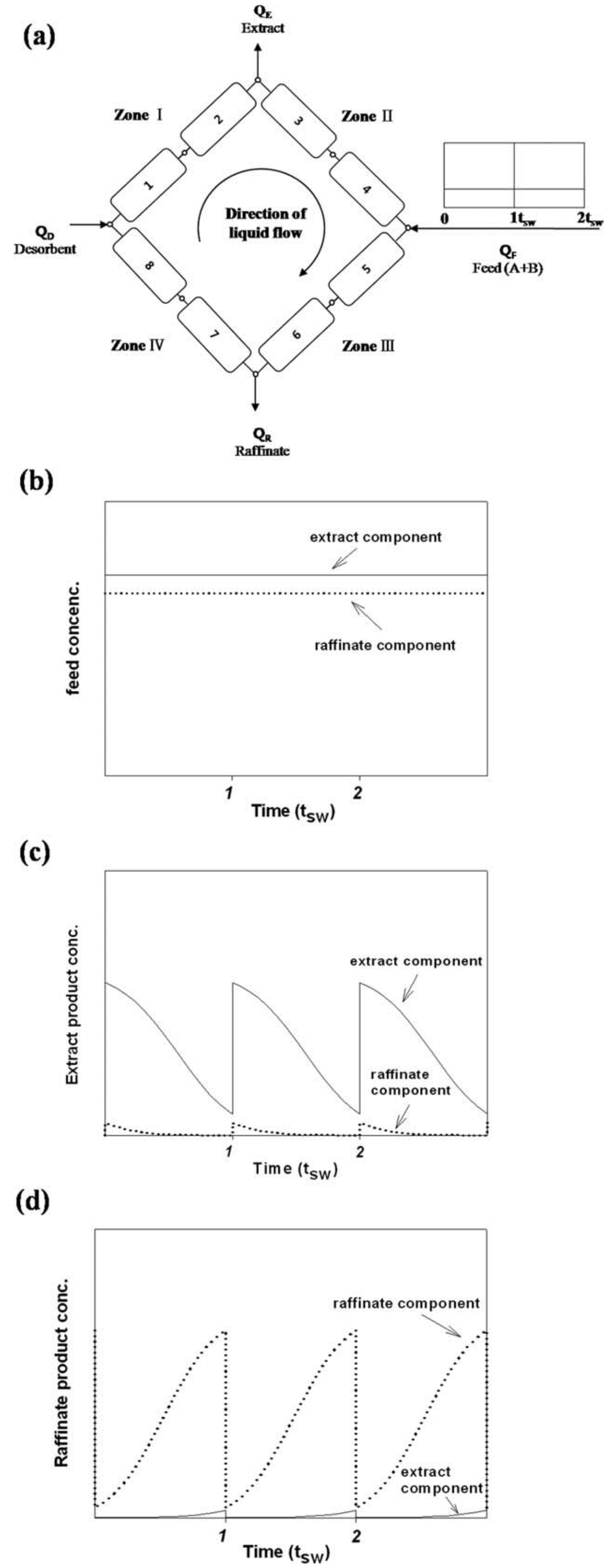

Figure 1. Conventional SMB: (a) schematic of the conventional SMB operation, (b) feed concentration profile, (c) extract product concentration profile, and (d) raffinate product concentration profile.

the SMB system during a switching period, as shown in Figure 1b. Major impurities from both product ports (extract and raffinate) incline to one side during a switching period. A large portion of the impurities (raffinate component) exist in the extract product at the initial part of the switching period, as shown in Figure 1c. On the contrary, a large portion of the impurities (extract component) appear in the raffinate product concentration profile at the last stage of the switching period (Figure 1d).

The PD strategy,[22] which involves discarding the initial or last portion of product during a switching period, has been found to enhance purity, as can be seen in Figures 1c, d. However, this strategy is inevitably accompanied by a loss of recovery because a high concentration of product is discarded along with the impurities. Naturally, it is desirable that the SMB strategy should be able to improve product purity without sacrificing other performance parameters (recovery, productivity, and eluent consumption).

As an alternative, the feed can be modified by reducing the concentration of the extract and raffinate at the initial and last stages of the switching period, respectively. Then, the raffinate-rich feed at the initial stage of the switching period proceeds to the raffinate port while the extract-rich feed at the last stage goes to the extract port. This process improves product purity because the impurity profile at each product port in Figures 1c, d decreases. In this study, a new SMB operating concept using feed modified by a column (the ‘‘FeedCol’’ strategy) was developed. In this strategy, a short chromatographic column with the same selectivity as the SMB columns is added to the SMB unit. And the feed, modified by its passage through the column, is supplied to the SMB unit during a switching period.

Figure 2a is a schematic of the FeedCol strategy with a short chromatographic column (Column 9). To clearly describe the operating strategy used in this study, the term ‘‘rectangular pulse input’’ is used to indicate the input to the chromatographic column (Q_I in Figure 2a). The term ‘‘feed’’ is used to describe the input injected into the SMB system from the outlet of the chromatographic column (Q_F in Figure 2a). After the rectangular pulse input passes through a short chromatographic column, the concentration profile of the feed is changed to the shape of partially separated chromatographic peaks. If this modified concentration profile is injected directly into the SMB system, improved performance can be expected because the extract and raffinate in the initial and last parts of the feed, respectively, are reduced. We refer to the chromatographic column as the ‘‘feed column.’’ The ‘‘FeedCol’’ operation combines a chromatographic column as a feed column with the SMB system to create the ‘‘TMB effect’’. If the feed column is replaced by the glass bead column, the FeedCol operation becomes almost the same as the pulse feed operation except for the feed dispersion and retention time in the precolumn. Since a relatively short feed column is applied to the FeedCol operation in this study, the dispersion in the glass bed column may be very small.

As indicated in Figure 2b, an injection period consists of three parts (initial, middle, and last stages) due to the rectangular pulse input during a switching period. In addition, there is a time shift between the injection period and the switching period because the rectangular pulse input passes through the feed column. Here, the injection period must be equal to the switching period as shown in Figures 2b, c ($T_{inj} = T_{sw}$). To rigorously investigate the FeedCol strategy, we introduced two additional variables for rectangular pulse input: injection length and injection time (Figure 2b). Injection length is defined as the time duration of the pulse input of the feed, which is expressed as a fraction (%) of the injection period. Injection time is defined as the time gap between the beginning of each injection period and the center of each rectangular pulse input. The injection time is also expressed as a fraction (%) of the injection period. Equations for the injection length and injection time are provided below in Eqs. 1 and 2, respectively.

$$L_{inj}(\%) = \mathrm{T}_{inj,mid} \tag{1}$$

$$t_{inj}(\%) = \mathrm{T}_{inj,ini} + \frac{\mathrm{T}_{inj,mid}}{2} \tag{2}$$

In the equations above, L_{inj} is the injection length, and t_{inj} is the injection time. In addition, $T_{inj,i}$ is the ratio of i (i = ini, mid, last) part of one injection period ($T_{inj,ini} + T_{inj,mid} + T_{inj,last} = 100\%$). The subscripts (ini, mid, last) indicate the initial, middle, and last parts of one injection period.

In the FeedCol operation, a time gap between the injection period (Figure 2b) and the switching period (Figure 2c) occurs due to the separation time in the feed column as indicated in Figure 2. Hence, the time gap between both periods must be set first to alter the feed shape to that shown in Figure 2c.

The application of preparative high performance liquid chromatography (PHPLC) to separate crude material with an extremely large amount of by-compounds leads to two major problems: the accumulation of residents in the chromatographic column and column impediment due to an unnecessary load of material. It has been reported that a preadsorption process [preadsorption unit (PAU)] can be used to remove one or several by-compounds or at least reduce their amounts quite drastically.[25] Therefore, PAUs are not considered as precolumns in the PHPLC application. For the same reason, the role of the added column in the SMB process in the FeedCol strategy is different from that of a PAU and precolumn; the purpose of the added column in the SMB process is mainly to modify the feed shape during the SMB switching period, instead of directly discarding by-compounds.

Modeling of the Conventional SMB and FeedCol Operations

As shown in a schematic of the FeedCol operation in Figure 2a, it is possible to apply the FeedCol strategy to any SMB configuration. In this study, a four-zone SMB system with two columns per zone (2-2-2-2) was selected as a representative process to evaluate the performance of the FeedCol strategy because it is one of the most common SMB systems. Because the feed column operation is connected to the SMB operation, the configuration of the FeedCol strategy in Figure 2a can be considered to be a 1+2-2-2-2 operation.

The FeedCol strategy was applied to a binary system with low selectivity (α = 1.1 [-]) to clearly determine the

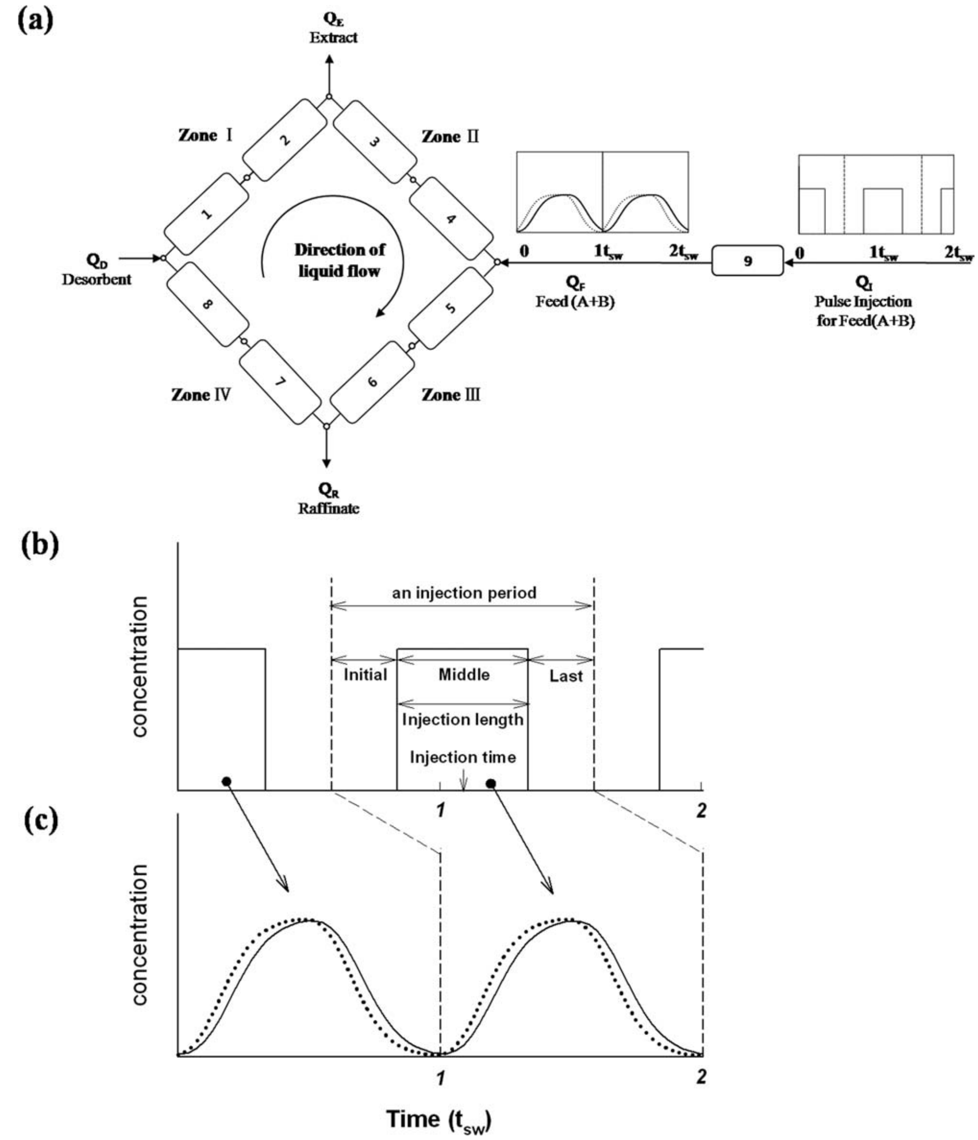

Figure 2. Principle of the FeedCol strategy: (a) schematic of the FeedCol operation, (b) the rectangular pulse inputs of feed injected into a feed column (solid line = both component), and (c) the feed profile modified by a feed column (dotted line = raffinate component, solid line = extract component).

performance difference between the proposed operation and the conventional SMB operation. To study the effect of kinetics on the FeedCol strategy, three systems (System-1, -2, and -3) with mass transfer coefficients of 0.2, 0.5, and 0.8 s^{-1}, respectively, were investigated. In addition, it was assumed that in the FeedCol operation, the eight columns of the SMB system have identical characteristics (column diameter, length, total porosity, and so forth) and that the additional feed column has identical characteristics to the eight SMB columns with the exception of diameter and length. The systems are summarized in Table 1.

Since the productivity in SMB processes increases with increasing feed concentration, it is attractive to choose the highest possible feed concentration for the best separation. However in many cases, this is not applicable to real fields because of the decrease of operational reliability with increasing feed concentration. That is, the system should be able to maintain an operating point in the presence of various disturbances. A higher feed concentration requires typically lower feed flow rate, which might be difficult to control. Therefore, small fluctuations of flow rates, temperature, or feed concentration may cause significant contamination of the products. As a result, a lower feed concentration is typically chosen, which is clearly below the solubility limitation.[19,20] Furthermore, the FeedCol strategy is applicable for nonlinear SMB system separations, where the feed concentration is restricted by technical reasons and not by the solubility of the components in the solvents used.

The FeedCol operation was compared with the conventional SMB based on the same amount of feed treatment, like the Modicon study.[19,20] In this study, the maximum feed concentration was limited to five times higher than the conventional SMB feed because some solute mixtures can lead to practical solubility limitation.

Table 1. System and Operating Parameters for Both Conventional SMB and Feed Column

Conventional SMB			Feed Column		
SMB system parameters			Feed column system parameters		
SMB configuration		2-2-2-2	D (column diameter) (cm)		0.55
D (column diameter) (cm)		2.6	L (column length) (cm)		4.0
L (column length) (cm)		10.5	ε (total porosity)		0.4
ε (total porosity)		0.4	N_{disp} (the number of dispersion units)		500
N_{disp} (the number of dispersion units)		500			
Mass transfer coefficient			Mass transfer coefficient		
k (both components) (s^{-1})	System-1	0.2	k (both components) (s^{-1})	System-1	0.2
	System-2	0.5		System-2	0.5
	System-3	0.8		System-3	0.8
Isotherm coefficient and selectivity			Isotherm coefficient and selectivity		
K_A (raffinate component)		2.000	K_A (raffinate component)		2.000
K_B (extract component)		2.200	K_B (extract component)		2.200
b_A (raffinate component) (L g^{-1})		0.030	b_A (raffinate component) (L g^{-1})		0.030
b_B (extract component) (L g^{-1})		0.040	b_B (extract component) (L g^{-1})		0.040
α (Selectivity)		1.10	α (Selectivity)		1.10
Operating parameters			Operating parameters		
$C_{i,F}$ (feed concentration) $i = A,B$ (g L^{-1})		1.0	$C_{i,I}$ (concentration of injection pulse) $i = A,B$ (g L^{-1})		variable
Q_F (feed flow rate) (mL min^{-1})		2.0	Q_I (flow rate of feed column)		2
Q_E (extract flow rate) (mL min^{-1})		5.46			
Q_R (raffinate flow rate) (mL min^{-1})		5.54			
Q_D (desorbent flow rate) (mL min^{-1})		9			
Q_1 (flow rate of zone1) (mL min^{-1})		58.33			
Q_2 (flow rate of zone2) (mL min^{-1})		52.87			
Q_3 (flow rate of zone3) (mL min^{-1})		54.87			
Q_4 (recycle flow rate) (mL min^{-1})		49.33			
T_{sw} (switching time) (s)		100.32			

Column model for the FeedCol operation

In this study, the internal concentration profile, feed concentration profile (feed shape), and product concentration profile (the transient variation in the extract and raffinate concentrations) in the FeedCol operation were predicted by the transport-dispersive model. In this model, the mass balance equation is combined with the kinetic equation, and it is assumed that the rates of adsorption-desorption are very fast but that the mass transfers are slow. Therefore, the mass transfer kinetics of the solute to the surface of the adsorbent are given by either the liquid film linear driving force (LDF) model or the solid film LDF model.[26]

The mass balance differential equation of each component for each column is expressed as follows:

$$\frac{\partial C_i}{\partial t} + u\frac{\partial C_i}{\partial z} + \frac{1-\varepsilon}{\varepsilon}\frac{\partial q_i}{\partial t} = D_L\frac{\partial^2 C_i}{\partial z^2} \quad D_L = \frac{uL}{2N_{disp}} \tag{3}$$

where C_i and q_i are the liquid phase and solid phase concentrations of component i ($i = A$, B) in all columns, respectively, u is the liquid-phase interstitial velocity, ε is the total porosity, N_{disp} is the number of dispersion units, L is the length of a column, and D_L accounts for the axial dispersion.

The axial dispersion coefficient was assumed to be the same for all components and was constant for all columns. Furthermore, the pressure drop that stemmed from the addition of the feed column was neglected because a short column with the same bed properties as a SMB column was used in the FeedCol operation.

A simple liquid film LDF model was used to represent the overall mass transfer kinetic across the column:

$$\frac{\partial q_i}{\partial t} = k_i(q_i^* - q_i) \tag{4}$$

where k_i is the mass transfer coefficient and q_i* is the equilibrium solid phase concentration of component i. The mass transfer coefficient was assumed to be the same for all components.

A nonlinear adsorption equilibrium isotherm between the liquid and the solid phase was applied to the system. However, it is not necessary to apply nonlinear adsorption isotherms to the solutes in the FeedCol strategy because the benefits of the proposed strategy come mainly from the feed shape with partially separated chromatographic peaks.

The Langmuir-type isotherm parameters in Eq. 5 are summarized in Table 1.

$$q_i^* = f_i(C_1, C_2) = \frac{K_i C_i}{1 + \sum_{i=1}^{2} b_i C_i} \tag{5}$$

The initial and boundary conditions of all columns were used to solve the transport-dispersive model. At the start time of the system, pure solvent was assumed to be supplied through the feed inlet.

(1) The initial conditions for all columns were defined as:

$$\text{At } t = 0: \quad C_{i,j}(x,0) = 0, \; q_{i,j}(x,0) = 0 \tag{6}$$

The subscript i indicates the specific solute, and j is the column number (j = 1, 2,…,8 for the conventional SMB operation, or j = 1, 2,…,9 for the FeedCol operation).

(2) The boundary conditions[27] were defined as:

At the beginning of all columns ($z = 0$):

$$C_{i,j} = C_{i,j}^{in} + \frac{D_L}{u_j}\frac{\partial C_{i,j}}{\partial z} \tag{7}$$

At the end of each column:

for the end of Column 1 ($z = L_1$):

$$C_{i,1}^{\text{out}} \cdot Q_1 = C_{i,2}^{\text{in}} \cdot Q_2 \tag{8}$$

for the end of Column 2 ($z = L_2$):

$$C_{i,2}^{\text{out}} = C_{i,3}^{\text{in}} = C_{i,E} \tag{9}$$

for the end of Column 3 ($z = L_3$):

$$C_{i,3}^{\text{out}} \cdot Q_3 = C_{i,4}^{\text{in}} \cdot Q_4 \tag{10}$$

(For the conventional SMB operation:)

for the end of Column 4 ($z = L_4$):

$$C_{i,4}^{\text{out}} \cdot Q_4 + C_{i,F} \cdot Q_F = C_{i,5}^{\text{in}} \cdot Q_5 \tag{11-1}$$

(For the FeedCol operation:)

for the end of Column 4 ($z = L_4$), and of Column 9 (feed column, $z = L_9$):

$$C_{i,4}^{\text{out}} \cdot Q_4 + C_{i,9}^{\text{out}} \cdot Q_9 = C_{i,5}^{\text{in}} \cdot Q_5 \quad C_{i,9}^{\text{in}} \cdot Q_9 = C_{i,I} \cdot Q_I \tag{11-2}$$

for the end of Column 5 ($z = L_5$):

$$C_{i,5}^{\text{out}} \cdot Q_5 = C_{i,6}^{\text{in}} \cdot Q_6 \tag{12}$$

for the end of Column 6 ($z = L_6$):

$$C_{i,6}^{\text{out}} = C_{i,7}^{\text{in}} = C_{i,R} \tag{13}$$

for the end of Column 7 ($z = L_7$):

$$C_{i,7}^{\text{out}} \cdot Q_7 = C_{i,8}^{\text{in}} \cdot Q_8 \tag{14}$$

for the end of Column 8 ($z = L_8$):

$$C_{i,8}^{\text{out}} \cdot Q_8 + C_{i,D} \cdot Q_D = C_{i,1}^{\text{in}} \cdot Q_1 \tag{15}$$

where $C_{i,j}^{\text{in}}$ and $C_{i,j}^{\text{out}}$ are the inlet and outlet concentrations of component i in column j, respectively, Q_j is the flow rate of column j, $C_{i,\text{F}}$ is the concentration of the feed in SMB, and $C_{i,\text{I}}$ is the concentration of the rectangular pulse input.

Therefore, Eq. 11-2 was used as the boundary condition for the FeedCol operation instead of Eq. 11-1 as in conventional SMB.

Global node model in the FeedCol operation

Global node models[28-30] for the configuration of both operations in both Figures 1a and 2a are required. The models were expressed as the relationship equation of the volumetric flow-rate of each column, desorbent, feed, and product.

for the eluent node:

$$Q_8 + Q_D = Q_1 \tag{16}$$

for the mid-node between the desorbent and extract draw-off nodes:

$$Q_1 = Q_2 \tag{17}$$

for the extract draw-off node:

$$Q_2 - Q_{\text{E}} = Q_3 \tag{18}$$

for the mid-node between the extract draw-off and feed nodes:

$$Q_3 = Q_4 \tag{19}$$

(For the conventional SMB operation:)

for the feed node:

$$Q_4 + Q_F = Q_5 \tag{20-1}$$

(For the FeedCol operation:)

for the feed node and rectangular pulse injection node:

$$Q_4 + Q_9 = Q_5 \quad Q_9 = Q_I \tag{20-2}$$

for the mid-node between the feed and raffinate draw-off nodes:

$$Q_5 = Q_6 \tag{21}$$

for the raffinate draw-off node:

$$Q_6 - Q_R = Q_7 \tag{22}$$

for the mid-node between the raffinate draw-off and desorbent nodes:

$$Q_7 = Q_8 \tag{23}$$

Equation 20-2 was used for the feed node in the FeedCol operation instead of Eq. 20-1 that is used for conventional SMB.

The global node model combines the mass balance equations for the columns to produce a simulated countercurrent in the series of columns. All of the nodes were shifted to the next position along the fluid flow direction after a switching period. Because of the cyclic nature of the port switching for each node, the boundary conditions for each column were changed accordingly at the beginning of each switching period.

With the simulation package gPROMS Model-builder[21,31,32] used by many SMB researchers, the periodic discontinuities caused by discrete fluid port switching in the model were solved.

Chromatographic performance parameters

Four performance parameters (purity, recovery, productivity, and eluent consumption)[28,30] were used to investigate the performance of the FeedCol strategy.[33] These parameters were defined as follows:

purity (%):

$$(\text{Raffinate}): \frac{C_{A,\text{R}}}{C_{A,\text{R}} + C_{B,\text{R}}} \times 100; \quad (\text{Extract}): \frac{C_{B,\text{E}}}{C_{A,\text{E}} + C_{B,\text{E}}} \times 100 \tag{24}$$

recovery (%):

$$(\text{Raffinate}): \frac{C_{A,\text{R}} Q_{\text{R}}}{C_{A,\text{F}} Q_{\text{F}}} \times 100; \quad (\text{Extract}): \frac{C_{B,\text{E}} Q_{\text{E}}}{C_{B,\text{F}} Q_{\text{F}}} \times 100 \tag{25}$$

productivity [g/(a day)/(L of adsorbent)]:

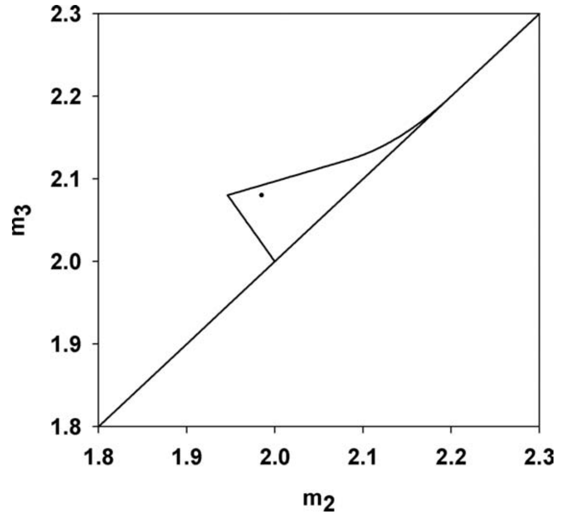

Figure 3. Triangle plot and operating condition with the racemic concentration of 1 g L^{-1}.

(For the conventional SMB operation:)

$$(\text{Raffinate}):\frac{C_{A,\text{R}}Q_\text{R}}{N_\text{column}(1-\varepsilon)V_\text{column}};\quad (\text{Extract}):\frac{C_{B,\text{E}}Q_\text{E}}{N_\text{column}(1-\varepsilon)V_\text{column}} \tag{26-1}$$

(For the FeedCol operation:)

$$(\text{Raffinate}):\frac{C_{A,\text{R}}Q_\text{R}}{N_\text{column}(1-\varepsilon)V_\text{column}+(1-\varepsilon)V_\text{feedcolumn}}$$
$$(\text{Extract}):\frac{C_{B,\text{E}}Q_\text{E}}{N_\text{column}(1-\varepsilon)V_\text{column}+(1-\varepsilon)V_\text{feedcolumn}} \tag{26-2}$$

eluent consumption (L/g):

$$(\text{Raffinate}):\ \frac{Q_\text{D}+Q_\text{F}}{Q_\text{R}C_{A,\text{R}}};\ (\text{Extract}):\ \frac{Q_\text{D}+Q_\text{F}}{Q_\text{E}C_{B,\text{E}}} \tag{27}$$

In the above equations, A (raffinate) is the component less retained, and B (extract) is the component more retained. In addition, $C_{i,j}$ (g cm^{-3}) is the average fluid phase concentration of component i (i =A, B) in the inlet or outlet ports j (j = F, E, R) during a switching period, and Q_j is the flow rate in the inlet or outlet ports j. The subscripts F, E, and R indicate the feed, extract, and raffinate, respectively, N_column is the number of columns in the SMB system, ε is the overall porosity of the adsorbent, and V_column and $V_\text{feedcolumn}$ represent the volume of an SMB column and the volume of a feed column, respectively. The performance parameters were calculated for each switching period from startup to steady state. In this study, the steady-state condition was defined as the state in which there was less than a 0.001% change between the performance profiles in two consecutive tacts.

System Design and Operating Conditions for the FeedCol Operation

In this study, the operating conditions for the SMB process were determined by the triangle theory.[34] The triangle theory is based on the equilibrium theory model where mass transfer resistances are neglected. In this study, we are explicitly considering mass transfer resistances; therefore, our calculated purities and other performance parameters will be inferior to those predicted by the triangle theory. Furthermore, the lower the mass transfer coefficient, the poorer the performance parameters will be compared with those predicted by the triangle theory. To compare the performance of FeedCol to that of SMB, the operating conditions were selected, for which a product with a purity of greater than 93% was obtained from both the extract and raffinate products using the conventional SMB with System-2. The triangle plot with the operating point is shown in Figure 3.

Table 2. Performance Parameters in SMB Systems 1–3 for Conventional SMB

		Case T1	Case T2	Case T3
Conventional SMB		1*	2*	3*
Purity (%)	A(Ra.)	79.48	93.32	97.59
	B(Ex.)	80.04	93.27	96.87
Recovery (%)	A(Ra.)	80.23	93.28	96.96
	B(Ex.)	79.29	93.31	97.58
Productivity [g (day*L)$^{-1}$]	A(Ra.)	8.63	10.04	10.44
	B(Ex.)	8.53	10.04	10.50
Eluent consumption (L g^{-1})	A(Ra.)	6.86	5.90	5.67
	B(Ex.)	6.94	5.89	5.64

*1, 2, and 3 are the systems.

All operating conditions and system parameters used in conventional SMB are presented in Table 1. The performance results from the conventional SMB systems (System-1, -2, and -3) with low selectivity are illustrated in Table 2. Figure 4 shows a wider concentration profile for each component with a decrease in the mass transfer coefficient. Therefore, the performance parameters deteriorated at a lower mass transfer coefficient because the impurity component can be contaminated easily in each product node. These

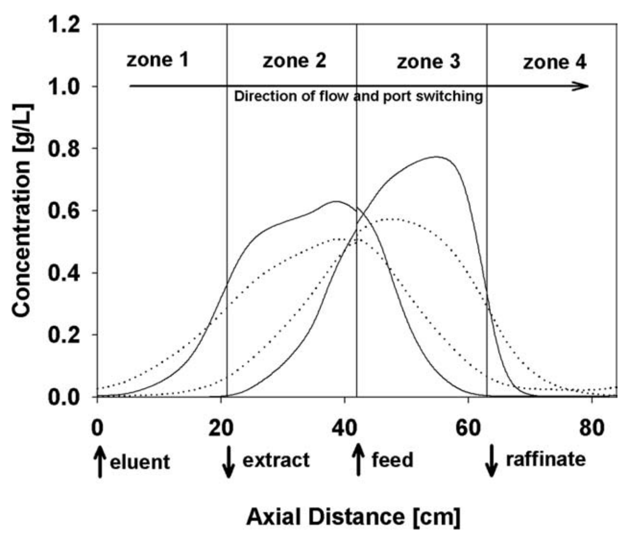

Figure 4. Internal concentration profiles of conventional SMB at the cyclic steady-state (dotted line: mass transfer coefficient = 0.2 s^{-1}, solid line: mass transfer coefficient = 0.8 s^{-1}).

results were used as a standard for comparison with the results obtained using the FeedCol operation.

To apply the FeedCol strategy to SMB, the operating conditions and system parameters of the feed column have to be determined. In the feed column, the rear part of an elution profile (extract-rich) can mix with the front part of the next elution profile (raffinate-rich) if the length of the elution peak is longer than the switching period. Hence, in the FeedCol operation, it is necessary to make the most of elution peak within the switching period by choosing a shorter feed column than in the SMB process.

To compare the FeedCol performance with the conventional SMB performance for the same amount of feed per time (switching time), the following relations were used for the rectangular pulse input for the FeedCol operation:

$$\begin{aligned} C_{i,\mathrm{I,ini}} &= 0 \\ C_{i,\mathrm{I,mid}} &= \frac{C_{i,\mathrm{F}} T_{\mathrm{sw}}}{L_{\mathrm{inj}} T_{\mathrm{inj}}} = \frac{C_{i,\mathrm{F}}}{L_{\mathrm{inj}}} \\ C_{i,\mathrm{I,last}} &= 0 \end{aligned} \tag{28}$$

In the equations above, the subscripts ini, mid, and last refer to the initial, middle, and last stages in an injection period, respectively (Figure 2). In addition, T_{sw} is the switching period in the conventional SMB operation, L_{inj} is the injection length of a rectangular pulse feed input, and T_{inj} is the injection period in the FeedCol operation.

Results and Discussion

Standard FeedCol operation at fixed operating conditions

In the FeedCol operation, a time gap between the injection period and the switching period occurs due to the separation time in the feed column. Therefore, it is necessary to fix the time gap to allow performance comparison with standard operation conditions (injection length and time). The time gap can be affected by various variables. However, because the feed flow rate, feed column, and adsorption isotherms were fixed in this study, the variation of the standard time gap in the FeedCol strategy was studied in three systems with mass transfer coefficients of 0.2, 0.5, and 0.8 s^{-1}, respectively.

To determine the standard FeedCol operation for each system, an injection time of 50% was first selected as the standard injection time. Then, the injection length of each system was determined as the length at which the time from the beginning to the end of the elution profile through the feed column was almost equal to a switching period. Therefore, the injection length must be less than 100% of T_{sw} in order for the entire elution profile to fit within one switching period. However, it is very hard to determine the exact condition of such injection length because elution peaks have a long tail. In this study, the injection length of the standard FeedCol operation was selected as the length at which over 99% of the elution profile was included within one switching period.

Figures 5a–c illustrate the rectangular pulse input and its elution profile for the standard FeedCol operation of each system in Table 3. The injection lengths satisfying the aforementioned condition were 20% for System-1, 50% for System-2, and 65% System-3. The figures show that the elution profile from the feed column was positioned within one switching period at a fixed injection time. The fixed time gap between the injection period and the switching period at

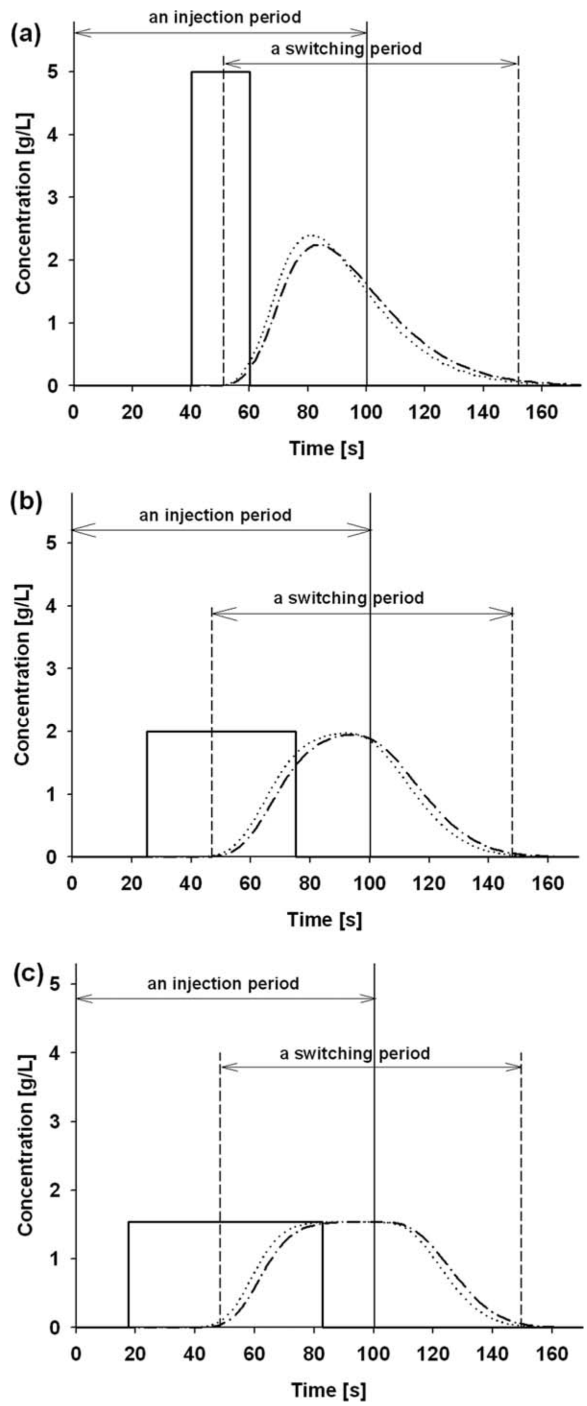

Figure 5. Elution profiles of each rectangular pulse input at standard FeedCol cases: (a) System-1, (b) System-2, and (c) System-3 (solid line: rectangular pulse input of feed, dotted line: elution profile of raffinate component, dash-dotted line: elution profile of extract component).

Table 3. Operating Conditions of Three Standard Cases in FeedCol Operation (System-1, -2, and -3)

		Case S1	Case S2	Case S3
FeedCol operation		1*	2*	3*
Mass transfer coeff.		0.2	0.5	0.8
Initial stage	T_{ini} (%)	30	25	17.5
Middle stage	T_{mid} (%)	40	50	65
Last stage	T_{last} (%)	30	25	17.5
$C_{i,I}$ (g L^{-1}) (During initial stage)		0	0	0
$C_{i,I}$ (g L^{-1}) (During middle stage)		2.5	2.0	1.54
$C_{i,I}$ (g L^{-1}) (During last stage)		0	0	0
Injection length (%)		40	50	65
Injection time (%)		50	50	50

*1, 2, and 3 are the systems.

each standard operation was 51.13 s for System-1, 47.08 s for System-2, and 48.56 s for System-3. In addition, because the same amount of feed used in the conventional SMB was applied to all the systems, the feed concentration for standard operation of each system differed among the different systems. Therefore, with an increase in the mass transfer coefficient, an increase in injection length and a decrease in feed concentration were observed. The time gap decreased in the range of mass transfer coefficient from 0.2 to 0.5 s^{-1} while it increased in the range of 0.5 to 0.8 s^{-1}. It was because the elution profile from the feed column was skewed to the front-side at a short injection length under the condition of low mass transfer coefficient as shown in Figure 5a. As a result, the adsorption isotherm and mass transfer coefficient can have a significant effect on the determination of standard conditions as shown by the skewed peak in Figure 5a.

Operating results of the FeedCol operation and the conventional SMB operation under the three sets of standard conditions (Table 3) are compared in Figure 6. As presented in Figure 6a, the purities of both products (extract and raffinate) were improved by the FeedCol strategy for all Systems. The improved level of extract was larger than that of raffinate. This is because the feed concentration profile in the SMB system became skewed, and the standard condition with lower mass transfer coefficient was shown more clearly (Figure 5a). Because of the front-tilted asymmetric feed, more feed was injected into the SMB system in the early stage of a switching period.

Figure 7 shows the variation of the internal concentration profiles of System-1 (mass transfer coefficient = 0.2 s^{-1}; Case T1 and S1) and System-3 (mass transfer coefficient =

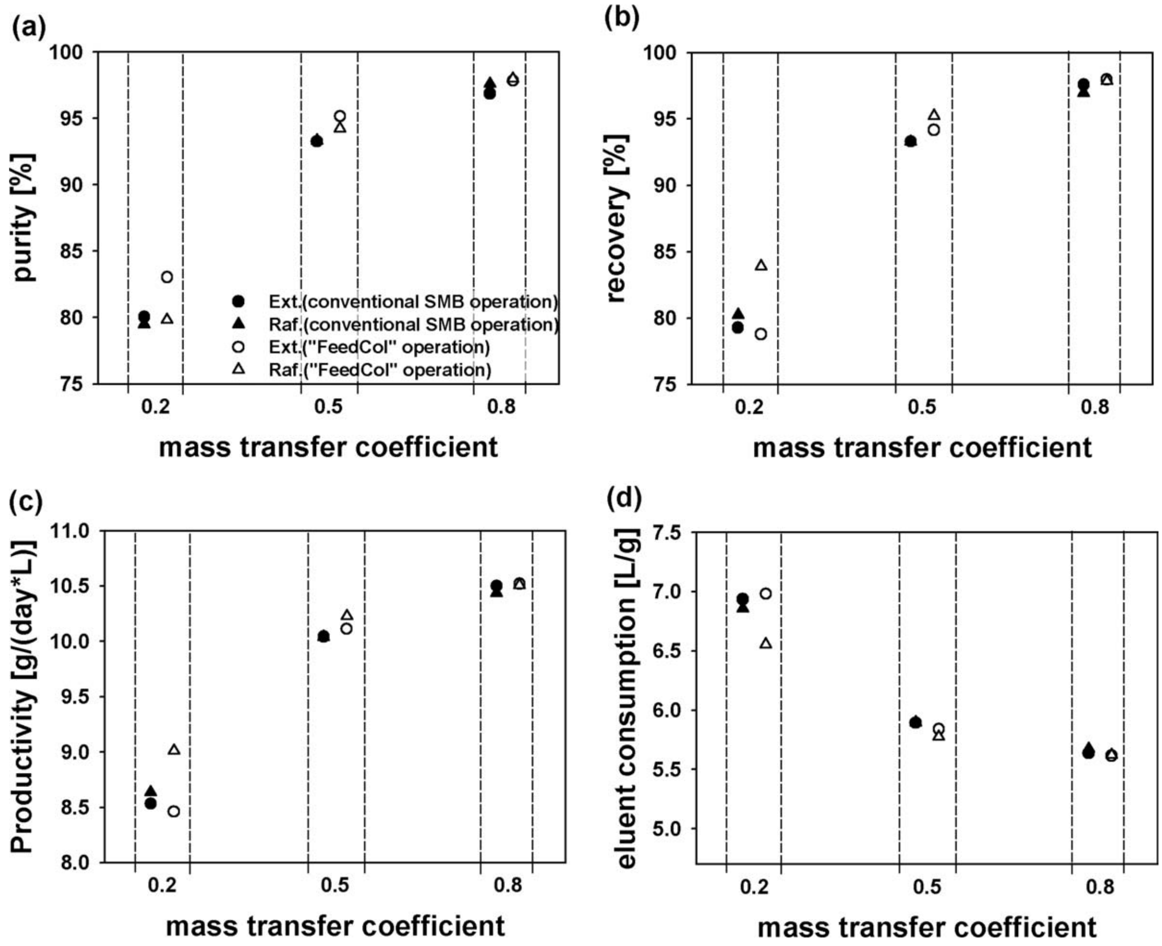

Figure 6. Comparison of conventional operation and FeedCol standard operation at three systems: (a) purity, (b) recovery, (c)productivity, and (d) eluent consumption.

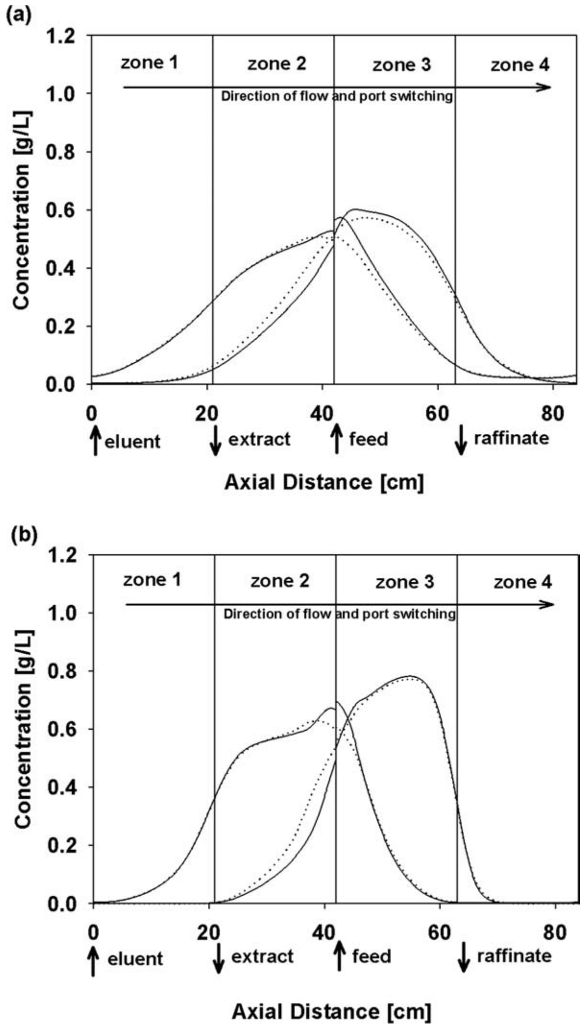

Figure 7. Internal concentration profiles at the cyclic steady-state: (a) mass transfer coefficient = 0.2 s^{-1} (dotted line: conventional SMB, solid line: FeedCol operation) and (b) mass transfer coefficient = 0.8 s^{-1} (dotted line: conventional SMB, solid line: FeedCol operation).

0.8 s^{-1}; Case T2 and S2) in the FeedCol operation. In both systems, the concentration of major component at each product node increased while the impurity decreased successfully. However, the concentration difference between the conventional SMB and FeedCol operation was observed at the extract and raffinate nodes in System-1, whereas it was hardly shown at the raffinate node in System-3. Because of the skewed peak of feed in System-1 (Figure 5), the head of each component in System-1 moved more to the direction of the raffinate node than in System-3. Therefore, the extract component can easily reach the raffinate node while most of the raffinate component can go far from the extract node. Simultaneously, more raffinate product can be obtained in System-1. As a result, the front-tilted asymmetric feed is advantageous to the extract purity and raffinate recovery but disadvantageous to the raffinate purity and extract recovery.

As shown in Figures 6b–d, the FeedCol strategy also improved the recovery, productivity, and eluent consumption of both products in System-2 and System–3, when compared with the conventional SMB operation. In System-1, in contrast to the other two systems, the extract recovery, productivity, and eluent consumption deteriorated slightly while the raffinate results showed relatively high enhancement.

This result had the same basis as the purity result discussed above: a greater amount of feed was injected at the initial stage of a switching period due to the asymmetric feed. In the FeedCol operation, because one additional feed column was added to the conventional SMB, more adsorbent was used. However, our results indicate that improved purity and recovery can lead to improved productivity and eluent consumption under appropriate operating conditions of the FeedCol operation.

Effects of operating parameters on the FeedCol strategy

As mentioned previously, the FeedCol strategy has two additional operating variables: injection length and injection time. By adjusting these two parameters, the feed concentration profiles (feed shapes) that pass through the feed column are changed during a switching period, and the results of the performance parameters (purity, recovery, productivity, and eluent consumption), therefore, differ. In this section, System-2 was selected as a representative system, and the effects of these two operating variables on the FeedCol operation for this system were studied in detail.

Effects of Injection Length. As summarized in Table 4, we designed various cases (H1–H7) in System-2 to investigate the effect of injection lengths, ranging from 20 to 80% at a fixed injection time of 50%.

Figure 8 shows the comparison of the feed concentration profiles (feed shapes) for each case; these were obtained by passing different rectangular pulse inputs through the feed column. The feed concentration profile became gradually

Table 4. Operating Condition of Each Injection Length in FeedCol Operation (System-2)

Case		H1	H2	H3	H4*	H5	H6	H7
Initial stage	T_{ini} (%)	40	35	30	25	20	15	10
Middle stage	T_{mid} (%)	20	30	40	50	60	70	80
Last stage	T_{last} (%)	40	35	30	25	20	15	10
$C_{i,I}$ (g L^{-1}) (During initial stage)		5.00	3.34	2.50	0	1.67	1.43	1.25
$C_{i,I}$ (g L^{-1}) (During middle stage)					2.00			
$C_{i,I}$ (g L^{-1}) (During last stage)					0			
Injection length (%)		20	30	40	50	60	70	80
Injection time (%)					50			
Feed shape (during switching time)		Figure 8a	Figure 8b	Figure 8c	Figure 8d	Figure 8e	Figure 8f	Figure 8g

*Standard case of System-2.

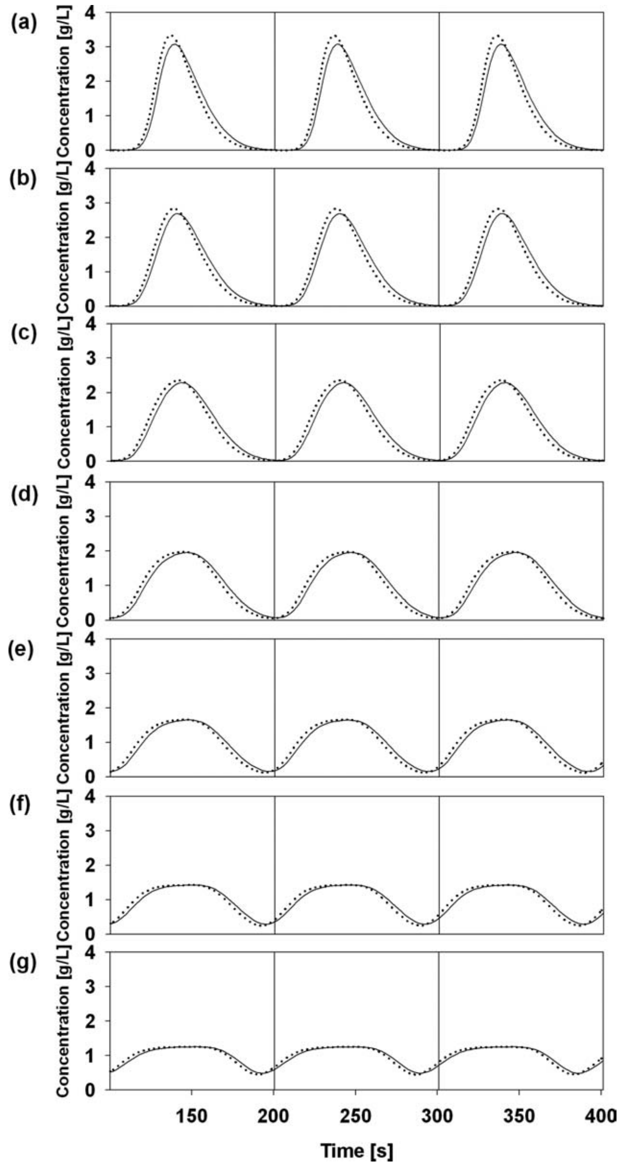

Figure 8. Effect of injection length on feed shape (feed concentration profile) at injection time of 50% in System-2: (a) injection length = 20%, (b) injection length = 30%, (c) injection length = 40%, (d) injection length = 50%, (e) injection length = 60%, (f) injection length = 70% and (g) injection length = 80% (dotted line: raffinate component, solid line: extract component).

skewed with a decrease in the injection length because higher concentrated pulse input was injected to the feed column at a shorter injection length. As shown in Figures 8a–g, raffinate-rich profiles appeared at the initial stage of a switching period while extract-rich profiles formed at the last stage of a switching period. Because the principle of the FeedCol strategy can be applied to all the cases, as described before, the modified feed can contribute to the improvement of SMB performance.

Figure 9 shows the variation in the performance parameters of the FeedCol operation brought about by changing the injection length. Figure 9a shows that the purities of both raffinate and extracts in all cases were higher than those in the conventional SMB operation and the improvement in purity of the extract became greater than that of the raffinate. The extract purity increased steadily with a decrease in the injection length, while the small variation of the raffinate purity followed the parabolic shape with the maximum value at the injection length of 50–60%. As shown in Figure 8, a greater amount of feed was injected to the SMB at the initial stage of the switching period under the condition of short injection length (as an example, Figure 8a). As a result, the concentrated raffinate was produced at the raffinate node with relatively high concentrated extract. On the other hand, because the extract was obtained from the tailing rear-profile of asymmetric peak, the extract purity could always be higher than the raffinate purity, and the extract product concentration became lower than the raffinate product concentration.

For the FeedCol strategy, the variation in recovery, productivity, and eluent consumption with injection length shows a trend in Figures 9b–d. As can be expected from Figures 8 and 9a, the improvement level of these three performance parameters for the raffinate from the conventional SMB was higher than that for the extract. These three performance parameters of raffinate improved as the injection length decreased while the variation of these parameters of extract was almost constant showing a minute parabolic shape. From the results, it can be expected that all the performance parameters of FeedCol operation in a linear system can be improved more clearly with a decrease in the injection length. If the injection length of 100% is applied to the FeedCol operation, it will be the same as the conventional SMB operation. But it will naturally lead to a decrease in the productivity of FeedCol operation due to the extra adsorbent.

Figure 10 shows a comparison of two product concentration profiles at the cyclic steady states of Case H1 (FeedCol operation at 50% injection time and 20% injection length in Table 4) and Case T2 (conventional SMB operation in Table 2). The dotted line and solid line in Figure 10 indicate the concentration profiles in the product ports of Case T2 and Case H1, respectively. At the extract node in the FeedCol operation (Figure 10a), the raffinate (impurity) concentration was reduced successfully from the result of conventional SMB while the extract (product) concentration was almost the same in both operations. In contrast, at the raffinate node, the raffinate (product) concentration was higher in the FeedCol than in the conventional SMB while the difference in the extract (impurity) concentration in both operations was trivial (Figure 10b). These figures clearly illustrate why both recovery and purity were better at both the raffinate and extract product ports in the FeedCol operation than in the conventional SMB operation.

When using the FeedCol strategy, the appropriate choice of injection length is very important. If the injection length is longer than 50%, the end part of the feed concentration profile overlaps with the beginning part of the next one, as shown in Figures 8f, g. Hence, a part of the extract-rich mixture was injected at the initial stage of a switching period. As a result, the impurity (extract) increased considerably at the raffinate product port. For the same reason, a part of the

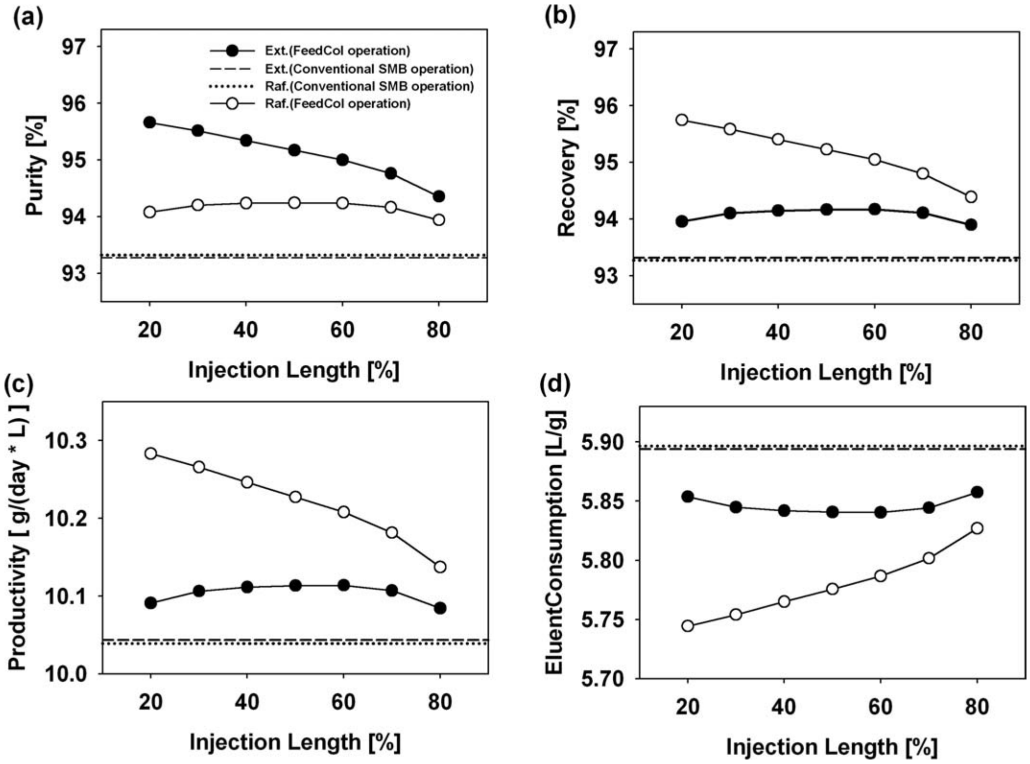

Figure 9. Effect of injection length on performance parameters at injection time of 50% in System-2: (a) purity, (b) recovery, (c) productivity, and (d) eluent consumption.

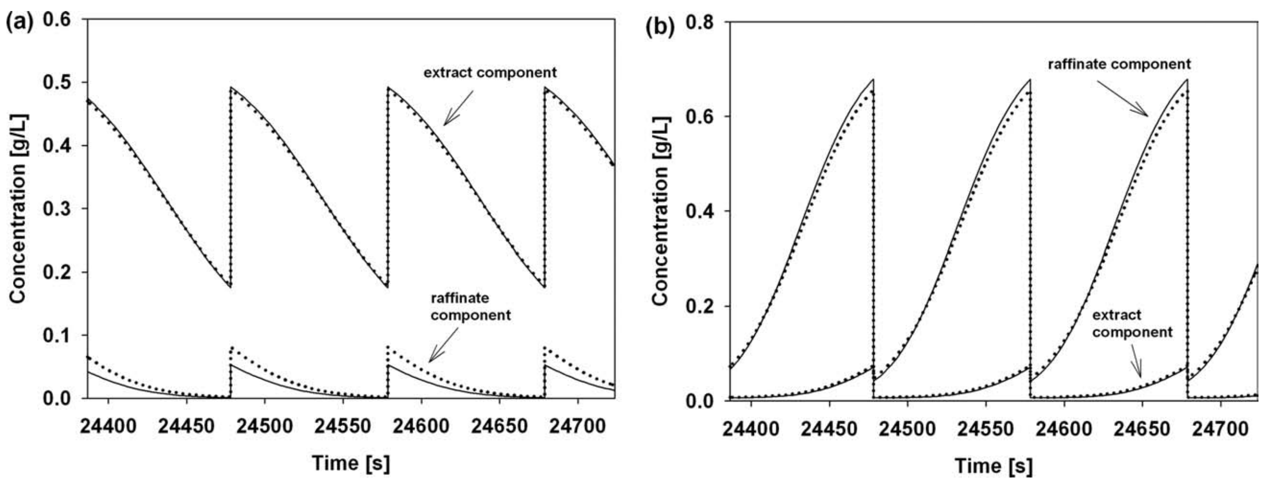

Figure 10. Product concentration profiles at the cyclic steady-state of System-2 for both case T2(conventional SMB operation) and case H1("FeedCol" operation): (a) product concentration profile at extract port and (b) product concentration profile at raffinate port (solid line: Injection length = 20%, dotted line: conventional SMB).

Table 5. Operating Condition of Each Injection Time in FeedCol Operation (System-2)

Case		H8	H9	H10	H11	H12	H13	H14	H15
Initial stage	T_{ini} (%)	10	15	20	30	40	50	60	70
Middle stage	T_{mid} (%)	20	20	20	20	20	20	20	20
Last stage	T_{last} (%)	70	65	60	50	40	30	20	10
$C_{i,\mathrm{I}}$ (g L^{-1}) (during initial stage)		0							
$C_{i,\mathrm{I}}$ (g L^{-1}) (during middle stage)		5.00							
$C_{i,\mathrm{I}}$ (g L^{-1}) (during last stage)		0							
Injection length (%)		20							
Injection time (%)		20	25	30	40	50	60	70	80
Feed shape (during switching time)		Figure 11a	Figure 11b	Figure 11c	Figure 11d	Figure 11e	Figure 11f	Figure 11g	Figure 11h

raffinate-rich mixture was introduced at the last stage of a switching period, and the amount of impurities (raffinate) at the extract product port increased. In addition, a longer injection length had a negative influence on the performance of the FeedCol operation, as shown in Figure 9. Thus, if an injection length of 100% is applied to the FeedCol operation, the advantages of introducing a feed column will disappear, and the operation will return to conventional SMB.

Effects of Injection Time. It is highly possible that feed concentration profiles modified by the feed column exist within a switching period if a shorter feed length is applied, regardless of the injection time. Therefore, to investigate the influence of injection time on the FeedCol operation, we designed various cases (H8–H15) in System-2, as listed in Table 5, where the injection time varied from 20 to 80% of injection time under the condition of short injection length (20%).

The comparisons of the feed concentration profiles (feed shapes) for each case obtained by passing different rectangular pulse inputs through the feed column are shown in Figure 11. In cases with injection times of shorter than 50% (Cases H8–H11, Figures 11a–d), the positions of the feed shape shifted toward the initial stage in a switching period, while the positions of the feed shape moved toward the last stage in a switching period in cases with injection times of longer than 50% (Cases H13–H15, Figures 11f–h).

Figure 12 shows the effect of the position of the feed shape according to the injection time on the performance in the FeedCol operation (circle symbols). In Figure 12a, the raffinate purity of the FeedCol operation was higher than that found in the conventional SMB (Case T2) when the injection time was longer than around 45%. In contrast, the extract purity in the FeedCol operation was higher than that found for in the conventional SMB (Case T2) when the injection time was shorter than around 75%. These results imply that the purity of one of the two products (raffinate or extract) can be worsened by the FeedCol operation if an excessively short or long injection time is used. In addition, the improvement level of extract purity reached a maximum at an injection time of about 30% and decreased at lower injection times (Case H8–H10). This implies that, if an excessively large amount of raffinate exists at the last stage of a switching period (as in Figure 11a), it can mix with the extract as an impurity at the extract product port.

In Figure 12b, the recovery showed results opposite to those found at purity. As the injection time decreased, the recovery of extract decreased, while the recovery of raffinate increased. In addition, as shown in Figures 12c, d, the other two performance parameters (productivity and eluent consumption) showed trends similar to those of the recovery.

Depending on the injection time, the performance parameters of FeedCol operation may be worse than those of conventional SMB operation. Furthermore, the sensitivity of the performance parameters to injection time is greater than for injection length because a part of each feed concentration profile carries over to the next or previous switching period when the injection time is changed. However, if only one product is valuable, a short or long injection time would be more favorable than a 50% injection time (Case H11) with respect to purity. Simultaneously, as shown in Figure 12, the other performance parameters (recovery, productivity, and eluent consumption) can be worse than those of conventional SMB, except for purity.

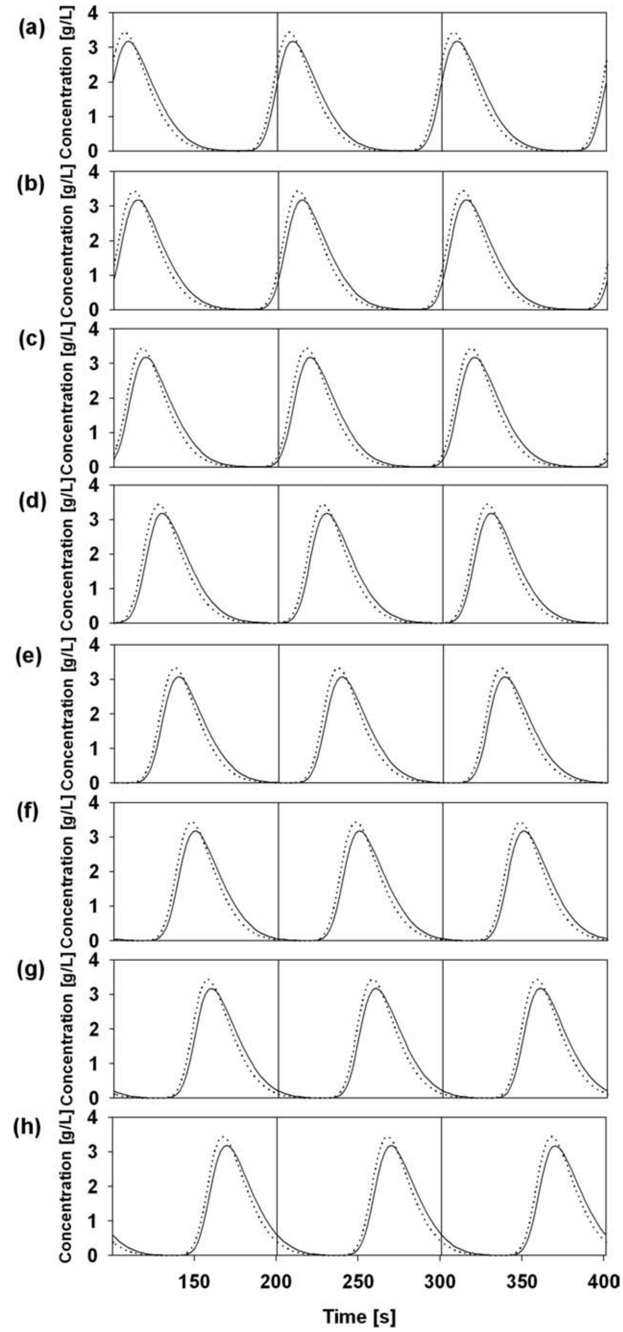

Figure 11. Effect of injection length on feed shape (feed concentration profile) at injection length of 20% in System-2: (a) injection time = 20%, (b) injection time = 25% (c) injection time = 30%, (d) injection time = 40%, (e) injection time = 50%, (f) injection time = 60%, (g) injection time = 70% and (h) injection time = 80% (dotted line: raffinate component, solid line: extract component).

Figure 12 also presents the comparison between FeedCol and pulse feed operations (pulse feed operation: the feed in the form of pulse is introduced directly to the SMB unit at a

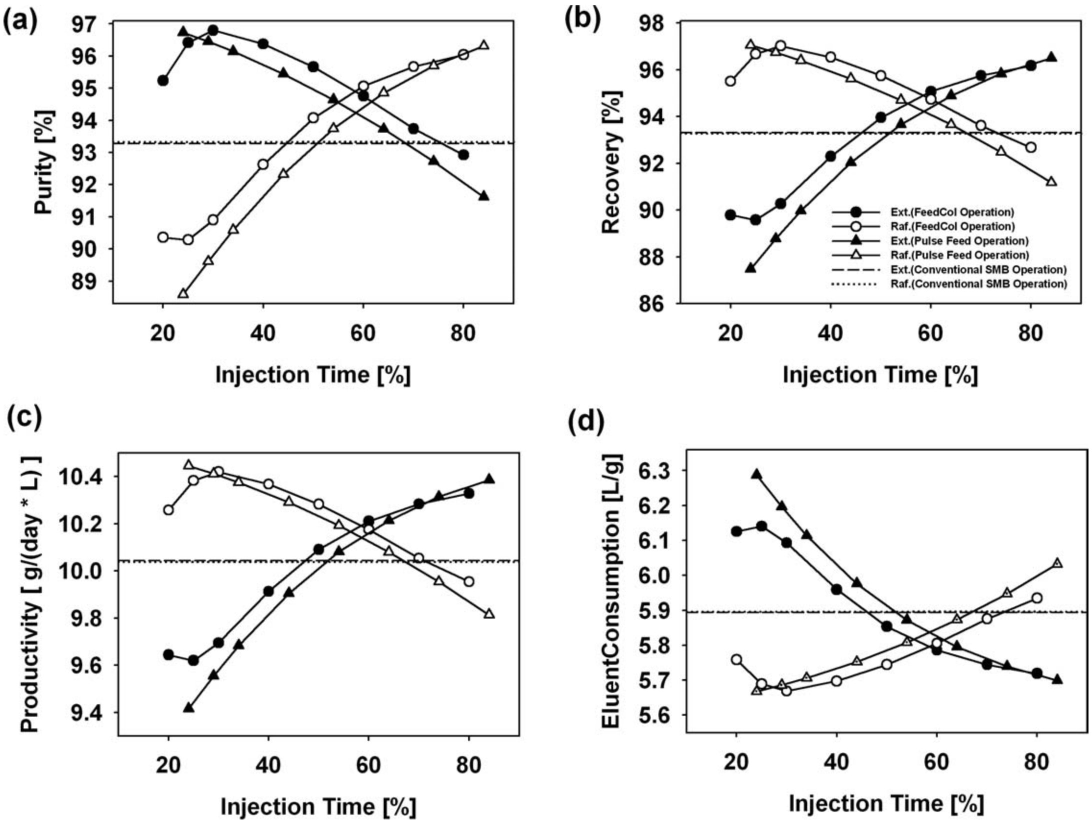

Figure 12. (Comparison of FeedCol with ModiCon): Effect of injection time on performance parameters at the injection length of 20% in both FeedCol and Pulse Feed operations of System-2: (a) purity, (b) recovery, (c) productivity and (d) eluent consumption (Here, all the performance results of Pulse Feed operation were shifted to the right by + 4% injection time.).

different time position within a switching period). The corresponding feeds of Cases H8–H15 in Table 5 were used as pulse feeds.

The pulse feed in the FeedCol is related to the injection period, whereas the pulse feed in the pulse feed operation is related to the switching period. Therefore, these two operating strategies cannot be compared with each other at the same injection time directly (shown in Figure 11e) due to the skewed elution profile through the feed column. Therefore, with respect to the injection time, the performance applied by a shorter injection time in the Pulse Feed operation should be compared with the result in the FeedCol. In Figure 12, if the 4% injection time is shifted in the pulse feed operation, the location of the pulse feed can be almost similar to that in the FeedCol.

As shown in Figure 12, the feed column contributed to the separation performance due to preseparation of feed. Because the low selectivity ($\alpha = 1.1$) condition was selected in the study, the simultaneous improvement of both products by the pulse feed operation was limited (1 to 1.5%) from the conventional SMB results. However, the FeedCol operation could achieve additional improvement of both products from the pulse feed operation (1 to 2% considering 4% injection time shift). Compared with the conventional SMB operation, the other performance parameters in the FeedCol operation were higher than that in the pulse feed operation. Therefore, it can be expected that the performance by the FeedCol operation can improve more with higher selectivity condition because of the separation in the feed column.

Figure 13 shows the internal concentration profiles in the SMB zones of the FeedCol operations for various injection times. At the cyclic steady state in the middle of a switching period, the front part of the extract profile and the rear part of the raffinate profile in Case H10 (injection time = 30%) shifted considerably toward the raffinate port, when compared with Case H12 (injection time = 50%). This is because a greater amount of feed was introduced at the initial stage of the switching period (Figure 11c). Therefore, for short injection times in the FeedCol operation, the extract purity was improved, but the raffinate purity became worse, as shown in Figure 12a.

Figure 13b shows a comparison of the internal column profiles of Case H12 (injection time = 50%) and Case H14 (injection time = 70%). In contrast to Figure 13a, the front of the extract concentration profile and the rear of the raffinate concentration profile shifted considerably toward the extract outlet when the operating conditions changed from Case H12 to Case H14. Hence, when a long injection time was applied to the FeedCol operation, the raffinate purity increased, while the extract purity decreased.

In this study, another case study was performed to confirm the validity of the FeedCol strategy at a high purity condition. A more favorable system with selectivity of 1.25 was selected and the operating conditions of conventional SMB

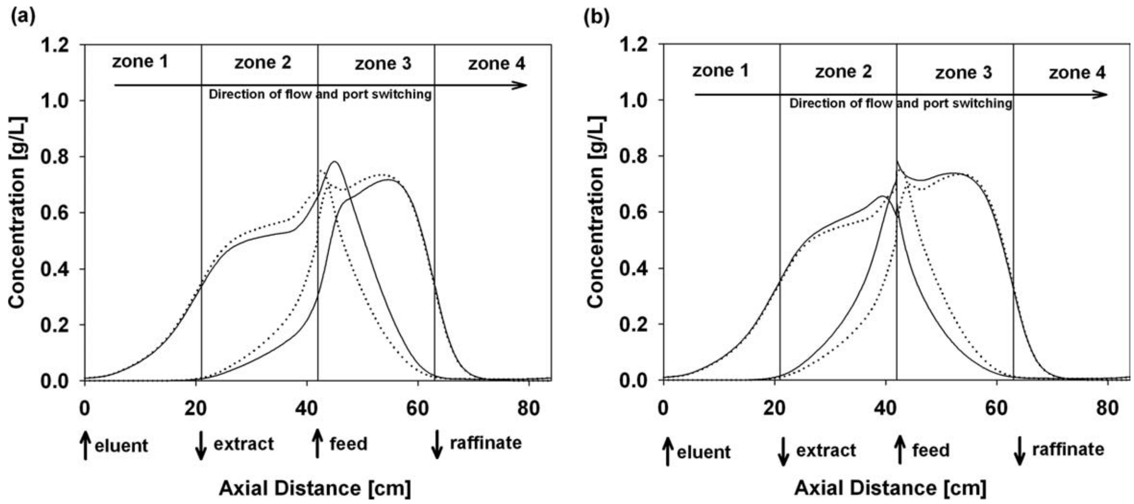

Figure 13. Internal SMB column profiles at the cyclic steady-state of System-2 in "FeedCol" strategy: (a) case H10 and case H12 (solid line: injection time = 30%, dotted line: injection time = 50%) and (b) case H14 and case H12 (solid line: injection time = 70%, dotted line: injection time = 50%).

were determined by a triangle theory (Table 6). In the conventional SMB operation, purities of both extract and raffinate were 98.83% and 98.85%, respectively. In this case study, a longer feed column than that in the previous case was selected. As mentioned before, the standard operation of the FeedCol strategy for the new system was first determined to the injection length and injection time of 50%. And the time gap between the injection period and the switching period was fixed to 100 s.

As shown in Figure 14a, the separation of raffinate and extract was more clearly presented through the feed column due to the higher selectivity of the system and the longer feed column. And the injected feed shifted to the right during a switching period with increasing injection time. The variation of purity and productivity in Figures 14b and c with injection time was similar to the previous case.

The extract purity of the FeedCol operation was always higher than that of the conventional SMB in the range of 40–70% injection time. However, the injection time of longer than 55% should be applied to improve the raffinate purity. The purity improvement at the intersection of both extract and raffinte purity was about 0.7% from the conventional SMB purity. Even though a longer feed column was applied to the system, the productivity in the range of the injection time, which could produce improved purity, was equivalent to the conventional SMB. The results imply that the FeedCol strategy is also valid at the condition of high purity requirement.

Table 6. Parameters for Both Conventional SMB System and Feed Column With 1.25 Selectivity

Conventional SMB		Feed Column	
SMB system parameters		Feed column system parameters	
SMB configuration	2-2-2-2	D (column diameter) (cm)	0.55
D (column diameter) (cm)	2.6	L (column length) (cm)	8.0
L (column length) (cm)	10.5	ε (total porosity)	0.4
ε (total porosity)	0.4	N_{disp} (the number of dispersion units)	500
N_{disp} (the number of dispersion units)	500		
Mass transfer coefficient		Mass transfer coefficient	
k (both components) (s^{-1})	0.2	k (both components) (s^{-1})	0.2
Isotherm coefficient and selectivity		Isotherm coefficient and selectivity	
K_A (raffinate component)	1.800	K_A (raffinate component)	1.800
K_B (extract component)	2.250	K_B (extract component)	2.250
b_A (raffinate component) (L g^{-1})	0.066	b_A (raffinate component) (L g^{-1})	0.066
b_B (extract component) (L g^{-1})	0.100	b_B (extract component) (L g^{-1})	0.100
α (Selectivity)	1.25	α (Selectivity)	1.25
Operating parameters		Operating parameters	
$C_{i,F}$ (feed concentration) $i = A,B$ (g L^{-1})	1.0	$C_{i,I}$ (concentration of injection pulse) $i = A,B$ (g L^{-1})	variable
Q_F (feed flow rate) (mL min^{-1})	2.0	Q_I (flow rate of feed column)	2
Q_E (extract flow rate) (mL min^{-1})	5.32		
Q_R (raffinate flow rate) (mL min^{-1})	3.43		
Q_D (desorbent flow rate) (mL min^{-1})	6.75		
Q_1 (flow rate of zone1) (mL min^{-1})	24.34		
Q_2 (flow rate of zone2) (mL min^{-1})	19.02		
Q_3 (flow rate of zone3) (mL min^{-1})	21.02		
Q_4 (recycle flow rate) (mL min^{-1})	17.59		
T_{sw} (switching time) (s)	252.9		

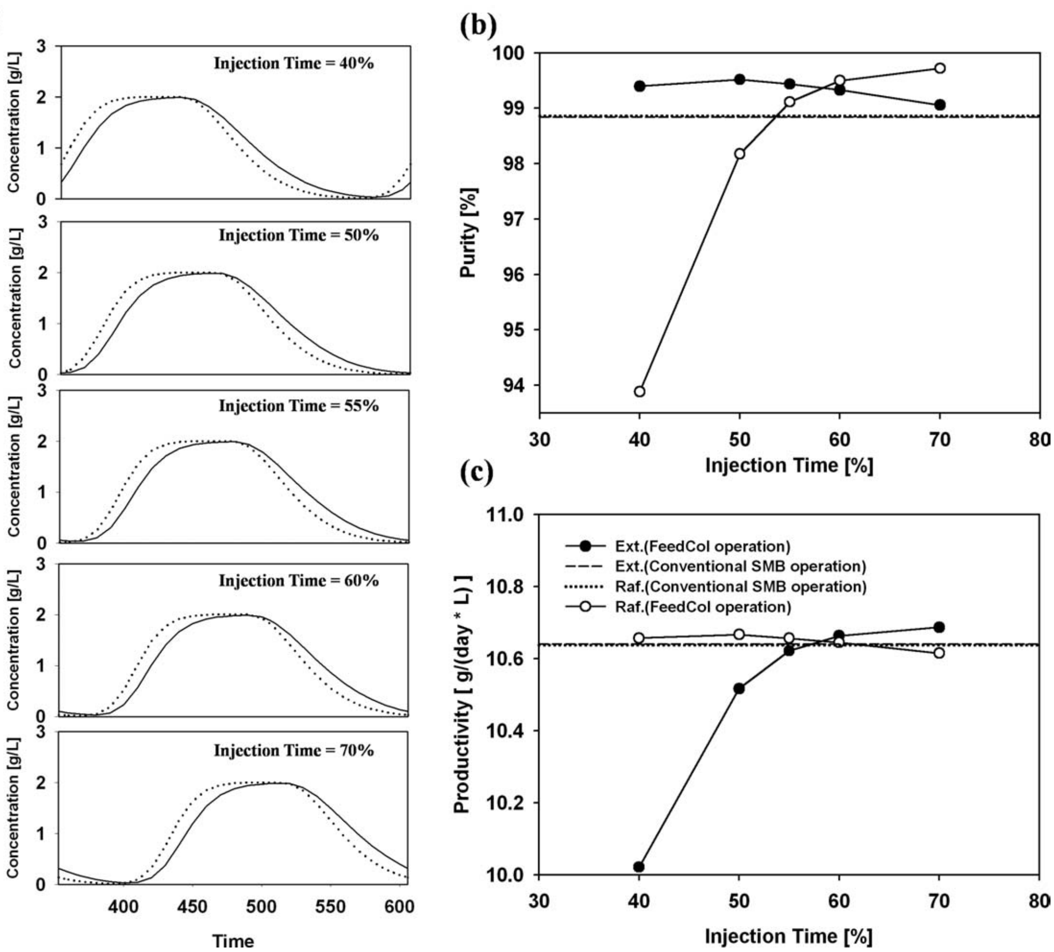

Figure 14. Effect of injection time on performance parameters at injection length of 50% in the system with 1.25 selectivity (Table 6): (a) feed shape, (b) purity, and (c) productivity.

However, an experimental study in specific systems is needed for validation of the FeedCol strategy. In addition, because the additional two operating parameters, injection length and injection time, and the chromatographic column are introduced to the conventional SMB process, an optimization study is also needed to compare the efficiency with other SMB processes.

Conclusions

We developed a new strategy, termed "FeedCol," to improve separation performance in SMB processes, which was a hybrid system of SMB separation and chromatographic separation. The desired shape of the feed supplied periodically to the SMB process can be achieved by feed pulse inputs through a chromatographic column, and FeedCol operation could reduce major impurities from both extract and raffinate ports, which incline to one side during switching period in conventional SMB operation. Therefore, performance parameters, especially purity, were improved over the conventional SMB process.

In this study, two additional operating variables, injection length and injection time, were introduced to assess the feed modified by the feed column because the feed through the feed column was synchronized with a switching period in the SMB unit. At a fixed injection time, shorter injection length improved the purity of extract and the recovery, productivity, and eluent consumption of raffinate while the variation of other performance parameters with the injection length was relatively small. However, all the performance parameters were improved compared with conventional SMB results. Furthermore, we found that, at a fixed injection length, the injection time could be adjusted to optimize the performance of FeedCol. In contrast, when the injection time for highest-purity product was used in the FeedCol operation, the other performance parameters decreased, when compared with conventional SMB. Therefore, using the FeedCol strategy, if the injection time and length are chosen carefully, purity can be improved without sacrificing other performance parameters.

With a short injection length, the mass injected into the SMB circuit is confined to a length shorter than an SMB column. However, in conventional SMB, the injected mass is evenly distributed over the entire length of an SMB column and is therefore mixed with more of the circulating SMB profile. Thus, with a shorter injection length, the FeedCol process is more similar to TMB chromatography in which the feed is injected at a single point in the TMB profile. The improvement due to this "TMB effect" would be in addition to the improvement caused by the partial resolution of the feed pulse caused by the feed column. It would be interesting to isolate this "TMB effect" in the modeling by having a short injection time but no resolution prior to injection in the SMB system. This would establish how much of the improvement with the FeedCol process was due to increased resolution of the injection pulse and how much was due to the shorter length of the injection pulse.

In this study, the FeedCol strategy was applied to a four-zone SMB chromatographic process, with two columns per zone; however, it can be used for any SMB configuration because the FeedCol operation can be implemented easily by adding a chromatographic column to all existing SMB units without additional pumps. In addition, the performance of the FeedCol operation can improve significantly with higher selectivity condition. Because the feed concentration profiles can be controlled by both injection length and time, the additional chromatographic column can be shorter and smaller than the SMB columns. Adjustment of the injection length and injection time applied for the chromatographic column acts as an important factor for the performance of the FeedCol strategy. However, due to the practical restrictions such as the solubility of the feed, controlling the injection length, unlike the injection time, may be limited in the application of some SMB processes. Therefore, the FeedCol strategy is needed for an experimental study as well as for an optimization study in near future.

Notation

b_j = second Langmuir isotherm parameter of component i (L g^{-1})
C_i = liquid phase concentration of component i (g L^{-1})
$C_{i,\mathrm{F}}$ = concentration of feed in the SMB (g L^{-1})
$C_{i,\mathrm{I}}$ = concentration of rectangular pulse input (g L^{-1})
$C_{i,j}^{\mathrm{out}}$, $C_{i,j}^{\mathrm{in}}$ = concentrations of component i at the outlet and the inlet of column j (g L^{-1})
D_L = the axial dispersion coefficient (m^2 s^{-1})
D = diameter of a column (cm)
K_i = first Langmuir isotherm parameter of component i (-)
k = mass transfer coefficient (1 s^{-1})
L = length of a column (cm)
L_inj = injection length of a rectangular pulse input (%)
N_disp = the number of dispersion units (-)
N_column = number of columns of the SMB system (-)
q_i = solid phase concentration of component i (g L^{-1})
q_i* = equilibrium solid phase concentration of component i (g L^{-1})
Q_j = flow rates of zone or column j (mL min^{-1})
Q_D, Q_E, Q_F, Q_R = desorbent, extract, feed, and raffinate flow rates (mL min^{-1})
Q_I = flow rate through feed column (mL min^{-1})
t = time (s)
t_inj = injection time of a rectangular pulse input (%)
T_sw = switching period in the conventional SMB operation (s)
T_inj = an injection period at the "FeedCol" operation (s)
$T_{\mathrm{inj},i}$ = i (i = ini, mid, last) part of one injection period (%)
u = the liquid-phase interstitial velocity (cm s^{-1})
V_column = volume of one column in SMB (L)
$V_\mathrm{feedcolumn}$ = volume of one feed column (L)

Greek letters

α = selectivity
ε = total column porosity

Subscripts

D = Desorbent
E = Extract
F = Feed
I = Rectangular pulse input
i (A, B) = Components
j = Column or inlet/outlet ports
R = Raffinate

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