Improving the Performance of One Column Analogs to SMBs

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A simple unmixed reservoir was developed for the one column chromatograph with recycle analogous to an SMB (Analog) to replace mixed tanks or a complicated unmixed reservoir. Separation of the 1,1′ bi-2-naphthol enantiomers was studied. In the linear range the purity index (PI) of the Analog with mixed tanks is 87.5, PI = 94.8 for the unmixed reservoir Analog, and PI = 96.9 for the SMB. SMB scaling rules, extended to Analogs, are used to increase the product purities of the unmixed reservoir Analog to match SMB purities but with lower productivity. Then productivity is increased at constant purity by operating at the maximum allowable pressure drop (15 bar) in each step. After scaling, the unmixed reservoir Analog's productivity was higher than the productivity of a standard SMB (one recycle pump) at the same purities (PI = 96.9), and the mixed tanks Analog's productivity was 3.5 times higher than the standard SMB, but with a significantly lower purity. © 2006 American Institute of Chemical Engineers *AIChE J,* 52: 2461–2472, 2006
Keywords: SMB, Analog, scaling, pressure drop, unmixed reservoirs

Introduction

Simulated moving bed chromatography (SMB) has seen an increased use in industry in recent years. It was first commercialized by UOP in the 1960s[1] for use in petrochemical and sugar separations. Since then its use has been extended to the pharmaceutical and fine chemicals industries.[2] A variety of novel operating methods, including partial[3] and power feed,[4] VARICOL,[5] two-feed systems,[6] and 3-zone[7] and 2-zone[8] SMBs have been developed and extensively studied.

Single column systems that mimic SMB operation have also been developed in recent years. Steady-state recycle (SSR) was first introduced by Grill[9]; it is a modified recycle chromatography system. It consists of a single column, where, like in the SMB, a fresh feed sample is injected into the interior of the circulating chromatographic profile. The cycle consists of several steps, which include a fresh feed injection, a fresh desorbent injection, two product stream collection steps, and two waste stream collections. SSR has been shown to be capable of achieving purities close to those of SMB systems but with the use of larger amounts of desorbent.[9,10]

Another single column system is the single column chromatograph with recycle stored for an appropriate lag time so that it is analogous to an SMB (the "Analog").[11] It has been shown, using complete computer simulations, that the Analog can mimic any SMB configuration and achieve reasonable separation.[6,11–13] Experiments have also been performed that show that it is feasible to operate the Analog and have shown close agreement between the simulations and the experiments.[13] Because the early simulations and experiments used stirred tanks for storage, mimicking complicated SMBs such as partial feed (or power-feed),[12] VARICOL,[12] and the use of two feeds,[6] the use of one tank per column of the SMB was not sufficient. Use of multiple storage tanks per SMB column retained the improvement achieved with the more complicated configuration, but the Analog becomes more complex and expensive as additional tanks are added.

Mota and Araujo[14] replaced the Analog's mixed tanks with a single unmixed or plug-flow reservoir equipped with a piston to adjust for the varying flow rates during the SMB cycle. The reservoir used compressible packing to minimize mixing. Use of a single unmixed reservoir reduces the number of valves and

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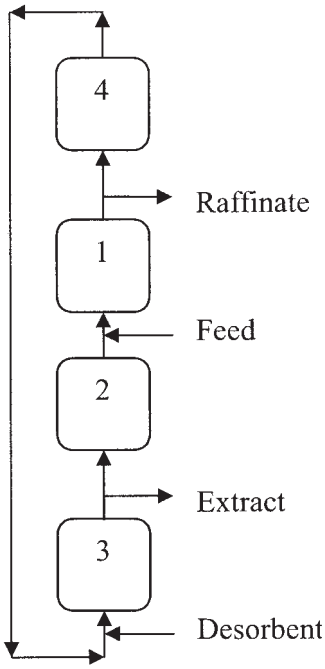

Figure 1. Four-zone (1,1,1,1) SMB.

tees while increasing product purities. Their theoretical analysis showed that this Analog gave higher purities than an Analog with one mixed tank per column but because of dispersion in the reservoir did not quite reach the product purities of the SMB.

Unmixed Reservoir System

We have developed a similar but simpler plug-flow reservoir that can be used when there is a small number of columns in the SMB, such as the (1,1,1,1) SMB (Figure 1). In this design a single unmixed tank packed with an inert packing (nonporous beads in this example) is used (Figure 2); however, the volume of the tank is constant and the variation in flow rates entering and exiting the column are accounted for by splitting the inlet and outlet streams into two different streams.

$$F = F_1 + F_2 \tag{1a}$$

$$D = D_1 + D_2 \tag{1b}$$

$$E = E_1 + E_2 \tag{1c}$$

$$R = R_1 + R_2 \tag{1d}$$

Subscript 1 indicates that the stream enters or leaves the adsorption column; subscript 2 indicates that the stream enters or leaves the unmixed reservoir (Figure 2); and F, D, R, and E are the feed, desorbent, raffinate, and extract flow rates from the SMB. For constant flow rates into and out of the reservoir,

$$T_1 + R_2 = T_4 + D_2 = T_3 + E_2 = T_2 + F_2 \tag{1e}$$

where T_i, the flow rate exiting the corresponding tank in the Analog with mixed tanks, can be calculated from simple mass balances.[12]

Splitting flows increases the degrees of freedom in the system. In a perfect plug-flow reservoir it doesn't matter if, for example, feed is introduced into band T2 as it enters the column or as it enters the reservoir. A similar splitting holds for addition of desorbent and for the removal of extract and raffinate. In practice (and in the simulations), the reservoir is not perfect plug-flow and there is a slight purity penalty involved in splitting the flow.

In order for the design to work, the following practical inequalities must also be satisfied:

$$F \le R, \quad E \le D \tag{2}$$

For an Analog to an SMB with one column per zone, there is a range of possible solutions for Eqs. 1 and 2. The two extremes of this range are:

Case I. When $F_2 = E_2 = 0$ (Figure 3)

$$F_1 = F \tag{3a}$$

$$R_1 = F \tag{3b}$$

$$E_1 = E \tag{3c}$$

$$D_1 = E_1 = E \tag{3d}$$

$$R_2 = R - R_1 = R - F \tag{3e}$$

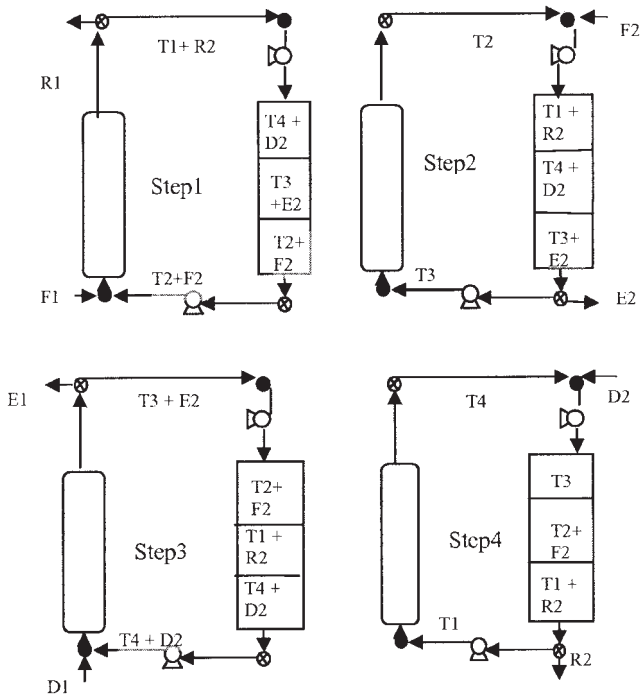

Figure 2. One column Analog with unmixed reservoir with all possible input and output streams.

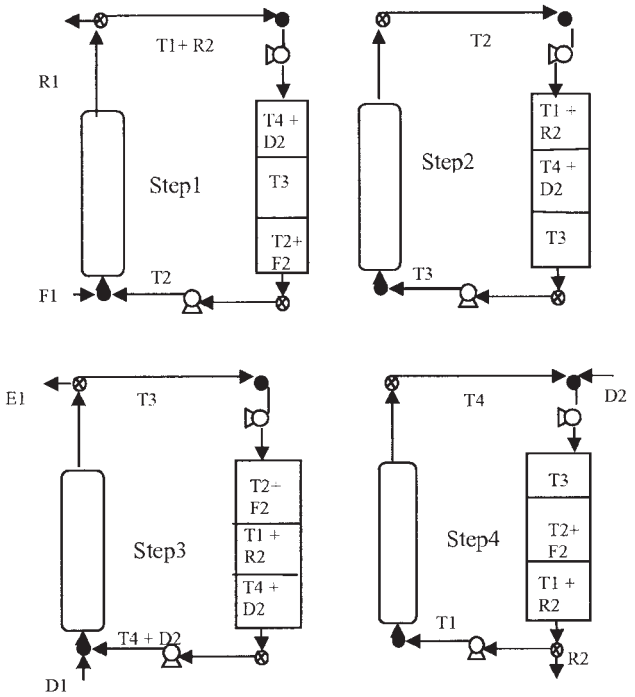

Figure 3. Analog with unmixed reservoir when $F_2 = E_2 = 0$.

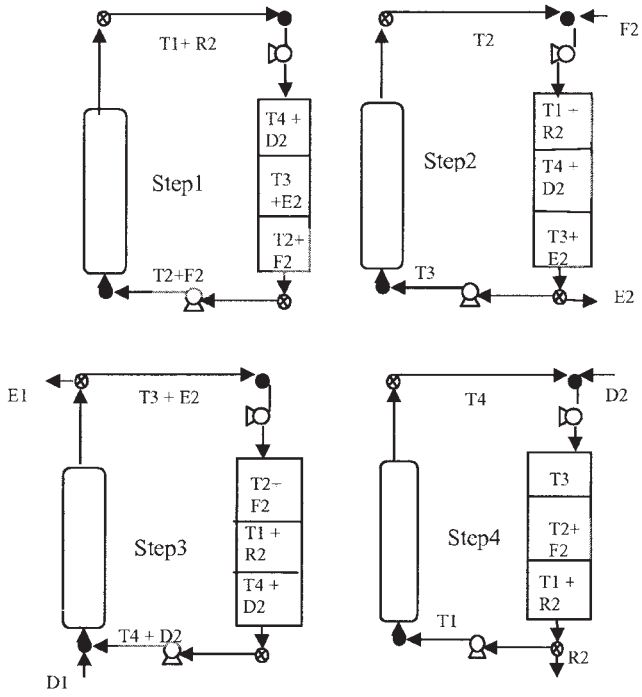

Figure 4. Analog with unmixed reservoir when $F_1 = R_1 = 0$.

$$D_2 = D - D_1 = R_2 \tag{3f}$$

$$\text{Volume of reservoir} = 3 * t_{sw} * (D_2 + \text{Recycle})$$
$$= 3 * t_{sw}(R - F + \text{Recycle}) \tag{3g}$$

Case II. $F_1 = R_1 = 0$ (Figure 4)

$$F_2 = F \tag{4a}$$

$$R_2 = R \tag{4b}$$

$$D_2 = R_2 = R \tag{4c}$$

$$D_1 = D - D_2 \tag{4d}$$

$$E_1 = D_1 \tag{4e}$$

$$E_2 = E - E_1 = F_2 \tag{4f}$$

$$\text{Volume of reservoir} = 3 * t_{sw} * (D_2 + \text{Recycle})$$
$$= 3 * t_{sw}(R + \text{Recycle}) \tag{4g}$$

The volume of the reservoir is smaller for Case I because D_2 is equal to only a fraction of the raffinate stream, while in Case II it is equal to the entire raffinate stream. For this reason the plug-flow setup in Case I will be used for further analysis.

This new unmixed reservoir design is limited to SMBs with a low number of columns because as the number of columns per zone increases, there are not enough variables (inlet and outlet streams) to keep the flow rate entering and exiting the unmixed reservoir equal while satisfying Eqs. 1a-e and 2. The (1,1,1,1) and (1,2,1,1) SMB configurations (Figures 1 and 5) can be mimicked. For Figure 5 the only set of equations satisfying Eqs. 1 and 2 is:

$$F_2 = E_2 = 0 \tag{5a}$$

$$F_1 = F \tag{5b}$$

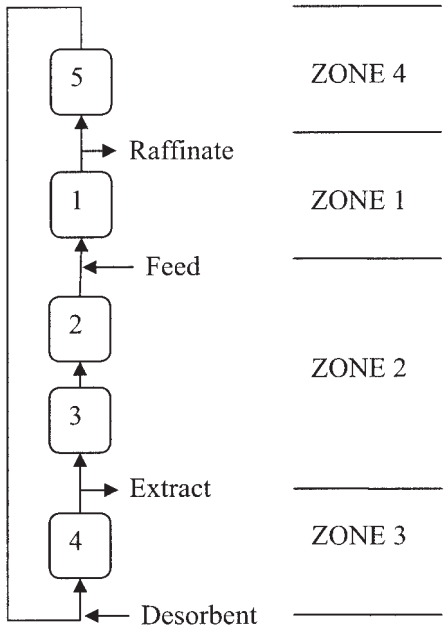

Figure 5. Four-zone (1,2,1,1) SMB.

Table 1. (1, 1, 1, 1) and (1, 2, 1, 1) SMB and Analog Column Specifications for the 1,1′ bi-2-Naphthol Systems[16]

System Parameters		
L_{col} (1, 11, 1)	21.0 cm	Length of columns
L_{col} (1, 2, 1, 1)	16.8 cm	Length of columns
D_{col}	26.0 cm	Diameter of columns
ε_e	0.40	External void fraction
ε_p	0	Internal void fraction
d_p	32 μm	Adsorbent particle diameter
ρ	0.6 g/mL	Liquid density
μ	0.876 cP	Liquid viscosity
$k_m a_p$ (A)	0.5 1/s	Mass-transfer coefficient
$k_m a_p$ (B)	0.5 1/s	Mass-transfer coefficient
L_{res}	75 cm	Length of reservoir
D_{res}	47.2 cm	Diameter of reservoir
$d_{p,res}$	100 microns	Particle diameter in reservoir
Operation Parameters		
Concentration of feed, $c_{F,i}$ i = A, B	2.9 & 10.0 g/L	Feed concentrations for all configurations
Feed flow rate	364 cm^3/min	Feed flow rate for all configurations
Feed purity	50% A, 50% B	

$$R_1 = F_1 = F \tag{5c}$$

$$E_1 = E \tag{5d}$$

$$D_1 = E_1 = E \tag{5e}$$

$$D_2 = D - D_1 \tag{5f}$$

$$R_2 = R - R_1 = D_1 \tag{5g}$$

$$\text{Volume of reservoir} = 4 * t_{sw} * (D_2 + \text{Recycle}) \tag{5h}$$

Other reservoir arrangements are under development.

These Analogs retain the advantage for operation of campaigns noted for the original design.[11] The chromatographic column and perhaps the reservoir will need to be repacked for each new campaign. This is simpler than for an SMB, where a number of chromatographic columns need to be repacked and must have identical residence times.

Simulations

The separation of the 1,1′ bi-2-naphthol enantiomers is used to study this new Analog. This is a system with nonlinear isotherms given by[15]:

$$q_A^* = \frac{2.69c_A}{1 + 0.0336c_A + 0.0466c_B} + \frac{0.10c_A}{1 + c_A + 3c_B} \tag{6a}$$

$$q_B^* = \frac{3.73c_A}{1 + 0.0336c_A + 0.0466c_B} + \frac{0.30c_A}{1 + c_A + 3c_B} \tag{6b}$$

The new analog design was tested in both the linear and nonlinear regions of these isotherms. Simulations were run using Aspen Chromatography v12.1 for the SMBs with one column per zone in the linear (c_f = 2.9 g/l) and nonlinear (c_f = 10.0 g/l) ranges at a D/F value of 5.56. The design and operating conditions followed those set by Jin and Wankat[16] (Tables 1 and 2). Analogs with mixed tanks and an unmixed reservoir were designed and simulated using the optimized SMB flow rates.

Table 2. (1, 1, 1, 1) and (1, 2, 1, 1) SMB and Analog Operating Conditions for the 1,1′ bi-2-Naphthol Systems[16]

	Values	
Conc. (g/L)	2.9	10.0
Feed rate (cm^3/min)	364	364
Recycle rate (cm^3/min)	2338.70	2902.46
Switching time (min) (1, 1, 1, 1)	8.06	6.36
Switching time (min) (1, 2, 1, 1)	6.45	5.09
Desorbent rate (cm^3/min)	2143.96	2143.96
Flow rate in zone I (cm^3/min)	2338.70	2902.46
Flow rate in zone II (cm^3/min)	3178.01	3456.45
Flow rate in zone III (cm^3/min)	2814.01	3092.45
Flow rate in zone IV (cm^3/min)	4482.66	5046.42
Raffinate rate (cm^3/min)	839.31	553.99
Extract rate (cm^3/min)	1668.66	1953.97
ΔP in zone I (bar)	1.11	1.38
ΔP in zone II (bar)	1.51	1.64
ΔP in zone III (bar)	1.34	1.47
ΔP in zone IV (bar)	2.13	2.40
Total ΔP (bar)	6.10	6.90

The results for these simulations are presented in Tables 3 and 4. As these tables show, the Analog with the unmixed reservoir had much higher purities and recoveries than the Analogs with the mixed tanks even when those tanks were split in half. The increase in purity was higher for the Analog run in the nonlinear region because solute velocities are concentration dependent in the nonlinear range. The velocities for the SMB operation were optimized based on a concentration profile entering the column, and included the changes in solute velocities as the concentration changed. These velocities will not be optimum for the Analog with mixed tanks because a constant concentration entered the column at each step. In the Analog with an unmixed reservoir, a concentration profile enters the column and the operation conditions are closer to those in the

Table 3. Results from the SMB and the Analogs for the (1, 1, 1, 1) Configuration for the 1,1′ bi-2-Naphthol Separation

	SMB	Analog with 4 Mixed Tanks	Analog with 8 Mixed Tanks	Analog with Unmixed Reservoir
c_F = 2.9 g/l (linear range) (1, 1, 1, 1)				
A purity (% A)	96.0	86.1	91.3	93.3
B purity (% B)	97.7	88.9	93.4	96.3
PI	96.9	87.5	92.3	94.8
A recovery (% A)	97.8	89.2	93.5	95.7
B recovery (% B)	95.9	85.7	95.7	93.8
c_F = 10.0 g/l (non-linear range) (1, 1, 1, 1)				
A purity (% A)	92.4	83.4	89.0	91.2
B purity (% B)	95.1	81.5	88.2	92.4
PI	93.8	82.4	88.6	91.8
A recovery (% A)	95.3	80.9	88.0	92.6
B recovery (% B)	92.2	84.0	89.1	91.1

Productivity = 8.16e-3 1/min.

Table 4. Results from the SMB and Analogs for the (1, 2, 1, 1) Configuration for the Separation of the 1,1′ bi-2-Naphthol System

	SMB	Analog with 5 Mixed Tanks	Analog with Unmixed Reservoir
c_F = 2.9 g/l (linear range) (1, 2, 1, 1)			
A purity (% A)	94.8	84.3	91.2
B purity (% B)	100	94.2	99.1
PI	97.4	89.2	95.1
A recovery (% A)	99.8	95.0	99.2
B recovery (% B)	94.8	82.4	90.4
c_F = 10.0 g/l (nonlinear range) (1, 2, 1, 1)			
A purity (% A)	90.0	80.7	87.8
B purity (% B)	98.3	83.9	90.4
PI	94.1	82.3	89.1
A recovery (% A)	98.6	84.7	93.9
B recovery (% B)	89.3	79.7	86.3

Productivity = 8.16e-3 1/min.

SMB. The purities in this new design and in Mota and Araujo's[14] design are less than the SMB purity because of dispersion in the reservoir, which was calculated in this study using the Chung and Wen[17] correlation. The particle size used here, d_p = 100 microns, is a practical size to pack, and does not cause an excessive pressure drop.

Mota and Araujo's[14] extensive study of dispersion in the reservoir showed that decreasing reservoir dispersion (such as by using smaller particles) always increases the Analog's purity; however, reducing this additive term never makes the Analog purity equal to the SMB purity. When a data register was used to store concentrations from the analog (equivalent to a perfect plug-flow reservoir), analog purities were identical to SMB purities.[14] One of the contributions of this article is to show that SMB purity can be matched by taking advantage of the Analog's inherently lower pressure drop.

Scaling of Analogs with Mixed Tanks and Unmixed Reservoirs

Scaling rules allow approximate, but usually quite accurate, prediction of a new design's performance based on a fully investigated base case and simple algebraic rules. The base case is assumed to have been designed either with detailed experiments or with appropriate techniques such as the Triangle theory[18] and simulations to obtain optimum or near optimum values of all flow rates. The scaling procedure is an appropriate next step since it explicitly includes mass transfer resistances and pressure drops. Scaling rules have been developed for chromatography[19] and the SMB.[20] Since the Analog is a cross between an SMB and a chromatograph, scaling rules for Analogs are expected to be similar. After developing the Analog scaling rules, these rules will be used to predict conditions necessary to first increase the purity of the Analog and then to increase the productivity. Complete simulations will then be used to check the results.

In order to scale any system, there must be an acceptable base case. Then by comparing the base case to the new case, the column dimensions, productivity, and so forth can be determined. The following assumptions were made for the adsorption column[20]:

- Axial dispersion due to eddy and molecular diffusivities (the $\partial^2 c/\partial z^2$ term in the mass balance) is negligible compared to the mass transfer resistances. Usually this assumption is close to valid in liquid systems.
- The particles in the adsorption column are rigid and have a constant porosity. This assumption can be relaxed if necessary.
- Constant physical properties.
- Properties of the adsorbent are not a function of particle size. This is not always true in practice.

Since the Analog was designed to mimic an SMB, the scaling rules are essentially identical to those used for SMBs.[20] The dimensions of the reservoirs (either mixed or unmixed) will be adjusted based on the flow rates, but the particle size in the unmixed reservoir was not scaled. A more detailed analysis is presented elsewhere.[21] First, the following ratios are defined for the adsorption column:

$$a = \frac{d_{p,new}}{d_{p,old}}, \quad b = \frac{L_{j,new}}{L_{j,old}}, \quad c = \frac{D_{col,new}}{D_{col,old}}, \quad g = \frac{Q_{j,new}}{Q_{j,old}} \quad \text{(7a-d)}$$

Then, for example, the velocity ratio can be calculated as:

$$\frac{v_{s,j,old}}{v_{s,j,new}} = \frac{Q_{j,old}}{Q_{j,new}}\left(\frac{D_{col,new}}{D_{col,old}}\right)^2 = \frac{c^2}{g} \quad \text{(7e)}$$

If ΔP is calculated using the Carmen-Kozney equation, then the ratio of pressure drops is:

$$R_p = \frac{\Delta P_{j,new}}{\Delta P_{j,old}} = \frac{bg}{a^2 c^2} \quad \text{(8a)}$$

If $R_P = 1$ the pressure drop in the new and base designs will be the same.

Since a simple relationship for the purity has not been identified, the fractional bed use in the adsorption column will be used as a surrogate. Fractional bed use is a function of the ratio of the bed length to the length of the mass transfer zone (L/L_{MTZ}). The value of the L_{MTZ} can be readily determined for nonlinear systems, which leads to the following rule:

$$R_N = \frac{(L/L_{MTZ})_{j,new}}{(L/L_{MTZ})_{j,old}} = \left(\frac{v_{s,j,old}}{v_{s,j,new}}\right)\left(\frac{L_{j,new}}{L_{j,old}}\right)\frac{(k_m a_p)_{new}}{(k_m a_p)_{old}} \quad \text{(8b)}$$

If $R_N = 1$ the fractional bed use will be the same in both the new and old design and, thus, product purities will be the same. The mass transfer coefficient $k_m a_p$ can often be correlated by[22]:

$$k_m a_p = k\,\frac{v_s^{1-n}}{d_p^{1+n}} \quad \text{(8c)}$$

where k is a constant. For pore diffusion control, which is very common in liquid systems, $n = 1$. Substituting Eq. 8c with $n = 1$ into 8b, R_N becomes:

$$R_N = \frac{(L/L_{MTZ})_{j,new}}{(L/L_{MTZ})_{j,old}} = \left(\frac{v_{s,j,old}}{v_{s,j,new}}\right)\left(\frac{L_{j,new}}{L_{j,old}}\right)\frac{(k_m a_p)_{new}}{(k_m a_p)_{old}}$$
$$= \left(\frac{v_{s,j,old}}{v_{s,j,new}}\right)\left(\frac{L_{j,new}}{L_{j,old}}\right)\left(\frac{d_{p,old}}{d_{p,new}}\right)^2 = \frac{bc^2}{a^2 g} \quad (8d)$$

The ratio of the adsorbent volumes in the new and old designs is:

$$R_V = \frac{(\text{adsorbent volume})_{j,new}}{(\text{adsorbent volume})_{j,old}} = bc^2 \quad (8e)$$

The switch time must also be scaled to keep the relative movements of the solutes equal. The ratio is a function of the velocities in the new and old designs:

$$R_{tsw} = \frac{t_{sw,new}}{t_{sw,old}} = \frac{(L_j/v_{s,j})_{new}}{(L_j/v_{s,j})_{old}} = \frac{bc^2}{g} = \frac{R_V}{g} \quad (8f)$$

The dead volume also affects the separation in an SMB[20,23] and must be scaled in the same way as the adsorbent volume:

$$R_D = \frac{(Q_j t_{sw}/V_D)_{new}}{(Q_j t_{sw}/V_D)_{old}} \quad (8g)$$

In the simulations used here, the dead volume was set equal to zero although it can easily be included. It may be difficult to set $R_D = 1$ if the new column uses a much smaller particle size than the old column because the smaller switching time t_{sw} in the new column will require a decrease in the dead volume.

The validity of applying these scaling rules to SMB systems was illustrated with a large number of simulations.[20] The validity of these rules for both the Analog with mixed tanks and the Analog with an unmixed reservoir was tested using the separation of the 1,1′ bi-2-naphthol enantiomers. The separations in Tables 1 and 2 were used as the base cases. Since the SMBs used for comparison follow standard practice and have only one pump in the recycle stream, the maximum allowable pressure drop for the SMB is the sum of the pressure drops in all the columns. The use of an unusual pump arrangement that places additional pumps in the SMB's recycle stream is explored in detail by Jin and Wankat.[16] The column dimensions, particle size, pressure drop, flow rates, and switching time were varied using the rules in Eqs. 8a-g while keeping $R_N = 1$. The results of these simulations are given in Table 5. Because of the way the systems are scaled, the volume of fluid that is processed per cycle remains constant, and the volumes of the mixed tanks and unmixed reservoirs do not change. This holds for all of the scaling procedures used in this article.

For cases 1 and 2 in Table 5, the column dimensions and pressure drop were scaled. The results of the simulations show that there was very little change in the purity indices. Case 3 shows the effect of changing the column dimensions, pressure drop, particle size, and switch time; again, there was little change to the purity indices. Cases 4 and 5 show that there was little effect on the separation when large changes were made to the switching times, column dimensions, and velocity. Therefore, it can be concluded that the scaling rules are valid for the Analogs with mixed tanks and unmixed reservoirs within the variable range considered.

Table 5. Results of Applying General Scaling Rules to the Analogs for the Separation of the 1,1′ bi-2-Naphthol System, $R_N = 1.0$

Case	Basis	1	2	3	4	5
$a = d_{p,new}/d_{p,old}$	1	1	1	0.954	2	0.5
$b = L_{new}/L_{old}$	1	0.707	0.354	1	4	5
$c = D_{col,new}/D_{col,old}$	1	1.189	1.682	1	1	2.236
$g = Q_{new}/Q_{old}$	1	1	1	1.1	1	100
R_p	1	1/2	1/8	1.21	1	1
$t_{sw,new}/t_{sw,old}$	1	1	1	0.909	4	0.25
c_F = 2.9 g/l Mixed Four Tanks (linear region) (1, 1, 1, 1)						
A purity (%)	86.1	86.0	86.1	86.4	86.2	86.3
B purity (%)	88.9	89.0	88.2	89.0	89.2	89.1
PI	87.5	87.5	87.1	87.7	87.7	87.7
c_F = 10 g/l Mixed Four Tanks (non-linear region) (1, 1, 1, 1)						
A purity (%)	83.4	83.3	83.5	83.5	83.5	83.5
B purity (%)	81.5	80.9	80.9	81.5	81.7	81.8
PI	82.4	82.1	82.2	82.5	82.6	82.7
c_F = 2.9 g/l Unmixed Reservoir (linear region) (1, 1, 1, 1)						
A purity (%)	93.3	93.9	94.0	94.0	94.1	94.0
B purity (%)	96.3	96.3	96.0	96.3	96.4	96.4
PI	94.8	95.1	95.0	95.1	95.2	95.2
c_F = 10 g/l Unmixed Reservoir (linear region) (1, 1, 1, 1)						
A purity (%)	91.2	91.1	91.5	91.2	91.3	91.2
B purity (%)	92.4	92.4	92.1	92.4	92.5	92.5
PI	91.8	91.8	91.8	91.8	91.9	91.9

The scaling rules were also used to improve the separation in the Analogs with the unmixed reservoir so that they matched the separation in the SMBs in Tables 3 and 4. First, a series of scaled simulations was done to relate R_N to the purity index (Figure 6), and the value of R_N required to match the SMB purity index was determined from this figure. Then the system was scaled with the required value of R_N while keeping the particle size and column dimensions constant, that is, $a = b = c = 1$. Substituting $a = b = c = 1$ into Eqs. 8a-g gives $R_N = R_{tsw} = 1/g$ and $R_p = g$. Comparing the scaled results in Table 6 to those for the SMBs in Tables 3 and 4, it can be seen that the purity indices match closely; however, the productivities in the Analogs are now significantly lower than that of the corresponding SMBs. This reduction in productivity will next be eliminated at constant purity by taking advantage of the maximum available pressure drop.

Utilization of Available Pressure Drop in Analogs

In the standard SMB with one pump in the recycle stream, the feed end of zone 3 (Figure 1) can be designed to operate at the pressure limit, but none of the other zones are operating at the maximum allowable pressure. The Analog, on the other hand, has only one column and the reservoir and the total pressure drop can be used. This will increase productivity without any effect on the product purities if correct scaling is used (Eqs. 8a-j). Additional increases in ΔP and, hence, productivity can be obtained be adding a booster pump immedi-

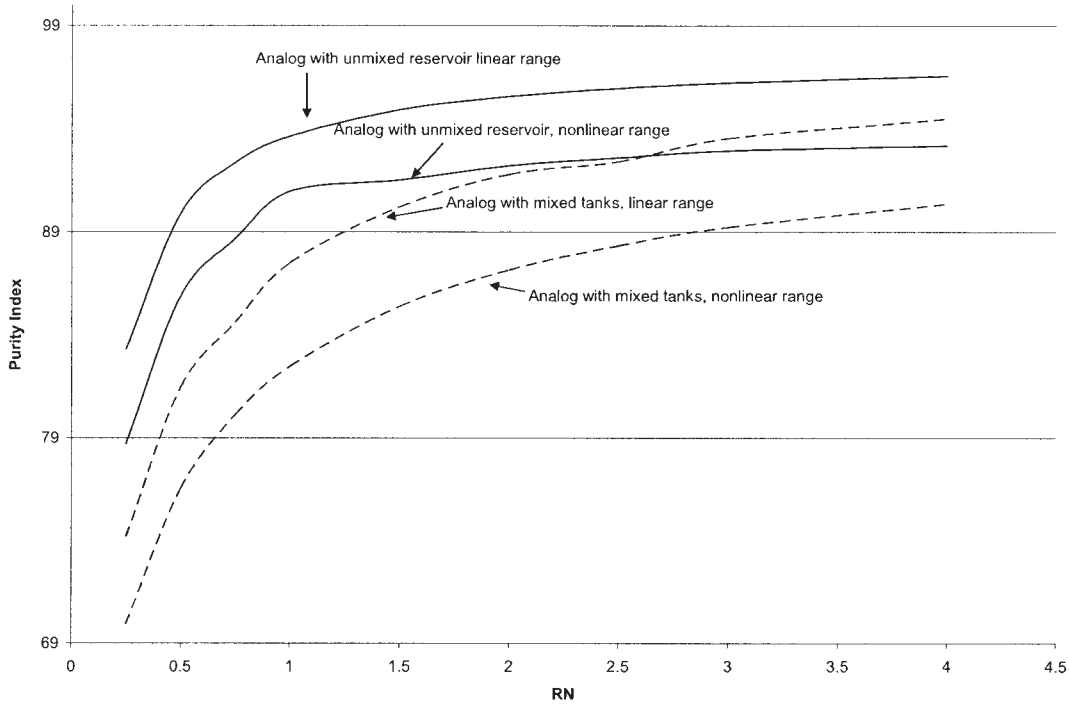

Figure 6. R_N versus Purity Index ($a = b = c = 1$) for Analogs separating 1,1′ bi-2-naphthols.

ately before the reservoir. When this was done, the reservoirs never reached their pressure drop limits in any of the calculations in this article.

Jin and Wankat[16] applied a similar idea to a 4-zone SMB and a 2-zone SMB that has two steps per switching time. With two recycle pumps for the 2-zone SMB and four recycle pumps for the 4-zone SMB, they showed a significant increase in productivity for both systems. Since the standard SMB operates with a constant switching time and the flow rates in each zone are different, only the zone with the highest flow rate can be operated at the maximum pressure drop. The two-zone SMB has the advantage that each step can have a different period, which allows each step to operate at the maximum allowable pressure drop and, hence, the maximum velocity. Scaling the 2-zone SMB for this asymmetric cycle required use of heuristic scaling rules, but allowed it to match the product purities of the corresponding 4-zone SMB with higher productivity. A 4-zone SMB with two columns per zone and eight pumps in the recycle line was able to produce higher purities than the 2-zone SMB.[16] Heuristic scaling rules will also be developed for Analogs with asymmetric cycles.

Table 6. Scaling of Analogs with Unmixed Reservoirs to Match the SMB Purities for the Separation of the 1,1′ bi-2-Naphthol System

Case	Linear (1, 1, 1, 1)	Nonlinear (1, 1, 1, 1)	Linear (1, 2, 1, 1)	Nonlinear (1, 2, 1, 1)
$a = d_{p,new}/d_{p,old}$	1	1	1	1
$b = L_{new}/L_{old}$	1	1	1	1
$c = D_{col,new}/D_{col,old}$	1	1	1	1
$g = Q_{new}/Q_{old}$	0.333	0.286	0.333	0.143
R_p	0.333	0.286	0.333	0.143
R_N	3	3.5	3	7
$t_{sw,new}/t_{sw,old}$	3	3.5	3	7
$R_{productivity}$	0.333	0.286	0.333	0.143
ΔP_1 (bar)	0.498	0.464	0.498	0.232
ΔP_2 (bar)	0.440	0.415	0.440	0.208
ΔP_3 (bar)	0.702	0.677	0.702	0.339
ΔP_4 (bar)	0.366	0.389	0.366	0.195
Productivity (1/min)	2.72e-3	2.33e-3	2.72e-3	1.17e-3
A purity (%)	96.4	92.8	95.0	90.0
B purity (%)	97.6	94.7	99.8	97.6
Purity index	97.0	93.8	97.4	94.2
A recovery (%)	97.6	94.8	99.8	97.9
B recovery (%)	96.3	92.6	94.7	89.9

See also Figure 6.

Increasing the Pressure Drop in Zone 3 to the Maximum Pressure Drop

In the 4-zone SMBs (Figures 1 and 5) and their corresponding Analogs, zone 3 (the desorption zone) has the highest pressure drop. In order to ensure that none of the zones operate above the maximum pressure drop allowable, the Analog will first be scaled to have zone 3 operating at this maximum pressure. The pressure drop for the reservoir is supplied by the booster pump. Since we assume an existing system or off-the-shelf equipment is being used, the column dimensions are constant, but the adsorption columns can be packed with any size packing. The base cases for the Analogs with the mixed tanks are the cases in Tables 3 and 4, and for the Analogs with the unmixed reservoir the base cases are those in Table 6. The maximum pressure drop ΔP_{max} was arbitrarily set at 15 bars.

The scaling procedure is as follows.

First, substitute $R_{N,3} = 1$, $b = 1$, and $c = 1$ into Eqs. 8a and 8d:

$$R_{P,3} = \frac{\Delta P_{MAX}}{\Delta P_3} = \frac{g_3}{a^2} \tag{9}$$

Table 7. Results of Scaling SMBs to Operate so That $\Sigma\Delta P_i = \Delta P_{max}$ and Analogs so That Zone 3 Operates at Maximum Pressure Drop of 15 Bars for the 1,1′ bi-2-Naphthol Separation

Case	Analog Linear Mixed (1, 1, 1, 1)	Analog Nonlinear Mixed (1, 1, 1, 1)	Analog Linear Unmixed (1, 1, 1, 1)	Analog Nonlinear Unmixed (1, 1, 1, 1)	Scaled SMB (1, 1, 1, 1) $\Sigma\Delta P_i = \Delta P_{max}$ (Linear)	Scaled SMB (1, 1, 1, 1) $\Sigma\Delta P_i = \Delta P_{max}$ (Nonlinear)
$a = d_{p,new}/d_{p,old}$	0.612	0.630	0.465	0.461	0.799	0.823
$b = L_{new}/L_{old}$	1	1	1	1	1	1
$c = D_{col,new}/D_{col,old}$	1	1	1	1	1	1
$g_3 = Q_{new}/Q_{old}$	2.67	2.52	4.62	4.71	$g = 1.57$	$g = 1.47$
R_{p3}	7.13	6.33	21.4	22.15	—	—
R_N	1	1	1	1	1	1
ΔP_1 (bar)	10.6	10.3	10.6	10.3	3.67	3.53
ΔP_2 (bar)	9.42	9.19	9.42	9.19	3.30	3.16
ΔP_3 (bar)	15	15	15	15	5.20	5.15
ΔP_4 (bar)	7.83	8.63	7.83	8.63	2.70	2.96
$R_{productivity}$	2.67	2.51	1.54	1.34	—	—
$t_{sw,new}$, min	9.07	8.84	5.22	4.72	5.14	4.31
Productivity (1/min)	0.0218	0.0205	0.0126	0.011	0.0128	0.0120
A purity (%)	86.2	83.5	96.4	92.8	96.0	92.4
B purity (%)	89.0	81.6	97.6	94.7	97.7	95.1
PI	87.6	82.5	97.0	93.8	96.9	93.8

$$R_{N,3} = 1 = \frac{1}{a^2 g_3} \tag{10}$$

Solving simultaneously gives:

$$a = (1/R_{P,3})^{(1/4)} \tag{11}$$

$$g_3 = 1/a^2 \tag{12}$$

Substitute Eq. 10 into 8f:

$$t_{sw,new} = \frac{1}{g_3} t_{sw,old} \tag{13}$$

The productivity ratio can be defined to compare the productivity of the Analogs to the corresponding SMBs. For the Analogs with mixed tanks:

$$R_{productivity} = \frac{F_{new}}{F_{old}} = g_{3,mixed} \tag{14}$$

For the Analogs with an unmixed reservoir, we want to compare to the original SMB and not to the Analog scaled to match the SMB purities; therefore:

$$R_{productivity} = \frac{F_{new,Analog}}{F_{SMB}} = g_{3,unmixed} \tag{15}$$

Scale all the flow rates using g_3 with a constant switch time. The results of applying this scaling to the Analogs to the 4-zone SMB with one column per zone are given in Table 7. The product purities (purity indices) are essentially identical to the base cases, with a significant increase in productivity. It should also be noted that the productivity in the Analogs with the unmixed reservoirs is now higher than that in the SMBs in Table 3 but slightly lower than the productivity of the SMB with one pump operating at ΔP_{max} (Table 7). However, the product purities are similar, significantly less equipment is required for the Analog, and the Analog is more flexible than an SMB.

Scaling Procedure for Increasing the Pressure Drop in All Zones to the Maximum Allowable Pressure Drop

It is possible to further increase the productivity of the Analog by scaling the flow rates so that each zone is operated at the maximum allowable pressure drop. Pressure drop can be increased by reducing the particle size and/or by reducing the step times for zones 1, 2, and 4, which causes the flow rates to increase during these steps. The scaling rules show how to balance the reduction in particle size and the increase in velocity to achieve the desired increase in pressure drop while keeping purity constant. Because the cycle is no longer symmetrical (step times are different), the scaling rules need to be modified. The following ratios will be defined:

$$R_{pi} = \left(\frac{\Delta P_{max}}{\Delta P_{i,old}}\right), \quad i = 1, 4 \text{ (because there are four zones)} \tag{16}$$

$$R_{Ni} = \left(\frac{(L/L_{MTZ})_{i,new}}{(L/L_{MTZ})_{i,old}}\right), \quad i = 1, 4 \tag{17}$$

$$g_i = \frac{Q_{i,new}}{Q_{i,old}}, \quad i = 1, 4 \tag{18}$$

The average R_N can be defined by either the arithmetic or geometric mean as follows:

$$R_{N,avg,arith} = \frac{R_{N,1} + R_{N,2} + R_{N,3} + R_{N,4}}{4} \tag{19a}$$

$$R_{N,avg,geom} = R_{N,1} \times R_{N,2} \times R_{N,3} \times R_{N,4} \tag{19b}$$

Substituting Eqs. 8a and 8d into Eqs. 16 and 17:

$$R_{Pi} = \frac{bg_i}{a^2c^2}, \quad i = 1, 4 \tag{21}$$

$$R_{Ni} = \frac{bc^2}{a^2g_i}, \quad i = 1, 4 \tag{22}$$

The step time can now be calculated using:

$$R_{t,i} = \frac{t_{i,new}}{t_{sw,old}} = \frac{bc^2}{g_i}, \quad i = 1, 4 \tag{23}$$

Since the new design proposed here will use the same equipment as the old design, $b = c = 1$, then:

$$g_i = a^2R_{Pi}, \quad i = 1, 4 \tag{24}$$

$$R_{Ni} = a^2g_i, \quad i = 1, 4 \tag{25}$$

Unfortunately, if $R_{N,I} = 1$, for i = 1,4, the system will be over constrained. Instead, require that the average $R_{N,avg,arith}$ or $R_{N,avg,geom} = 1$. Our hypothesis is that when $R_{N,avg} = 1$ the purities of the new design will match the purities of the old design. This constraint is a heuristic and is not guaranteed to keep the purity indices constant; however, the simulations show that this approximate procedure works for this example.

Since there are two different averages that can be used, there will be a different set of equations to solve for each case.

Procedure I: Using the arithmetic average, $R_{N,avg,arith}$:
Substituting Eq. 22 into Eq. 17:

$$\left(\frac{1}{4}\right) \times \left(\frac{1}{a^2g_1} + \frac{1}{a^2g_2} + \frac{1}{a^2g_3} + \frac{1}{a^2g_4}\right) = 1 \tag{26}$$

Substituting for g_i from Eq. 24 and solving for a gives:

$$a = \left[\frac{1}{4} \times \left(\frac{1}{R_{P,1}} + \frac{1}{R_{P,2}} + \frac{1}{R_{P,3}} + \frac{1}{R_{P,4}}\right)\right]^{1/4} \tag{27}$$

Then Eq. 18 becomes:

$$g_i = \left[\frac{1}{4} \times \left(\frac{1}{R_{P,1}} + \frac{1}{R_{P,2}} + \frac{1}{R_{P,3}} + \frac{1}{R_{P,4}}\right)\right]^{1/2} R_{P,i} \tag{28}$$

And the step time is calculated by:

$$t_i = \left[\left[\frac{1}{4} \times \left(\frac{1}{R_{P,1}} + \frac{1}{R_{P,2}} + \frac{1}{R_{P,3}} + \frac{1}{R_{P,4}}\right)\right]^{1/2} R_{P,i}\right]^{-1} \times t_{sw,old} \tag{29}$$

Procedure II: Using the geometric mean, $R_{N,avg,geom}$
Substituting Eq. 22 into Eq. 17 gives:

$$\frac{1}{a^2g_1} \times \frac{1}{a^2g_2} \times \frac{1}{a^2g_3} \times \frac{1}{a^2g_2} = 1 \tag{30}$$

Substituting for g_i from Eq. 24 and solving for a gives:

$$a = \left(\frac{1}{R_{P,1} \times R_{P,2} \times R_{P,3} \times R_{P,4}}\right)^{1/16} \tag{31}$$

Then Eq. 18 becomes:

$$g_i = \left(\frac{1}{R_{P,1} \times R_{P,2} \times R_{P,3} \times R_{P,4}}\right)^{1/8} R_{P,i} \tag{32}$$

And the step time can be calculated using:

$$t_i = \left[\left(\frac{1}{R_{P,1} \times R_{P,2} \times R_{P,3} \times R_{P,4}}\right)^{1/8} R_{P,i}\right]^{-1} \times t_{sw,old} \tag{33}$$

Both of the procedures were applied to the Analog with an unmixed reservoir in the linear range. The purity index was 96.8 for both procedures, while the purity index of the base case was 96.9. Procedure (II) was arbitrarily chosen. The results of the application of the scaling using procedure (II) on the Analogs with unmixed reservoirs for both the (1,1,1,1) and (1,2,1,1) configurations are given in Table 8. Comparison of the results for the (1,1,1,1) configuration in Table 8 for the Analog with the SMB results in Table 7 shows that now the productivity in the Analogs is higher than in the standard SMBs by 15.6% for the linear results and by 11.7% in the nonlinear range while the purities remained essentially constant. It is also interesting to compare these results to a scaled SMB with four pumps in the recycle line so that zone 3 operates at a pressure drop of 15 bar. In the linear region with 19.7 μm particle diameter Jin and Wankat[16] obtained PI = 97.3 with productivity = 0.0217 min^{-1} and in the nonlinear region with 20.2 μm particle diameter, PI = 94.5 with productivity = 0.0204. Thus, the more complicated SMB with additional pumps in the recycle line has slightly higher PI and significantly higher productivities.

Comparison of the results for the (1,2,1,1) configuration for the Analog and the SMB, both presented in Table 8, show the Analog productivity is higher (15.6 and 16.1%, in the linear and nonlinear ranges, respectively) but the PI values are slightly lower than the SMB values (0.2 and 0.3%).

The asymmetric scaling procedure was also applied to the Analog with mixed tanks.[21] The use of one tank per SMB column was not sufficient and a huge reduction in the product purities resulted. When the tanks were split in half, the purity indices closely matched the base analogs (Table 3), and the productivity of the scaled Analogs increased by a factor of approximately 3.8 for both the linear and nonlinear ranges. We were unable to match the purity of the SMB with Analogs with two mixed tanks per SMB column.

Jin and Wankat[16] showed that it is possible to increase the productivity in the SMB by adding booster pumps in the recycle stream while scaling to keep purity constant. It does not appear possible to scale the Analog with an unmixed reservoir to match the productivity of the SMB with four booster pumps;

Table 8. Results of Scaling the SMB to Operate so That $\Sigma\Delta P_i = \Delta P_{max}$ and Analogs with Unmixed Reservoirs so That They Operate at $\Delta P_{max} = 15$ Bar in Each Step for the 1,1′ bi-2-Naphthol System

Case	Analog Linear (1, 1, 1, 1)	Analog Nonlinear (1, 1, 1, 1)	Analog Linear (1, 2, 1, 1)	Analog Nonlinear (1, 2, 1, 1)	Scaled SMB (1, 2, 1, 1) $\Sigma\Delta P_i = \Delta P_{max}$ (Linear)	Scaled SMB (1, 2, 1, 1) $\Sigma\Delta P_i = \Delta P_{max}$ (Nonlinear)
$a = d_{p,new}/d_{p,old}$	0.424	0.422	0.424	0.355	0.799	0.823
$b = L_{new}/L_{old}$	1	1	1	1	1	1
$c = D_{col,new}/D_{col,old}$	1	1	1	1	1	1
$g_1 = Q_{new,1}/Q_{old,1}$	5.43	5.75	5.43	8.14	$g = 1.57$	$g = 1.47$
$g_2 = Q_{new,2}/Q_{old,2}$	6.14	6.43	6.14	9.09	—	—
$g_3 = Q_{new,3}/Q_{old,3}$	3.85	3.94	3.85	5.57	—	—
$g_4 = Q_{new,4}/Q_{old,4}$	7.38	6.85	7.38	9.69	—	—
R_{p1}	30.1	32.3	30.1	64.7	3.67	3.53
R_{p2}	34.0	36.1	34.0	72.3	3.30	3.16
R_{p3}	21.4	22.1	21.4	44.3	5.20	5.15
R_{p4}	41.0	38.5	41.0	77.0	2.70	2.96
R_{Nt}	1	1	1	1	1	1
$R_{productivity}$	1.81	1.64	1.81	1.16	—	—
$t_{sw,new,1}$, min	4.45	3.87	4.45	5.48	5.14	4.31
$t_{sw,new,2}$, min	3.94	3.45	3.94	4.90	5.14	4.31
$t_{sw,new,3}$, min	6.29	5.65	6.29	7.97	5.14	4.31
$t_{sw,new,4}$, min	3.26	3.25	3.26	4.59	5.14	4.31
Productivity	0.0148	0.0134	0.0148	0.00947	0.0128	0.00816
A purity (%)	96.3	92.9	94.8	90.8	94.8	90.0
B purity (%)	97.4	94.4	99.7	97.3	100	98.3
PI	96.9	93.7	97.2	93.8	97.4	94.1
A recovery (%)	97.4	94.5	99.7	97.6	99.8	98.6
B recovery (%)	96.2	92.7	94.6	90.0	94.8	89.3

however, an SMB with four booster pumps is a more complicated system requiring novel engineering design. Because of the significant differences in the systems, a fair comparison will require a detailed economic analysis.

Application of Scaling Procedure to Glucose-Fructose Separation

Table 9 gives the operating conditions for the separation of glucose from fructose. This system has linear isotherms, $q = Kc$, where q and c are in g/l, the mass transfer driving force is Δc, and the initial particle size is large compared to the size used in the separation of the 1,1′ bi-2-naphthol enantiomers (200 microns versus 32 microns). An Analog with an unmixed reservoir was designed for this system. The results for the SMB and the Analog are in Table 10. The same procedure used for the 1,1′ bi-2-naphthol system was used here; the Analog was scaled to increase the purity index to match the SMB purity index but at lower productivity (Table 11), and then procedure (II) was used to scale each step so that it operates at the maximum pressure drop (15 bar) to increase productivity (Table 12). The SMB was scaled for standard operating procedure (one pump in the recycle line) with the sum of column pressure drops equal to 15 bar. The scaling procedure increased the productivity in the Analog so that it is significantly higher than the SMB while keeping the average purity constant, and the particle size is still reasonably large at about 100 microns.

Discussion and Conclusions

It has been shown that an Analog with a single unmixed reservoir can be designed for SMBs with a low number of columns. The unmixed Analog has higher purities than the Analog with mixed tanks; however, due to dispersion in the unmixed reservoir, the purities are less than the corresponding SMBs. The purity index of the SMB can be matched by reducing the flow rates, and thus the productivities, in the unmixed Analogs using the scaling rules. We can then increase this productivity so that it is higher than that of the standard SMB without changing the PI by using the scaling rules a second time to allow each step of the Analog to operate at the maximum pressure drop allowable.

Table 9. Operating Conditions for the Separation of a 50%–50% Mixture of Glucose and Fructose[16]

4-Zone SMB Configuration	1, 1, 1, 1
Columns length, L (cm)	100
Column diameter, D_{col} (cm)	60
d_p (μm)	200
$k_m a_p$ (Glucose) (1/s)	0.045
$k_m a_p$ (Fructose) (1/s)	0.032
K_{GL}	0.18
K_{FR}	0.50
ε_e	0.4
ε_p	0.1
ρ_l (g/mL)	1.0
μ (cP)	0.8
L_{res} (cm)	200
D_{res} (cm)	83.2
$d_{p,res}$ (micron)	200
Switch time t_{sw} (s)	84
Feed concentration c_F (g/L)	40
Feed flow rate (L/min)	14.03
Desorbent flow rate (L/min)	55.35
Recycle flow rate (L/min)	100.18
Raffinate flow rate (L/min)	30.30
Extract flow rate (L/min)	39.07
D/F	3.9
R_{p1} (bar)	0.640
R_{p2} (bar)	0.572
R_{p3} (bar)	0.763
R_{p4} (bar)	0.492

Table 10. Results of the Separation of Glucose from Fructose in a (1, 1, 1, 1) SMB and Its Analog With an Unmixed Reservoir Before Scaling

	SMB	Analog with Unmixed Reservoir
Raffinate (% glucose)	79.1	77.6
Extract (% fructose)	91.2	87.4
PI	85.2	82.5
Glucose recovery (%)	92.9	89.3
Fructose recovery (%)	75.4	74.2

Productivity = 0.0124e (1/min).

This new Analog design is promising because it greatly reduces the amount of equipment used and retains most of the flexibility of the Analog with mixed tanks, while achieving the same PI as the standard SMB at productivities that are 11 to 15% higher than standard SMBs that have one pump in the recycle stream and a sum of column pressure drops equal to 15 bar.

If the Analog with mixed tanks is to be used in campaigns, it is quite simple to design it so that it will work for several different separations where the flow rates may change. Simply design the tanks so that their volumes are large enough to accommodate the highest flow rates that will be used in any of the campaigns, with some room for adjustment of these flow rates if need be. The larger tanks will not affect the separation. In the case of the unmixed reservoir, a flexible design is trickier. Table 13 shows the ratio of the reservoir volume to the feed flow rate versus the ratio of F_1/F_2 for the 1,1′ bi-2-naphthol system operating in the linear range. As was noted earlier, depending on how the streams are split, the volume of the reservoir changes. If all the feed were added to the column or to the reservoir, it would be difficult to account for small changes in the feed flow rate without changing the reservoir volume. It would, therefore, be good practice to design the Analog so that the reservoir is the average volume. For example, if the Analog was designed with both an F_1 and F_2 stream, then if the feed flow rate was reduced by 5%, and only the raffinate stream was affected by this change, all one would need to do would be to reduce both F_1 and R_1 by 0.05F, and the volume of the reservoir would be unaffected. If, however, a more drastic change in flow rates occurs, such as is likely when a new campaign is conducted, the volume of the reservoir would have to be changed. This is easily accomplished if the reservoir is designed as a column with a movable piston so that the packed volume can be adjusted. When the reservoir volume is changed, the reservoir would have to be repacked to the desired volume.

Obviously, one expects to change the packing and repack the chromatographic column for a new campaign. When this is done for an SMB, all columns have to have essentially identical retention times, which may require significant effort. The Analog column has to be well-packed, but since the same column is used for all steps it is automatically identical in all steps. Thus, Analogs with either mixed or unmixed reservoirs are a flexible system that should be useful in campaigns.

Table 11. Scaling of Analog with Unmixed Reservoir to Match SMB Purities for the Glucose-Fructose Separation

Case	
$a = d_{p,new}/d_{p,old}$	1
$b = L_{new}/L_{old}$	1
$c = D_{col,new}/D_{col,old}$	1
$g = Q_{new}/Q_{old}$	0.714
R_p	0.714
R_N	1.4
$R_{productivity}$	0.715
$t_{sw,new}/t_{sw,old}$	1.4
ΔP_1 (bar)	0.915
ΔP_2 (bar)	0.817
ΔP_3 (bar)	1.09
ΔP_4 (bar)	0.702
ΔP_{total} (bar)	3.52
Productivity, min^{-1}	0.00886
Glucose purity (%)	81.6
Fructose purity (%)	89.1
PI	85.3
Glucose recovery (%)	90.3
Fructose recovery (%)	79.5

Table 12. Results of Scaling the SMB to Operate so That $\Sigma\Delta P_i = \Delta P_{max}$ and Analog with an Unmixed Reservoir to Operate at the Maximum Pressure Drop in Each Step for the Glucose-Fructose Separation

Case	Unmixed Analog	Scaled SMB (1, 1, 1, 1) $\Sigma\Delta P_i = \Delta P_{max}$
$a = d_{p,new}/d_{p,old}$	0.490	0.760
$b = L_{new}/L_{old}$	1	1
$c = D_{col,new}/D_{col,old}$	1	1
$g_1 = Q_{new,1}/Q_{old,1}$	3.95	$g = 1.73$
$g_2 = Q_{new,2}/Q_{old,2}$	4.42	—
$g_3 = Q_{new,3}/Q_{old,3}$	3.31	—
$g_4 = Q_{new,4}/Q_{old,4}$	5.14	—
R_{p1}	16.4	$R_p = 15$
R_{p2}	18.4	—
R_{p3}	13.8	—
R_{p4}	21.3	—
R_{Nt}	1	1
$R_{productivity}$	2.82	
$t_{sw,new,1}/t_{sw,old}$	0.253	0.808
$t_{sw,new,2}/t_{sw,old}$	0.226	0.808
$t_{sw,new,3}/t_{sw,old}$	0.302	0.808
$t_{sw,new,4}/t_{sw,old}$	0.194	0.808
Productivity, min^{-1}	0.0350	0.0215
Glucose purity (%)	81.5	79.1
Fructose purity (%)	89.1	91.2
PI	85.3	85.2
Glucose recovery (%)	90.3	92.8
Fructose recovery (%)	79.5	75.6

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Table 13. Effect of Flow Rates on the Volume of the Unmixed Reservoir for the Separation of the 1,1′ bi-2-Naphthol System in the Linear Range

Volume of Reservoir/Feed Rate	F_1/F_2
187	Infinity
190	7
193	3
195	1
202	0.6
205	0.333
208	0.143
211	0

Notation

a, b, c, g = ratios defined in Eqs. 7a-d
c_i = concentration of species *i* (g/l)
D = desorbent flow rate, cm^3/min
D_{col} = column diameter, cm
d_p = particle diameter, cm
E = extract flow rate, cm^3/min
F = feed flow rate, cm^3/min
$k_m a_p$ = lumped parameter mass transfer coefficient, 1/min
L_j = column length, cm
L_{MTZ} = Length of the mass transfer zone, cm
q_i = amount of species *i* adsorbed
Q_j = flow rate in zone j, cm^3/min
R = raffinate flow rate, cm^3/min
Recycle = recycle flow rate, cm^3/min
R_D = ratio of dead volumes, Eq. 8g
R_N = ratio of the L/L_{MTZ}
$R_{N,\ avg,\ arith}$ = arithmetic average of R_N defined in Eq. 19a
$R_{N,\ avg,\ geom}$ = geometric average of R_N defined in Eq. 19b
R_P = ratio of pressure drops, Eq. 8a
$R_{productivity}$ = ratio of productivities, Eq. 14
R_{tsw} = ratio of switch times, Eq. 8f
R_V = ratio of adsorbent volumes, Eq. 8e
t_{sw} = switch time, min
T_i = flow rate exiting corresponding tank in Analog, cm^3/min
V_D = dead volume, cm^3
v_s = superficial velocity, cm/min
ΔP = pressure drop, bar

Definitions

Productivity = feed flow rate/adsorbent volume
Purity index (PI) = (% A in Raffinate + % B in Extract)/2
% increase in purity = 100* (new purity − base purity)/base purity

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