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Use of Two Feeds in Simulated Moving Beds for Binary Separations

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Abstract−Simulated moving bed (SMB) and Analog systems with two-feeds are proposed to increase the separation performance. Operation with both total and partial feeds is studied. When the two feeds have different compositions, the proposed SMB system often showed better performance than conventional SMB and Varicol systems and the Analog system with two-feeds typically achieved higher purities compared to the Analog for conventional SMB and Varicol when the number of tanks was increased. Partial-feed operation strategy for SMB and Analog systems with two-feeds often showed significant performance improvement compared to conventional SMB plus partial feed and Varicol plus partial feed. When the two feeds are identical, partial feed operation of the two-feed SMB becomes identical to partial feed operation of Varicol.

Key words: Simulated Moving Bed, Analog, Two Feeds, Partial Feed

INTRODUCTION

Simulated moving bed (SMB) technology was first introduced by Universal Oil Products, UOP [Broughton et al., 1961]. This now conventional SMB process with four zones and continuous feed has been effective for the separation of binary mixtures and has attracted considerable attention in the fine chemical, pharmaceutical, and food industries for production of high value added products. Most of the studies for this technology are focused on the design and optimization of operating conditions. Recently, studies of new process developments [Abunasser et al., 2003, 2004; Kim et al., 2003, 2004; Mota et al., in press; Pais et al., 2003] and operating strategies have appeared [Ludemann-Hombourger et al., 2002; Zang et al., 2002; Zhang et al., 2003, 2004]. One column chromatography columns are useful for obtaining the data needed to design an SMB column [Kim et al., 2001]. The one column analog [Abunasser et al., 2003, 2004; Mota et al., 2005], which goes further and mimics the operation of an SMB with a single chromatographic column, is also studied in this paper.

The SMB technique involves simulated countercurrent contact between the mobile fluid phase and the stationary phase. The performance of a true moving bed is more closely approached when the SMB has multiple columns per zone [Broughton et al., 1961]. The UOP design for petrochemical separations successfully uses this principle. On other hand, since the adsorbent and columns used for chiral separation are quite expensive, those SMB processes are designed with few columns per zone [Ludemann-Hombourger et al., 2002; Pais et al., 2003; Zhang et al., 2003, 2004]. Two four-zone SMBs using five columns for binary separation are shown schematically in Fig. 1. Component A (the less adsorbable component) tends to be carried by mobile phase, while component B (the more adsorbable component) tends to be retained by the stationary phase. In the SMB process, each zone of the unit plays a specific role. The separation is performed in the two central zones. Consider an SMB

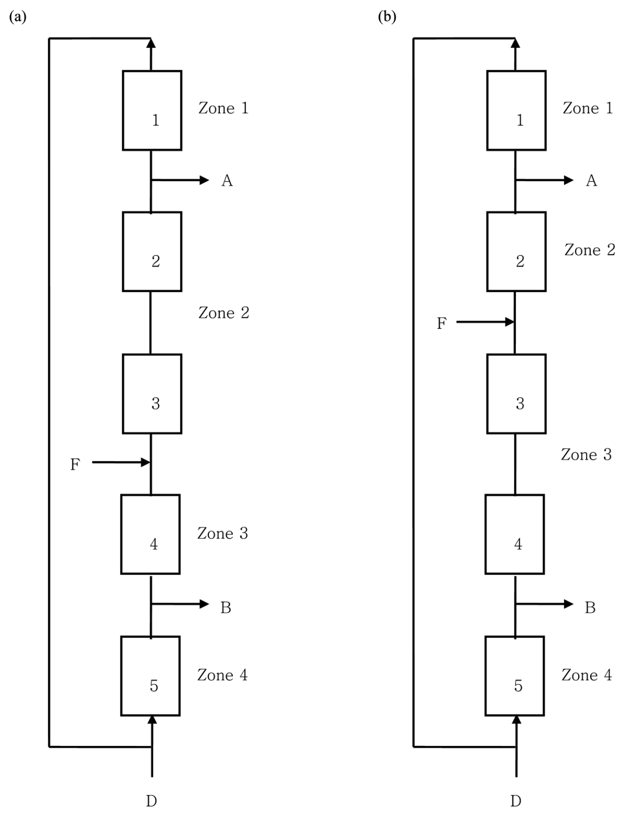

Fig. 1. Five-column SMB systems. Column switching not shown.
(a) Configuration: 1-2-1-1, (b) Configuration: 1-1-2-1

system with the (1,2,1,1) configuration (Fig. 1a). At the beginning of each switch time interval, all inlet and outlet streams will jump one column forward, in the direction of the liquid flow. This jump is synchronous, so, for this example, zones 1, 3, and 4 will always have one column, while zone 2 will always have two. The SMB in Fig. 1b is in the (1,1,2,1) configuration. These two configurations tend to have relatively similar separation characteristics, and detailed simulations are required to determine which is better. The (2,1,1,1)

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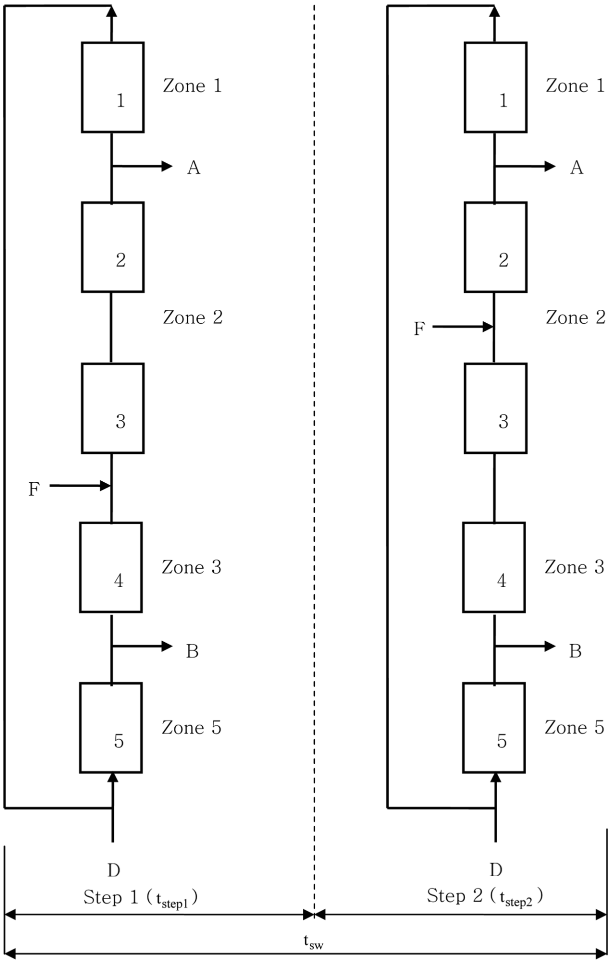

Fig. 2. Five-column varicol system. Column switching not shown.

or (1,1,1,2) configurations can also be used, but they normally result in less separation than Fig. 1a or b.

Varicol is a new continuous chromatographic process [Kim et al., 2004; Pais et al., 2003; Zhang et al., 2004] that modifies the classic SMB operation by introducing an asynchronous shift of the inlet and outlet ports. Fig. 2 shows an illustrative example of Varicol operation. This system does not keep the (1,2,1,1) or (1,1,2,1) configurations until the end of the switch time interval. Therefore, the configuration is neither (1,2,1,1) nor (1,1,2,1). During the entire switch time interval, the Varicol system has two different SMB configurations. In step 1, the Varicol system has the SMB (1,2,1,1) configuration and in step 2, it has the SMB (1,1,2,1) configuration. Therefore, the Varicol system operates with a variable number of columns per zone.

The goal of this research is to improve the separation performances of SMB and Analog systems. This is achieved by proposing SMB and Analog systems with two-feeds. First, detailed simulations are used to show that if two feeds of different composition are simultaneously fed into an SMB with a large number of columns, better separation is often achieved than one obtains by mixing the two feeds and using this as the feed to a normal single feed SMB. Then the separation performances of the newly proposed SMB and Analog systems are compared to the conventional four-zone SMB systems and a Varicol system with five columns each. Finally, the separation performance is increased further by using the partial feed strategy.

Since Zhang et al. [2004] studied the combinations of Powerfeed and Varicol, Modicon and Varicol, and Power feed and Modicon for single-feed SMB systems with 5, 3, and 4 columns, there is some overlap with our research. However, the strategies differ. They reported that these processes achieve better performance than standard SMBs, because the availability of more degrees of freedom in the operating conditions results in better optimization. The extra degrees of freedom come from choices made in conducting the asynchronous switches for Varicol, and changing flowrates or feed concentration during the switching interval for PowerFeed or ModiCon, respectively. We look at the problem starting with two feeds of different concentrations and purities and look at configurations of these two feeds with both five and ten columns. We will show that the two-feed and Varicol approaches coincide when the two feeds are identical and partial (or Power) feed is used for both two-feed and Varicol.

SINGLE-CASCADE SMB AND ANALOG DESIGN WITH TWO-FEEDS

Distillation, the most widely used method for liquid separations, has been extensively studied. The weak analogy between distillation and SMB systems can be used to develop new SMB systems and qualitatively predict their behavior for the separation of mixtures. The use of two feeds in distillation (Fig. 3a) when the feeds are different compositions can be traced at least as far back as McCabe and Thiele's classic paper [McCabe et al., 1925]. Wankat and Kessler

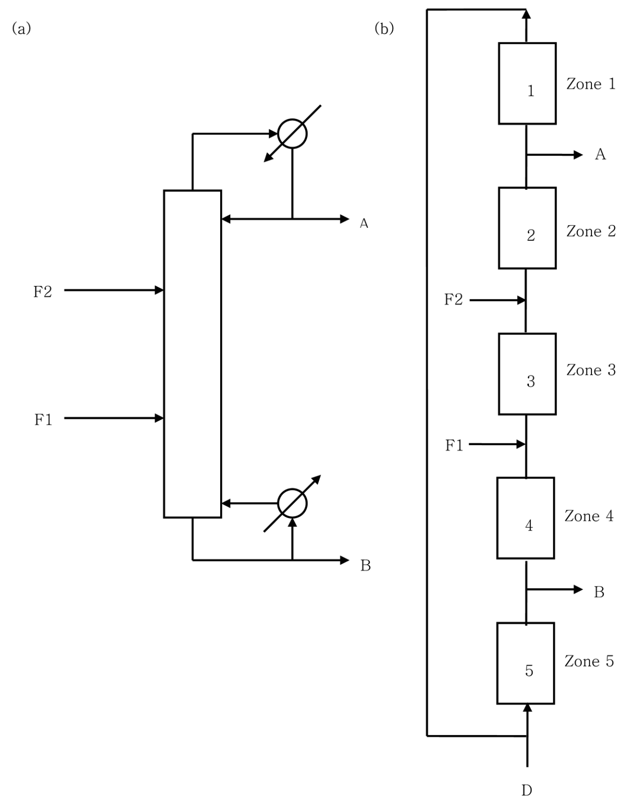

Fig. 3. Single-cascade distillation and SMB system with two-feeds. (a) Distillation tower, (b) SMB, (1, 1, 1, 1, 1) configuration

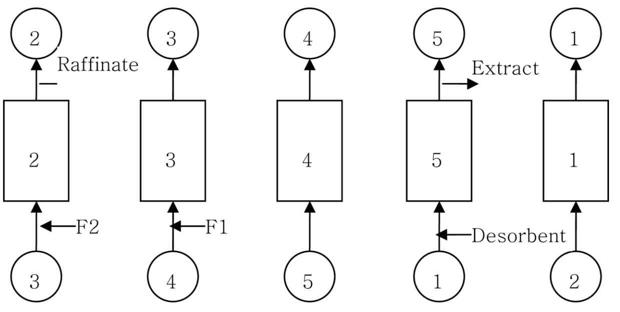

Fig. 4. One-column analogue to a five-zone SMB with one column per zone and two-feeds (1,1,1,1,1 configuration). One tank per step.

[1993] showed that two-feed distillation is also useful if both feeds are of the same composition but are at different enthalpies.

In this paper, an SMB with two feeds of different compositions (Fig. 3b) is proposed to increase separation performance. A variety of configurations of the two-feed SMB are studied for systems with a total of 10 columns, which closely mimics countercurrent operation and for the (1,1,1,1,1) configuration for 5 column systems, which has much more of a chromatographic character.

To allow comparisons the sum of the two-feed flowrates is set equal to the feed flowrate of the single-feed SMBs in Figs. 1 and 2. When F1=0, the two-feed SMB (Fig. 3b) reverts to the (1,1,2,1) configuration (Fig. 1b). When F2=0, the two-feed SMB system reverts to the (1,2,1,1) configuration (Fig. 1a). Also, we will show that the two-feed SMB system becomes a modification of the Varicol system (Fig. 2) if partial feed [Zang et al., 2002] is used for each of the two feeds.

Analog systems [Abunasser et al., 2003, 2004; Mota et al., in press] were also designed and compared for the SMB systems in Figs. 1 to 3 for 5 column systems. The basic configuration of the Analog (Fig. 4) has one adsorption column connected to several tanks, with one tank for each column in the SMB configuration being studied. The Analog system has the advantage of flexibility; since there is only one column to repack it should be useful when a plant operates campaigns.

LOCAL EQUILIBRIUM MODEL AND ASPEN CHROMATOGRAPHY

The local equilibrium model [Wankat, 1990] is a method for performing calculations on adsorption systems using simplified forms of the mass and energy balances to enable analytical calculations. For linear equilibrium this model is equivalent to the triangle theory [Migliorini et al., 1998]. The solid and fluid are assumed to be locally in equilibrium. The mass and energy balances for fixed bed adsorption can be derived by writing differential balances around the solid and fluid phases. If one assumes that radial gradients are negligible, no chemical reactions, linear equilibrium, mass transfer is extremely rapid and there is no axial dispersion, the mass balances can be solved for the solute wave velocity:

$$u_{s,i}(T)=\frac{v_j}{1+[(1-\varepsilon_e)/\varepsilon_e]\varepsilon_p K_d+[(1-\varepsilon_e)/\varepsilon_e](1-\varepsilon_p)\rho_s K_i} \tag{1}$$

The average velocity of port movement is

$$u_{port}=L/t_{sw} \tag{2}$$

For Fig. 3a the condition to have A exit in the A product is,

$$u_{A2},\ u_{A3},\ u_{A4}\geq u_{port}\geq u_{A1} \tag{3}$$

To have solute B exit in the B product, the condition is

$$u_{B5}\geq u_{port}\geq u_{B2},\ u_{B3},\ u_{B4} \tag{4}$$

In isothermal systems, Eqs. (3) and (4) are essentially satisfied by varying the velocities in each zone.

To compare the performance of SMB systems, the purity index (PI), the average purity of the major components in the two products, and the productivity are defined as,

$$\text{Purity index (PI)}=\frac{\text{Purity of A (\%) in A product}+\text{Purity of B (\%) in B product}}{2} \tag{5}$$

$$\text{Productivity}=\frac{\text{Volumetric flowrate of feed}}{\text{Total adsorbent volume}} \tag{6}$$

In order to examine separation performance of the new two-feed SMB, detailed simulations were run for various feed compositions and operating strategies (SMB, Analog, Varicol, SMB+partial feed, and Varicol+partial feed) using Aspen Chromatography, version 12.1. The simulations were done for the separation of enantiomers of 1,1'-bi-2-naphtol as a model system. The adsorbent is silica gel and the desorbent is a mixture of 72/28(v/v) heptane/isopropanol [Pais et al., 1998]. The simulation conditions are reported in Tables 1 to 7.

Aspen Chromatography calculates flow as convection with esti-

Table 1. Simulation results for SMB systems with two feeds, 5 zones and 10 columns for total feed operation

Run	Feed concentration (g/L)				Configuration: 2-2-1-3-2			Configuration: 2-2-2-2-2			Configuration: 2-3-1-2-2		
	F1		F2		Raffinate (A)	Extract (B)	PI	Raffinate (A)	Extract (B)	PI	Raffinate (A)	Extract (B)	PI
	$c_{A,F1}$	$c_{B,F1}$	$c_{A,F2}$	$c_{B,F2}$									
1	1.0	10.0	10.0	5.0	99.76	94.54	**97.15**	99.76	93.59	**96.68**	99.83	93.47	**96.65**
2	1.0	10.0	10.0	1.0	99.83	86.51	**93.17**	99.83	85.34	**92.59**	99.84	85.12	**92.48**
3a	5.0	10.0	10.0	5.0	99.71	94.11	**96.91**	99.73	92.40	**96.07**	99.86	92.43	**96.15**
3b	5.0	5.0	10.0	10.0	99.06	94.07	**96.57**	99.16	92.55	**95.86**	99.83	92.70	**96.27**
4	5.0	10.0	10.0	10.0	94.10	98.64	**96.37**	96.61	98.03	**94.58**	95.17	97.84	**96.51**

L=10.5 cm, D_c=2.4 cm, ε_e=0.4, ε_p=0.0, k=0.5 min^{-1}, Productivity=0.0077

$Q_{F1}=Q_{F2}$=1.82 cm^3/min, Q_R=6.8546 m^3/min, Q_E=20.0814 cm^3/min, Q_D=23.2960 cm^3/min, $Q_{Recycle}$=19.8290 cm^3/min, D/F_{total}=6.4

Table 2. Simulation results for standard SMB systems with one feed, 4 zones and 10 columns for total feed operation

Run	Concentration (g/L)		Purity (%)														
			Configuration: 2-1-5-2			Configuration: 2-2-4-2			Configuration: 2-3-3-2			Configuration: 2-4-2-2			Configuration: 2-5-1-2		
	$c_{A,F}$	$c_{B,F}$	A	B	**PI**	A	B	**PI**	A	B	**PI**	A	B	**PI**	A	B	**PI**
1	5.5	7.5	90.32	93.54	**91.93**	99.44	94.74	**97.09**	99.82	94.05	**96.94**	99.83	92.14	**95.99**	99.80	83.96	**91.88**
2	5.5	5.5	93.80	85.68	**89.74**	99.68	86.77	**93.23**	99.84	85.79	**92.82**	99.84	83.30	**91.57**	99.81	74.15	**86.98**
3	7.5	7.5	90.53	92.85	**91.69**	98.94	94.57	**96.76**	99.82	93.96	**96.89**	99.86	91.90	**95.88**	99.85	82.46	**91.16**
4	7.5	10.0	83.02	97.56	**90.29**	88.14	98.19	**93.17**	88.59	97.76	**93.18**	89.53	96.55	**93.04**	99.70	90.67	**95.19**

Feed is average of two-feeds showen in Table 6, L=10.5 cm, D_c=2.4 cm, ε_e=0.4, ε_p=0.0, k=0.5 min^{-1}, Productivity=0.0077
Q_F=3.64 cm^3/min, Q_R=6.8546 m^3/min, Q_E=20.0814 cm^3/min, Q_D=23.2960 cm^3/min, $Q_{Recycle}$=19.8290 cm^3/min, D/F$_{total}$=6.4

mated dispersion and the kinetic model was a linear lumped resistance with a ($q_i^*-q_i$) driving force.

The isotherms for binary separation are correlated as bi-Langmuir type [Pais et al., 1998]

$$q_A^* = \frac{2.69c_A}{1+0.0336c_A+0.0466c_B} + \frac{0.10c_A}{1+c_A+3c_B} \quad (7)$$

$$q_B^* = \frac{3.73c_A}{1+0.0336c_A+0.0466c_B} + \frac{0.30c_A}{1+c_A+3c_B} \quad (8)$$

where A and B are defined as the less- and more-retained components, respectively.

SIMULATION RESULTS: LARGE NUMBER OF COLUMNS IN SMB

When there are a large total number of columns (10 in this case) the SMB more closely approaches the behavior of true moving bed systems. Since previous research showed that neither Varicol [Ludemann-Hombourger et al., 2002; Zhang et al., 2004] nor partial feed [Zang et al., 2002] or Power feed [Zhang et al., 2003, 2004] results in significant improvement when there are multiple columns per zone, we only need to compare the two-feed SMB with total feed to single feed SMBs where the two feeds are mixed together.

Fig. 3 illustrates a distillation column with two-feeds and three sections, and a SMB cascade with two-feeds and five zones. The formal analogy with a distillation process in which zones 5 and 1 (Fig. 3b) play the roles of reboiler and condenser (Fig. 3a) is readily apparent. The analogy to SMB systems must be treated with caution since there are significant differences. In case of distillation columns, the optimal feed locations are readily calculated by using a McCabe-Thiele diagram [McCabe et al., 1925; Wankat et al., 1993]. The optimum feed locations for distillation can be determined according to the following rules:

(1) When the two feeds have different purities and the purity of component A in F2 is higher than that in F1, feed F2 should enter the column higher up than feed F1.

(2) When the two feeds have same purities and have different enthalpies (or phases), feed F1 should enter the column with higher enthalpy or as vapor, and feed F2 should enter the column with lower enthalpy or as liquid.

Rule 1 can be used directly for SMBs. Rule 2 needs to be translated to the SMB. By analogy, adding desorbent is equivalent to increasing enthalpy. Thus, for the SMB rule 2 becomes.

(2 SMB) When the two feeds have same purities and different concentrations, feed F1 with lower solute concentrations (more desorbent) is feed lower in the cascade (closer to desorbent addition) than feed F2.

Table 1 shows the simulation results for ten column SMB systems with two feeds for total feed operation. When $c_{A,F1}<c_{A,F2}$ and $c_{B,F1}<c_{B,F2}$ and $(c_{A,F1}+c_{B,F1})<(c_{A,F2}+c_{B,F2})$ (Run 1), and when $c_{A,F1}<c_{A,F2}$ and $c_{B,F1}>c_{B,F2}$ and $(c_{A,F1}+c_{B,F1})=(c_{A,F2}+c_{B,F2})$ (Runs 2 and 3a), the (2,2,1,3,2) configuration has a higher PI than the (2,2,2,2,2) and (2,1,3,2,2) configurations. These runs with different feed concentrations are analogous to normal two feed distillation [McCabe et al., 1925]. When $(c_{A,F1}/c_{B,F1})=(c_{A,F2}/c_{B,F2})$ and $(c_{A,F1}+c_{B,F1})<(c_{A,F2}+c_{B,F2})$ (Run 3b), the (2,2,1,3,2) configuration again has a higher PI. This is analogous to 2-enthalpy feed distillation [Wankat et al., 1993]. When $c_{A,F1}<c_{A,F2}$ and $c_{B,F1}=c_{B,F2}$ and $(c_{A,F1}+c_{B,F1})<(c_{A,F2}+c_{B,F2})$ (Run 4), the (2,3,1,2,2) configuration has higher PI than the (2,2,1,3,2) and (2,2,2,2,2) configurations. The (2,1,3,2,2) configuration was also tried for all the runs in Table 1, but never had the highest raffinate, extract or PI values.

Table 2 shows the simulation results for standard SMB systems with one feed for total feed operation and feed is the average of the two feeds for the corresponding runs in Table 1. Comparing the results in Table 1 and Table 2 shows that when $c_{A,F1}<c_{A,F2}$ and $c_{B,F1}=c_{B,F2}$ and $(c_{A,F1}+c_{B,F1})<(c_{A,F2}+c_{B,F2})$ (Run 4 in Table 1), the SMB system with two-feeds (configuration: 2,3,1,2,2) can achieve a significant performance improvement over the SMB with one feed. For 1 and 3a the 2-feed SMB was slightly superior to the single feed SMB, while for Runs 2 and 3b the single feed (2,2,4,2) and (2,3,3,2) configurations, respectively, were slightly superior.

SIMULATION RESULTS: LIMITED NUMBER OF COLUMNS IN SMB WITH TOTAL FEED OPERATION

Because of the expense of the adsorbent and columns used for separation of optical isomers, there has been considerable recent interest in SMB systems with a limited total number of columns. In order to evaluate the performance of the (1,1,1,1,1) SMB system with two feeds (Fig. 3b), it is compared to the five columns, four zone SMB systems with one feed (Fig. 1) and to Varicol (Fig. 2). The feed flowrate in the single feed SMBs and Varicol is the sum of the flowrates in the two feed system, and the feed concentrations in the single feed systems are the average of those in the

Table 3. Simulation conditions and results for VARICOL system (Fig. 2) for total feed operation. Effects of feed length and feed concentration

Run	Feed concentration (g/L)		Feed flowrate (cm^3/min)		Feed length (min)	Purity (%)		PI
	$c_{A,F}$	$c_{B,F}$	Q_{F1}	Q_{F2}	t_{step1}	Raffinate (A)	Extract (B)	
a	5.5	10.0	3.640	3.640	$0.2t_{sw}$	89.44	97.72	**93.58**
b					$0.4t_{sw}$	91.60	97.49	**94.55**
c					$0.6t_{sw}$	93.21	96.94	**95.08**
d					$0.8t_{sw}$	95.63	95.95	**95.79**
e	7.5	10.0			$0.2t_{sw}$	87.05	96.73	**91.89**
f					$0.4t_{sw}$	88.12	96.33	**92.23**
g					$0.6t_{sw}$	89.00	95.58	**92.29**
h					$0.8t_{sw}$	90.29	94.29	**92.29**
i	10.0	10.0			$0.2t_{sw}$	85.60	95.32	**90.46**
j					$0.4t_{sw}$	86.15	94.75	**90.45**
k					$0.6t_{sw}$	86.66	93.77	**90.22**
l					$0.8t_{sw}$	87.43	92.14	**89.79**

L=21.0 cm, D_c=2.4 cm, ε_e=0.4, ε_p=0.0, k=0.5 min^{-1}, t_{sw}=6.95 min, D/F=6.4, Productivity=0.0077
Flowrates: Q_R=6.8546 cm^3/min, Q_E=20.0814 cm^3/min, Q_D=23.2960 cm^3/min, $Q_{Recycle}$=19.8290 cm^3/min, D/F_{total}=6.4

two feed system.

The effects of step time and feed concentration for the simulation of Varicol are shown in Table 3. At a constant step time, the raffinate and extract purities decreased with increasing component A feed concentration because the solute wave velocity of component A is decreased. When feed concentration is constant, increasing feed length in the configuration (1-2-1-1), the raffinate purities increased and extract purities decreased because of the effect of the column distribution between zones during the switching time (configuration: 1-2-1-1>configuration: 1-1-2-1, see Fig. 2).

Table 4 shows the simulation conditions and results for the SMB system with two feeds, SMB systems with one feed and Varicol. The best simulation results for Varicol are selected from the runs in Table 3. The results of SMB system with two feeds show that when the concentration of component B in F1 and concentrations of components A and B in F2 are constant, the raffinate purities and extract purities decrease with increasing concentration of component A in F1 (runs 1a, 2a, and 3). Also, when the concentrations of components A and B in F1 and the concentration of component B in F2 are constant, the raffinate purities increased and the extract purities decreased slightly when the concentration of component A in F2 increased (runs 1b, 2b, and 3). From the results, when $c_{A,F1}<c_{A,F2}$

Table 4. Comparison of simulation results for total feed operation for five column systems

Run	Purity (%)											
	Two-feed SMB (1, 1, 1, 1, 1)			SMB (configuration: 1-2-1-1)			SMB (configuration: 1-1-2-1)			Varicol		
	Raffinate	Extract	PI	Raffinate	Extract	PI	Raffinate	Extract	PI	Raffinate	Extract	PI
1a	94.72	97.27	**96.00**	98.35	94.08	**96.22**	85.81	97.65	**91.73**	95.63	95.95	**95.79**
1b	81.65	91.35	**86.50**									
2a	93.35	94.53	**93.94**	92.74	92.12	**92.43**	85.06	96.79	**90.93**	90.29	94.29	**92.29**
2b	85.40	91.07	**88.24**									
3	87.76	90.62	**89.19**	88.92	89.41	**89.17**	84.56	95.56	**90.06**	85.60	95.32	**90.46**

L=21.0 cm, D_c=2.4 cm, ε_e=0.4, ε_p=0.0, k=0.5 min^{-1}, Productivity=0.0077, D/F_{total}=6.4

-Feed concentration in SMB with two-feeds (configuration: 1-1-1-1-1)

Run 1a: $c_{A,F1}$=1.0 g/L, $c_{B,F1}=c_{A,F2}=c_{B,F2}$=10.0 g/L, Run 1b: $c_{A,F1}=c_{B,F1}=c_{B,F2}$=10.0 g/L, $c_{A,F2}$=1.0 g/L,

Run 2a: $c_{A,F1}$=5.0 g/L, $c_{B,F1}=c_{A,F2}=c_{B,F2}$=10 g/L Run 2b: $c_{A,F1}=c_{B,F1}=c_{B,F2}$=10.0 g/L, $c_{A,F2}$=5.0 g/L, Run 3: $c_{A,F1}=c_{B,F1}=c_{B,F2}$=10.0 g/L

-Feed concentration in SMBs (configuration: 1-2-1-1 and 1-1-2-1) and VARICOL system

Feed is average of two-feeds

Runs 1a and 1b: $c_{A,F}$=5.5 g/L, $c_{B,F}$=10.0 g/L, Runs 2a and 2b: $c_{A,F}$=7.5 g/L, $c_{B,F}$=10.0 g/L, Run 3: $c_{A,F}=c_{B,F}$=10.0 g/L

-Operating conditions

SMB with two-feeds: F1=F2=1.82 cm^3/min

SMB (configuration: 1-2-1-1 and 1-1-2-1) and Varicol system: F=3.64 cm^3/min

Q_R=6.8546 cm^3/min, Q_E=20.0814 cm^3/min, Q_D=23.2960 cm^3/min, $Q_{Recycle}$=19.8290 cm^3/min, D/F=6.4, t_{sw}=6.95 min and $c_{B,F1}=c_{B,F2}$ (run 2a), the SMB system with two feeds has higher PI than the other SMB systems. The (1,2,1,1) SMB was best for runs 1a, 1b, and 2b, and Varicol was best for run 3.

LIMITED NUMBER OF COLUMNS IN SMB WITH PARTIAL FEED OPERATION

Zang and Wankat [2002] developed partial feed and Zhang et al. [2003, 2004] developed Powerfeed, which are essentially identical operating procedures. In the partial feed operation developed for two-feed SMB and Varicol in this paper, for simplicity, most of the variables are maintained constant, such as temperatures, pressures, switching time, etc. Obviously, these constraints can be relaxed. The feed flowrate changes from continuous constant flow in total feed to discontinuous pulse flow in partial feed (Fig. 5). The partial feed operation uses a larger feed rate, but the averages are the same.

Partial feed operation introduces two additional degrees of freedom: the feed length and the feed time. Feed length refers to the time duration of the feed (Fig. 5). Feed time defines the time at which the center of the feed pulse enters the column (Fig. 5). The feed length is expressed as a fraction of the switching time, and the feed time is the time gap from the beginning of each step to the feed center,

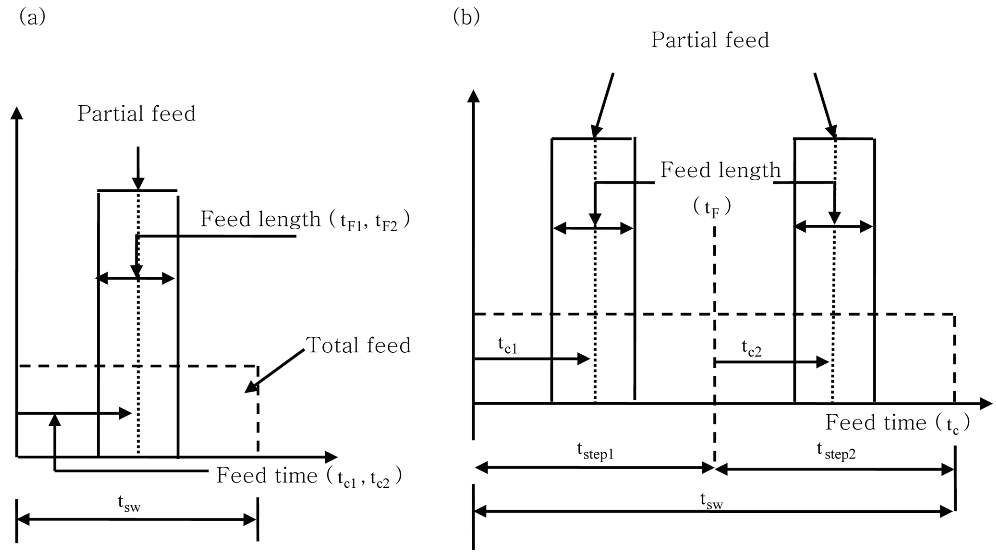

Fig. 5. Partial-feed strategy.
(a) SMB+partial feed. For a two-feed system with partial feed, both feeds are operated as partial feed. (b) Varicol+partial feed.

Table 5. Effect of feed length and feed time for the partial feed two-feed SMB system which is identical to partial feed Varicol system for feeds of same concentration

Run	Feed concentration (g/L)				Feed lengths	Feed times		Purities (%)		PI
	$c_{A,F1}$	$c_{B,F1}$	$c_{A,F2}$	$c_{B,F2}$	(t_{F1}/t_{sw}, t_{F2}/t_{sw})	t_{c1}/t_{sw}	t_{c2}/t_{sw}	Raffinate (A)	Extract (B)	
1							0.1	85.52	94.98	**90.25**
2						0.1	0.5	85.93	95.24	**90.59**
3							0.9	85.95	95.26	**90.61**
4							0.1	86.10	93.08	**89.59**
5					0.2	0.5	0.5	86.75	93.30	**90.03**
6							0.9	86.78	93.37	**90.08**
7							0.1	85.75	86.14	**85.95**
8	10.00	10.00	10.00	10.00		0.9	0.5	89.20	87.62	**88.41**
9							0.9	89.71	87.83	**88.77**
10							0.2	85.94	94.55	**90.25**
11						0.2	0.4	86.21	94.68	**90.45**
12							0.8	86.25	94.69	**90.47**
13					0.4		0.2	87.42	88.20	**87.81**
14						0.8	0.4	88.52	88.65	**88.56**
15							0.8	89.06	88.87	**88.97**

L=21.0 cm, D_c=2.4 cm, ε_e=0.4, ε_p=0.0, k=0.5 min^{-1}, t_{sw}=6.95 min, D/F_{total}=6.4
Q_E=20.0814 cm^3/min, Q_D=23.2960 cm^3/min, $Q_{Recycle}$=19.8290 cm^3/min

also expressed as a fraction of the switching time. The operation does not have to be symmetric. The separation efficiency of a partial feed SMB will depend on the choice of these two parameters.

The flowrates of the desorbent and the extract product are maintained constant at the same values as in total feed operation. Because of mass balance constraints, the raffinate product's flowrate changes according to the changes in the feed flowrate. Although the feed flowrate is changed, the operating method keeps the feed amount for each switching period the same as in total-feed operation

$$[(\text{feed flowrate})\times t_{sw}]_{total\,feed}=[(\text{feed flowrate})\times t_{feed}]_{partial\,feed},\quad t_{feed}\le t_{sw} \qquad (9)$$

Total feed operation can be considered as a special case of partial feed when $t_{feed}=t_{sw}$.

When the two feeds have identical concentrations and partial feed is applied to both feeds in Fig. 2 and to both feeds in Fig. 3b, the Varicol and two-feed systems are identical. They essentially merge into the same process. The optimum feed times for the two feeds are different. A number of simulations were run to compare the separation performance of a partial feed SMB system with two feeds/Varicol, and the partial feed operation of a (1,2,1,1) SMB. Table 5 shows the effects of feed length and feed time for the partial feed SMB system with two feeds/Varicol system. These results show that the optimum operation has relatively short feed lengths (0.2), early input of feed 1 (t_{c1}/t_{sw}=0.1) and late input of feed 2 (t_{c2}/t_{sw}= 0.9). These rules agree with results for partial feed [Zang et al., 2002] and can be predicted from the local equilibrium theory. This partial feed operation with equal concentration feeds gives slightly higher purity indexes (PI) than the total-feed operation (compare the results in Table 5 and run 3 in Table 4).

Table 6 shows the simulation conditions and results when the feeds have different concentrations (run 2a in Table 4). The purity index has a maximum value at a feed length of ~0.3 (run 2 in Table 6). Comparison of these runs shows that the partial-feed operation for SMB with two-feeds gives a significantly higher purity index (PI) than total-feed operation. Table 7 shows simulation conditions and results for the partial feed Varicol/2-feed SMB with the two feeds from run 2a mixed together. The results show the partial-feed operation strategy increases separation efficiency of Varicol with constant productivity. But the improved separation is very small (compare the results in Table 7 to the Varicol results for run 2 in Table 4). Comparing the best PI in Table 6 (95.30) to the best PI in Table 7 (93.38) shows that keeping the two feeds separate improves the separation when their concentrations are different.

Table 6. Simulation results and operating conditions for SMB system with two-feeds+partial feed strategy for feeds with different concentrations (Fig. 5b)

Run	Feed length		Purity (%)		PI
	t_{F1}/t_{sw}	t_{F2}/t_{sw}	Raffinate (A)	Extract (B)	
1	0.2	0.2	94.19	96.46	**94.33**
2	0.3	0.3	94.26	96.34	**<u>95.30</u>**
3	0.4	0.4	94.26	96.21	**95.24**
4	0.5	0.5	94.24	95.99	**95.12**
5	0.8	0.8	93.49	95.47	**94.48**

Conditions:
Feed time (t_{c1}/t_{sw}, t_{c2}/t_{sw})=0.5, L=21.0 cm, D_c=2.4 cm, ε_e=0.4, ε_p= 0.0, k=0.5 min^{-1}
Feed concentration: $c_{A,F1}$=5.0 g/L, $c_{B,F1}$=$c_{A,F2}$=$c_{B,F2}$=10.0 g/L (run 2a in Table 4), D/F_{total}=6.4, t_{sw}=6.95 min
Q_E=20.0814 cm^3/min, Q_D=23.2960 cm^3/min, $Q_{Recycle}$=19.8290 cm^3/min

Table 7. Simulation results and operating conditions for partial feed two-feed SMB/Varicol system for two feeds of same composition (Fig. 5). Feed time (t_c/t_{step1}, t_c/t_{step2})=0.5

Run	Step 1		Step 2	Purity (%)		PI
	t_{step1}/t_{sw}	(t_F/t_{step1})	t_F/t_{step2}	Raffinate (A)	Extract (B)	
1	0.2	0.2	0.2	87.22	96.83	**92.03**
2		0.5		87.19	96.85	**92.02**
3		0.8		87.23	96.82	**92.03**
4		0.2	0.4	87.22	96.84	**92.03**
5		0.5		87.25	96.83	**92.04**
6		0.8		87.26	96.82	**92.04**
7		0.2	0.8	89.32	90.87	**90.10**
8		0.5		88.99	91.64	**90.32**
9		0.8		88.71	92.10	**90.41**
10	0.5	0.2	0.2	88.23	96.40	**92.32**
11		0.5		88.32	96.29	**92.31**
12		0.8		88.43	96.15	**92.29**
13		0.2	0.4	88.24	96.40	**92.32**
14		0.5		88.33	96.29	**92.31**
15		0.8		87.87	95.84	**91.86**
16		0.2	0.8	88.76	96.71	**92.74**
17		0.5		90.45	96.31	**<u>93.38</u>**
18		0.8		91.45	93.47	**92.46**
19	0.8	0.2	0.8	88.82	96.24	**92.53**
20		0.5		89.78	95.94	**92.86**
21		0.8		92.38	94.12	**93.25**

L=21.0 cm, D_c=2.4 cm, ε_e=0.4, ε_p=0.0, k=0.5 min^{-1}, t_{sw}=6.95 min, Q_E=20.0814 cm^3/min, Q_D=23.2960 cm^3/min, $Q_{Recycle}$=19.8290 cm^3/min
Feed is average of two-feeds for Run 2a in Table 4. Average feed concentration: $c_{A,F}$=7.5 g/L, $c_{B,F}$=10.0 g/L, D/F_{total}=6.4

SIMULATIONS FOR ANALOG OPERATION

The one column analog system (Fig. 4) is a simpler process that will be more flexible when columns have to be repacked frequently; however, the product purities are typically lower than the product purities obtained with the corresponding SMB process. For the comparison of the Analogs to the different SMB configurations considered for the total feed operation so far, simulations were run for the conditions in Run 2a of Table 4. The results of these simulations can be seen in Fig. 6. When the simulations were run with the minimum number of tanks (five), the trend for the changes in the purity index for the Analogs (1,2,1,1>two feeds with partial feed>two feeds with total feed>Varicol) was not the same as for the corresponding SMBs (two feeds with partial feed>two feeds with total

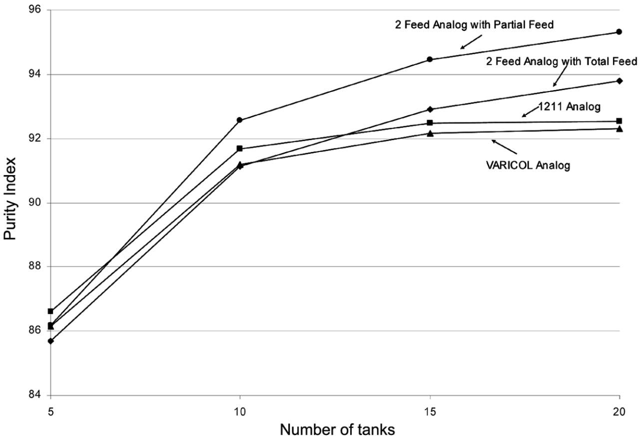

Fig. 6. Effect of the number of tanks for the analog systems for total feed operation.

feed>1,2,1,1>Varicol). This can be attributed to mixing in the tanks which tends to cause more reduction in separation for non-linear separations [Abunasser et al., 2004]. This reduction occurs because the solute velocities depend on concentration, which in turn affects the separation.

One solution to this mixing is to split the large tanks into several smaller tanks keeping the total volume constant. These smaller tanks will be emptied in the same order as they are filled. As the number of tanks becomes large, the storage for each step approaches plug flow and the separation in the Analog approaches that of the SMB [Abunasser et al., 2004]. Fig. 6 shows that when 15 tanks, or 3 smaller tanks per larger tank, are used the purity trend in the Analogs (two feeds with partial feed) becomes the same as the trend in the SMBs (two feeds with total feed>1,2,1,1>Varicol). When each large tank was split into four smaller tanks, this trend did not change but the purities continued to improve with the purity indices for the (1,2,1,1) Analog and Varicol Analog approaching the corresponding SMB values, while the two-feed Analogs still have room for improvement. The alternative to splitting the tanks into smaller tanks is the use of a plug-flow tank [Mota et al., in press].

DISCUSSION AND CONCLUSIONS

When the two feeds have different concentrations, partial feed operation of a two-feed SMB resulted in the highest purities. Based on the philosophical principle that since mixing is the reverse of separation, partially separated streams should not be mixed together, this result is not surprising.

When the two feeds are identical, the results do not show that one configuration is always superior. Detailed simulations are required to determine which configuration is optimum. When the two feeds are identical it is interesting to compare our results to those of Zhang et al. [2004]. Their results with five columns also showed that the combination of Varicol and partial feed (Power feed in their paper) is better than either Varicol or partial feed alone. Exact comparison of the numbers is not possible since the optimization strategy in this paper constrained D/F to a constant value, while Zhang et al. [2004] allowed D/F to vary.

In this work, we proposed both SMB and Analog systems with two-feeds and investigated their separation performance by using detailed simulations. Especially, when the compositions of two-feeds were different, the proposed SMB and Analog systems with total feed often produced better separations than other SMB processes (configurations: 1,2,1,1 and 1,1,2,1 and Varicol). The partial-feed operation strategy further increases product purities of the SMB and Analog systems with two-feeds and the Varicol system with constant productivity. Under partial feed operation with feeds of the same concentration, the two-feed SMB and Varicol become indistinguishable. When feed concentrations are different, the partial-feed operation strategy of SMB system with two-feeds can achieve a significant performance improvement over Varicol+partial feed using a mixed feed.

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NOMENCLATURE

c_i : concentration of species i in liquid [g/cm^3]
D : volumetric flow rate of fresh desorbent [cm^3/s]
F : volumetric flow rate of the feed [cm^3/s]
K_d : steric hindrance factor, K_d=0.0 if molecules are excluded from all pores and K_d=1.0 if molecules have free access to all pores
K_i : linear equilibrium constant, $q_i=K_ic_i$ [g of adsorbent/cm^3]
k_i : overall mass-transfer coefficient [s^{-1}]
L : length of each column [cm]
q_i : amount adsorbed [g of solute/g of adsorbent]
q_i^* : amount adsorbed in equilibrium with fluid
t_{feed} : feed time [s]
t_{sw} : switching time [s]
u_i : velocity of the solute [cm/s]
u_{port} : port velocity=L/t_{sw} [cm/s]
v_i : interstitial fluid velocity in zone j [cm/s]

Greek Letters

ε_e : external porosity
ε_p : particle porosity
ρ_s : solid density [kg/m^3]

Subscript

A, B : solutes

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