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Ternary Separations with One-Column Analogs to SMB

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Abstract: Analogs, recycled chromatography systems that mimic SMBs, for both a cascade of two four-zone SMBs and five-zone SMBs performing ternary separations are designed and analyzed. The basic Analog consists of one column and several mixed tanks equal to the number of columns in the mimicked SMB. Analogs with mixed tanks give lower purities than the SMBs because of mixing in the tanks. For example, the five-zone SMB with one column per zone achieved a purity index (PI) of 88.3, while the Analog with five mixed tanks has a PI of 83.4. If the tanks are divided into smaller tanks the purity improves, and for the Analog to be the five-zone SMB using 10 tanks the PI was 85.4. Analogs with a single unmixed reservoir were also designed for a cascade of two four-zone SMBs with one column per zone. This reservoir reduces the mixing and improves the separation. For example, a cascade of two four-SMBs with one column per zone achieved a PI of 86.7; the Analog to this SMB with 8 mixed tanks achieved a PI of 82.9, while the Analog with an unmixed reservoir achieved a PI of 84.6.

Keywords: SMB, analog, ternary separation, unmixed reservoir

INTRODUCTION

The Simulated Moving Bed (SMB) has become a widely used binary separation technique. First commercialized by UOP in the 1960s (1), it was originally used for the separation of petrochemicals (2) and sugars. However, in recent years the use of the SMB in industry has become more widespread and it is now used in the pharmaceutical and fine chemicals (3) industries.

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There have been several studies on the use of the SMB for ternary separations including easy-split SMB cascade designs, which separate the most strongly adsorbed species from the weakest adsorbed (4) and a design for a nine zone SMB (5). These SMB configurations follow from the weak analogy between the SMB and distillation. Another SMB configuration that has been extensively studied is the five-zone SMB, which is a single cascade that can perform ternary separations (6–8) when the separation is relatively easy.

One shortcoming of standard SMBs is that they are difficult to use in plants running campaigns because the large number of columns have to be repacked identically when campaigns are changed. An alternative to SMBs for binary separations is the one column chromatograph with recycle analogous to the SMB (9–12). This Analog consists of one column and at least one mixed tank per column in the SMB. The Analog can achieve the same purity as an SMB with approximately twice the desorbent usage (9). If mixing is reduced by splitting the tanks into several smaller tanks, high purities can be obtained with no increase in desorbent usage (10). In more recent studies, improved Analogs with a single unmixed reservoir were designed. Mota and Araujo (11) designed a variable volume reservoir that can be used for any SMB configuration. Abunasser and Wankat (12) designed a simpler constant volume reservoir that can be used for Analogs with a small number of steps. Both of these Analogs gave higher purities than the Analogs with mixed tanks.

This paper extends applications of the Analog to two SMB configurations performing ternary separations.

CASCADES OF TWO FOUR ZONE SMBs AND THEIR ANALOGS

An SMB configuration that is commonly used to separate ternary mixtures is a cascade of two four-zone SMBs. In this configuration (Fig. 1), one component is purified in the first SMB and taken as a product while the other two components are sent as a mixed stream to the second four-zone SMB, after collection in a well mixed tank, where a binary separation takes place. If the stream is not mixed before being sent to the second SMB, it will lead to a feed stream with a varying concentration; and to the flowrate of the feed to the second SMB being fixed at the flowrate of the product stream exiting the first SMB. A variable concentration feed stream can negatively affect the separation especially in the case of nonlinear adsorption isotherms where the solute velocities are a function of the concentration. Also having to design a separation without the freedom of choosing the feed flowrate can result in a less than optimum separation.

Since the least adsorbed component, A, is taken as a product in the first SMB in the configuration shown in Fig. 1, the A-B separation should be relatively easy compared to the B-C (C is the most strongly adsorbed) separation

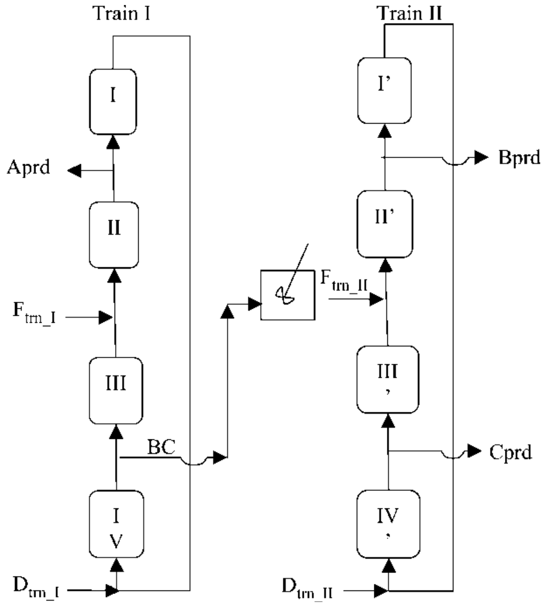

Figure 1. Cascade of two four-zone SMBs with one column per zone. A is least strongly adsorbed and C is most strongly adsorbed.

done in the second cascade. The mixed B-C stream is collected in a tank and is then fed to the second SMB. If the B-C separation is easier, then C is removed as a product from the first SMB and the A-B separation is done in the second SMB.

The Analogs are designed by following a single column of the SMB through a complete cycle (Fig. 2a) and then replacing the remaining columns with tanks (Fig. 2b) (9). The conditions for separation are identical to those for the SMB and the flowrates in and out of the tanks are calculated using simple mass balances.

The local equilibrium model is used to calculate the initial flowrates. In order for separation to occur in this system the following equations must be satisfied for systems with linear isotherms (4).

In Train I:

$$u_{A1} \leq u_{port} \tag{1a}$$

$$u_{A2} \geq u_{port} \tag{1b}$$

$$u_{B2} \leq u_{port} \tag{1c}$$

$$u_{A3} \geq u_{port} \tag{1d}$$

$$u_{B3} \leq u_{port} \tag{1e}$$

$$u_{C4} \geq u_{port} \tag{1f}$$

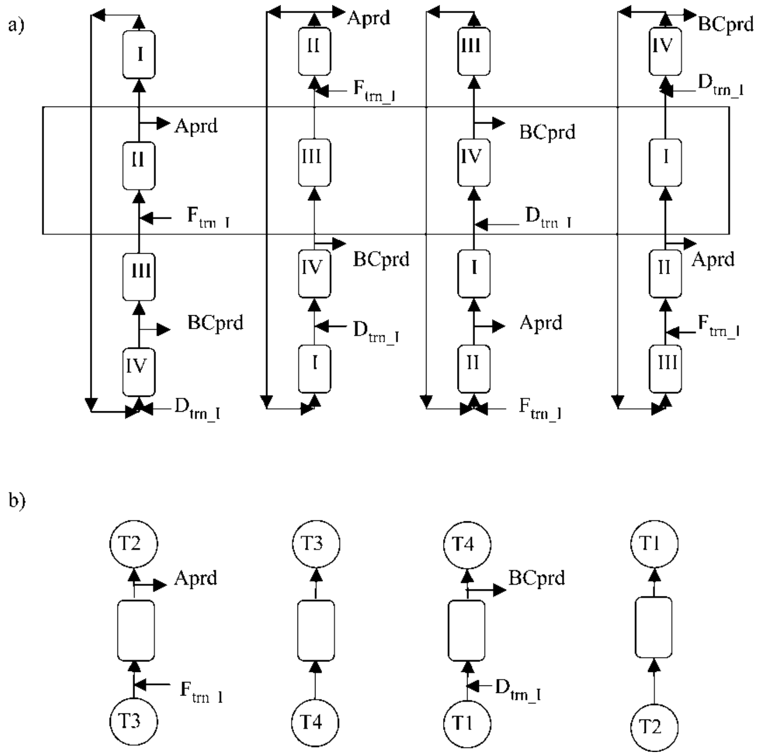

Figure 2. a) A complete cycle for a one column per zone SMB in Train I of Figure 1, b) a complete cycle for the Analog to a one column per zone SMB in Train I of Figure 1.

Train II is a binary separation,

$$u_{B1} \leq u_{port} \tag{2a}$$

$$u_{C2} \leq u_{port} \tag{2b}$$

$$u_{B3} \geq u_{port} \tag{2c}$$

$$u_{C4} \geq u_{port} \tag{2d}$$

where,

$$u_{i,j} = \frac{v}{\dfrac{1 + (1 - \varepsilon_e)\varepsilon_p}{\varepsilon_p K_d} + \dfrac{(1 - \varepsilon_e)(1 - \varepsilon_p)}{\varepsilon_e \ \rho_s K_i}} \tag{3}$$

Also, the feed flowrate into the Train II must be equal to the BC flowrate from Train I.

The separation of two ternary systems, three nucleosides, 2′-deoxyadenosine, 2′-deoxythymidine, and 2′-deoxycytidine (7) (dA, dT, and dC) and glucose, acetic acid, and sulfuric acid (5) were used to analyze the cascade of two four-zone SMBs and their Analog. Both of these systems have linear isotherms at low concentrations. Simulations were run on Aspen Chromatography v. 12.1 at three D/F values for SMBs with one and two columns per zone for the nucleosides and at 3 D/F values for SMBs with two columns per zone and their Analogs for the sugar and acids system. Analogs were designed for the SMBs with one column per zone with mixed tanks with both one (Fig. 2) and two (Fig. 3) columns per zone (9).

Analogs with unmixed reservoirs identical to those described by Abunasser and Wankat (12) (Fig. 4) were also designed for the SMBs with one column per zone. In this design, the mixed tanks are replaced by a single unmixed reservoir of constant volume packed with inert, nonporous beads. Although the flowrates entering and exiting the column vary, the reservoir flowrate is made constant by splitting each inlet and outlet stream into two different streams. The rational for splitting flows is that for a perfect plug-flow reservoir it does not matter if, for example, feed is introduced into band T_3 as it enters the column or as it enters the reservoir, where T_i is the flowrate exiting the corresponding tank in the Analog with mixed tanks. This also holds for the addition of desorbent and for removal of extract and raffinate.

There is a range of flowrates that will satisfy the mass balance when they are split. The two limiting cases are setting $F_1 = 0$ (no feed enters the column) and $F_2 = 0$ (no feed enters the reservoir). In the latter case the volume of the reservoir will be the smallest and therefore this case will be studied here. In order to design this Analog the following equations must be used for Train

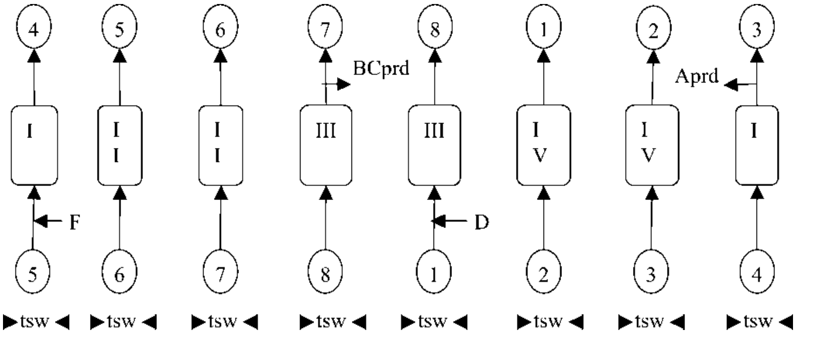

Figure 3. Analog to the SMB in Train I of Figure 1 with mixed tanks and two columns per zone.

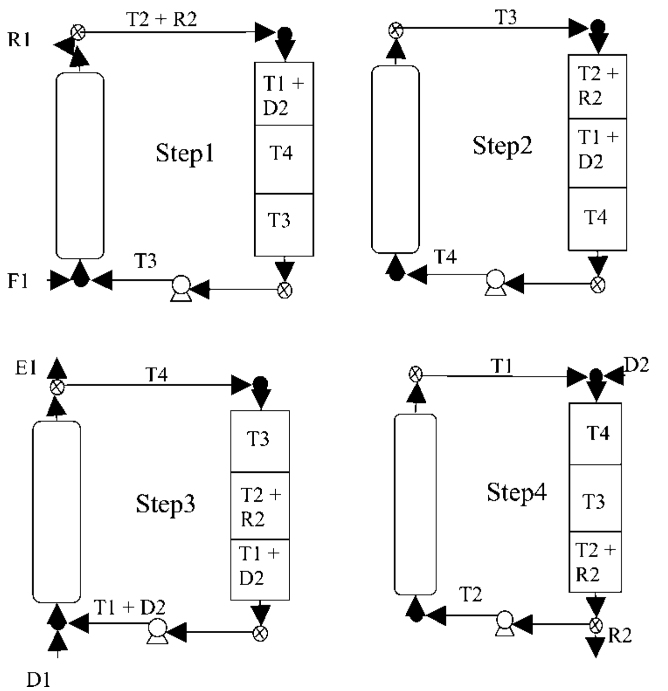

Figure 4. One column Analog to a four-zone SMB with an unmixed reservoir.

I of Fig. 1 (see Fig. 4):

$$F_1 = F_{trn\_I} \tag{4a}$$

$$R_1 = F_1 \tag{4b}$$

$$E_1 = BCprd \tag{4c}$$

$$D_1 = E_1 = BCprd \tag{4d}$$

$$R_2 = Aprd - R_1 = Aprd - F_{trn\_I} \tag{4e}$$

$$D_2 = D_{trn\_I} - D_1 = R_2 \tag{4f}$$

$$\text{Volume of tank} = 3^* t_{sw}^*(D_2 + \text{Recycle}) = 3^* t_{sw}(Aprd - F_{trn\_I} + \text{Recycle}) \tag{4g}$$

A similar set of equations is solved for Train II.

For the SMB with two columns per zone, only Analogs with mixed tanks were designed because this unmixed reservoir cannot be extended to the case of two columns per zone.

The simulation conditions for the separation of the nucleosides at the three D/F values and the isotherms for this system are given in Tables 1, 2 and 3. The very different K values show that this is an easy separation. The dispersion was estimated using the Chung and Wen equation (13). The solid

Table 1. Column specifications for the SMBs in Train I and II (Fig. 1) and their Analogs for the nucleoside separation. Values for ε_e, ε_p, K_i, and mass transfer are from reference (7). Reservoir dimensions are for Analogs with unmixed reservoirs

	Value	Unit	Description
L_{col} (4 columns)	25	cm	Column length (Train I and II)
L_{col} (8 columns)	12.5	cm	Column length (Train I and II)
d_{col}	4	cm	Column diameter (Train I and II)
d_p	30	micron	Particle size
ε_e	0.4	—	External void fraction
ε_p	0.67	—	Intraparticle void fraction
K_{dA}	27.7	—	Isotherm parameter
K_{dC}	3.15	—	Isotherm parameter
K_{dT}	9.6	—	Isotherm parameter
$k_m a_{p,\ dA}$	0.1	1/s	Mass transfer coefficient
$k_m a_{p,\ dC}$	1	1/s	Mass transfer coefficient
$k_m a_{p,\ dT}$	0.5	1/s	Mass transfer coefficient
Feed flowrate	8.0	cm^3/min	Feed flowrate
$d_{p,res}$	100	micron	Particle size in reservoir
$L_{res\_trn\_1}$	50	cm	Length of reservoir in train I
$D_{res\_trn\_I}$	9.15	cm	Diameter of reservoir in train I
$L_{res\_trn\_1I}$	50	cm	Length of reservoir in train II
$D_{res\_trn\_II}$	13.4	cm	Diameter of reservoir in train II

phase used is a reversed phase SOURCE™ 30RPC, the liquid phase is water with 6 vol% ethanol, and the mass transfer driving force is based on the concentration in the solid phase (7).

$$\frac{\partial q_i}{\partial t} = k_m a_p (q_i^* - q_i) \tag{5}$$

Table 2. Zone velocities in Train I (Fig. 1) at different D/F values studied for nucleosides

Train I	$D_T/F_{trn\_I} = 7.61$	$D_T/F_{trn\_I} = 9.23$	$D_T/F_{trn\_I} = 22.7$
F_{trn_I} (cm^3/min)	8.00	8.00	8.00
A product (cm^3/min)	8.00	8.73	9.71
BC product (cm^3/min)	30.4	34.9	39.3
D_{trn_I} (cm^3/min)	30.4	35.6	41.0
Recycle (cm^3/min)	8.93	10.2	10.8
v1 (cm/min)	1.78	2.03	2.16
v2 (cm/min)	3.37	3.76	4.09
v3 (cm/min)	1.78	2.17	2.50
v4 (cm/min)	7.83	9.11	10.3
t_{sw} (4 columns) (min)	50.1	43.1	39.2
t_{sw} (8 columns) (min)	25.1	21.5	19.6

Table 3. Zone velocities in Train II (Figure 1) at different D/F values studied for the nucleosides

Train II	$D_T/F_{trn\_I} = 7.61$	$D_T/F_{trn\_I} = 9.23$	$D_T/F_{trn\_I} = 22.7$
F_{trn_II} (cm^3/min)	30.4	34.9	39.3
B product (cm^3/min)	30.4	36.9	59.3
C product (cm^3/min)	30.4	36.2	121
D_{trn_II} (cm^3/min)	30.4	38.2	141
Recycle (cm^3/min)	23.0	27.8	47.5
v1 (cm/min)	4.57	5.53	9.46
v2 (cm/min)	10.6	12.9	21.2
v3 (cm/min)	4.57	5.93	13.4
v4 (cm/min)	10.6	13.1	37.5
t_{sw} (4 columns) (min)	37.0	29.9	15.7
t_{sw} (8 columns) (min)	18.5	15.0	7.86

The SMBs with two columns per zone were designed so that their productivities matched those of the SMBs with one column per zone by reducing the column length and switch times by half.

The results for Trains I and II for the case of one column per zone are given in Table 4 for the SMB, Analog with mixed tanks (one tank per column), and the Analog with the unmixed reservoir. The Analogs with mixed tanks achieved reasonably high purities for this system; this is probably a result of the easy separation. As expected, the Analogs with the unmixed reservoir gave higher purities than the Analogs with the mixed tanks, but were not quite as high as the SMB because of the dispersion in the unmixed reservoir. Also, for both of these Analogs the purities in Train II (B product and C product) were lower compared to the SMBs purities than what was seen with just binary separations. There is a cumulative effect here; since the separation in Train I was not as good as the SMB, the separation in Train II becomes even worse. This effect is reduced with the use of the unmixed reservoirs. For both Analogs the purity trends are the same as those in the SMB, i.e. the purities increase with increasing D/F.

The results for the simulations for the SMBs with two columns per zone and its Analog with mixed tanks for the nucleosides system are given in Table 5. Comparing the SMBs with one (Table 4) and with two columns per zone (Table 5), it is obvious that the purities increased when the number of columns was increased as expected. Also, the Analogs to the SMBs with two columns per zone had higher purities than the Analogs to the SMBs with one column per zone and they followed the same purity trends as the SMB, increasing purities with increasing D/F.

In this type of SMB cascade the total amount of desorbent used is very dependent on the isotherms and the operating conditions of Train II. If the BC stream is very dilute, the total amount of desorbent used increases

Table 4. Results of the separation in the SMBs with one column per zone in Figure 1and their Analogs for the nucleosides

	A product		B product		C product	
	Purity (%)	Recovery	Purity (%)	Recovery	Purity (%)	Recovery
$D_T/F_{trn\_I} = 7.61$						
SMB (1 column/zone)	88.4	0.909	79.8	0.854	91.8	0.829
Analog, mixed tanks	85.5	0.878	74.1	0.800	89.0	0.838
Analog, unmixed reservoir	87.1	0.881	77.1	0.825	89.5	0.820
$D_T/F_{trn\_I} = 9.23$						
SMB (1 column/zone)	91.5	0.932	82.5	0.900	93.9	0.838
Analog, mixed tanks	88.4	0.898	76.5	0.845	91.0	0.799
Analog, unmixed reservoir	89.8	0.901	79.0	0.877	91.2	0.833
$D_T/F_{trn\_I} = 22.74$						
SMB (1 column/zone)	92.6	0.958	93.9	0.936	98.2	0.953
Analog, mixed tanks	89.4	0.927	89.5	0.886	96.3	0.937
Analog, unmixed reservoir	90.4	0.927	89.6	0.886	96.9	0.937

Table 5. Results of the separation in the SMBs with two columns per zone and their Analogs for the nucleosides

	A product		B product		C product	
	Purity (%)	Recovery	Purity (%)	Recovery	Purity (%)	Recovery
$D_T/F_{trn\_I} = 7.61$						
SMB (2 columns/zone)	95.1	0.971	92.0	0.935	97.5	0.940
Analog, mixed tanks	91.1	0.932	83.3	0.873	93.9	0.871
D_T/F_{trn_I}–9.23						
SMB (2 columns/zone)	99.1	0.988	94.9	0.984	99.0	0.956
Analog, mixed tanks	94.6	0.955	86.2	0.925	95.9	0.880
$D_T/F_{trn\_I} = 22.74$						
SMB (2 columns/zone)	99.6	0.998	99.8	0.999	100	0.998
Analog, mixed tanks	95.4	0.976	96.8	0.953	99.1	0.983

rapidly with the slightest increase in D/F in the second train. Figure 5 illustrates this for the nucleosides system. Therefore, it might be desirable to concentrate the BC product before sending it as feed to the second SMB (4).

For the separation of glucose, acetic acid and sulfuric acid (5), the SMBs were designed with two columns per zone. The operating conditions are in Tables 6, 7, and 8. The mass transfer driving force for this system is Δc. This system is a more difficult separation than the nucleosides. For this system the separation in Train I was first optimized and then the separation in Train II was performed at three different D/F values. The results from the separation in Train I are given in Table 9. As expected the purities in the Analog were lower than the purities in the SMB. Since this system has two columns per zone, the unmixed reservoir discussed earlier does not work; therefore, to improve the Analog purities two of the larger tanks were split in half. The tanks that were chosen were Tanks 4 and 5 (Fig. 3) because in previous cases it was found that the tanks surrounding the feed have the largest effect on the separation (9). The results from this separation are also given in Table 9. As expected, there was a significant improvement in the separation in the Analog when more tanks are used.

Simulations were run for Train II at three D_{trn_II}/F_{trn_II} values for the SMB and the Analog. The results are shown in Figs. 6 and 7 for B product and C product, respectively. As in the case of Train I, the separation in the Analog with 8 tanks was quite a bit lower than the SMB. However, this separation improved when Tanks 4 and 5 were split in half. The separation occurring in the Analogs in Train II is still quite a bit lower than the SMB,

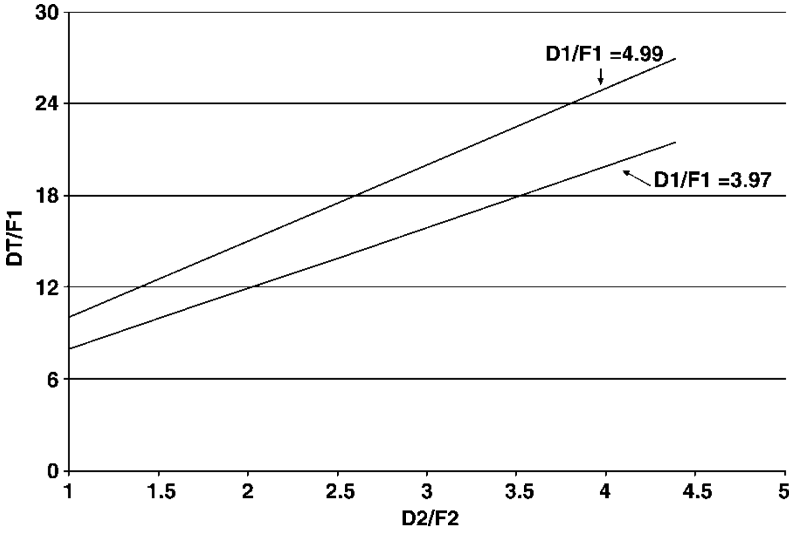

Figure 5. Effect of D/F in Train II on the total amount of desorbent ($D_T = D_{trn\_I} + D_{trn\_II}$) used in the SMBs in Figure 1.

Table 6. Column specifications for the Glucose-sulfuric acid-acetic acid separation. Values for ε_e, $k_m a_p$, and $K_{d,i}$ are from reference (5)

	Value	Unit	Description
L_{col}	250	cm	Column length (Train I and II)
d_{col}	7	cm	Column diameter (Train I and II)
d_p	320	micron	Particle size
ε_e	0.39	—	External void fraction
$K_{Sulfuric\ Acid}$	0	—	Isotherm parameter
$K_{Glucose}$	0.28	—	Isotherm parameter
$K_{Acetic\ Acid}$	0.7722	—	Isotherm parameter
$k_m a_{p,\ Sulfuric\ Acid}$	1.5	1/s	Mass transfer coefficient
$k_m a_{p,\ Glucose}$	3	1/s	Mass transfer coefficient
$k_m a_{p,\ Acetic\ Acid}$	10.5	1/s	Mass transfer coefficient
$K_{d,\ Sulfuric\ Acid}$	0.2437	—	Size exclusion factor
$K_{d,\ Glucose}$	0.4167	—	Size exclusion factor
$K_{d,\ Acetic\ Acid}$	0.4167	—	Size exclusion factor

because of the cumulative effect of the mixing in the tanks. Since the first separation was not as good as in the SMB, the second separation becomes even worse. Further splitting of tanks may improve this, or the use of an unmixed tank like that proposed by Mota and Araujo (11) could be used.

FIVE-ZONE SMB AND ITS ANALOG

The single cascade, five-zone SMB has been extensively studied (6–8). The configuration that works best for SMBs (8) removes the side stream (B

Table 7. Flowrates and zone velocities for the separation of Glucose-sulfuric acid-acetic acid in Train I of Fig. 1

	Value
Feed (cm^3/min)	60
A product (cm^3/min)	67.7
BC product (cm^3/min)	213.48
Desorbent (cm^3/min)	221.18
Recycle (cm^3/min)	165.93
v1 (cm/min)	11.05
v2 (cm/min)	15.67
v3 (cm/min)	11.57
v4 (cm/min)	25.79
t_{sw} (min)	21.94

Table 8. Flowrates and zone velocities for Train II of Fig. 1 for the glucose-acetic acid-sulfuric acid separation

	$D_T/F_1 = 7.244$	$D_T/F_1 = 7.76$	$D_T/F_1 = 8.62$
Feed (cm^3/min)	213.48	213.48	213.48
B product (cm^3/min)	213.48	221.94	247.53
C product (cm^3/min)	213.48	236.20	262.03
Desorbent (cm^3/min)	213.48	244.66	296.08
Recycle (cm^3/min)	398.5	414.28	462.05
v1 (cm/min)	26.55	27.60	30.78
v2 (cm/min)	40.77	42.39	47.28
v3 (cm/min)	26.55	28.17	33.05
v4 (cm/min)	40.77	43.90	50.51
t_{sw} (min)	13.54	12.76	11.09

product) below the feed (Fig. 8). For a successful separation in the SMB in Fig. 8 there must be an easy B-C separation. The alternative configurations (B product side stream removal above the feed) will always have A contaminating the B product.

The local equilibrium theory is used to calculate the initial separation conditions. In order for separation to occur the following equations must be satisfied (8):

$$u_{A1} = M_{A1}u_{port}, M_{A1} \leq 1 \tag{6a}$$

$$u_{A2} = M_{A2}u_{port}, u_{B2} = M_{B2}u_{port}, M_{A2} \geq 1, M_{B2} \leq 1 \tag{6b}$$

$$u_{A3} = M_{A3}u_{port}, u_{B3} = M_{B3}u_{port}, M_{A3} \geq 1, M_{B3} \leq 1 \tag{6c}$$

$$u_{B4} = M_{B4}u_{port}, u_{C4} = M_{C4}u_{port}, M_{B4} \geq 1, M_{C4} \leq 1 \tag{6d}$$

$$u_{C5} = M_{C5}u_{port}, M_{C5} \geq 1 \tag{6e}$$

If, in addition, the leading edge of the C band does not breakthrough into the B product, a purer B product will be obtained (8).

$$u_{C2} + u_{C3} + u_{C4} = M_{C,lead}u_{port}, M_{C,lead} \leq 1 \tag{7}$$

Table 9. Results for the separation in Train I of Fig. 1 for the sugar-acids system

D/F = 3.96		Acetic acid (%)	Glucose (%)	Sulfuric acid (%)
SMB	Aprd	0.03	0.37	99.6
	BCprd	49.75	49.59	0.66
Analog	Aprd	0.78	5.51	93.71
8 tanks	BCprd	48.79	46.55	4.66
Analog	Aprd	0.80	2.66	96.54
10 tanks	BCprd	48.22	47.36	4.42

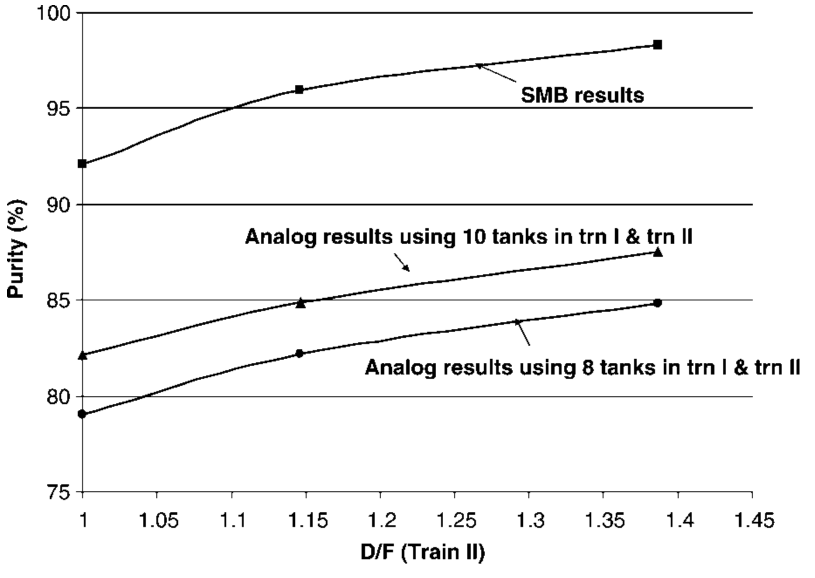

Figure 6. B product (Glucose) purities in Train II for glucose-acetic acid-sulfuric acid separation for the SMB and Analogs (8 and 10 tanks).

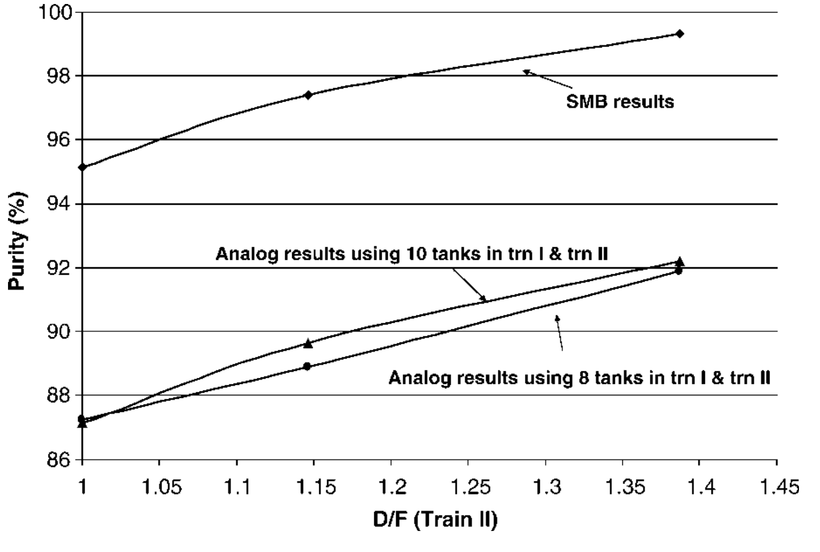

Figure 7. C product (Acetic Acid) purities in Train II for glucose-acetic acid-sulfuric acid separation for the SMB and Analogs (8 and 10 tanks).

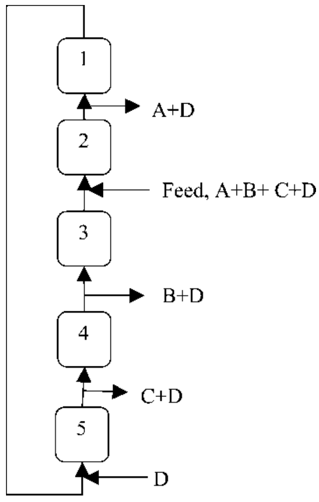

Figure 8. The five-zone SMB with one column per zone with B sidestream for ternary separations.

The characteristic diagram for this local equilibrium model is shown in Fig. 9 for the nucleoside system (7). Unfortunately, the combination of equations 1 and 2 can only be met when the B-C separation is very easy, which is the case for the nucleosides.

A one column Analog with mixed tanks can be designed for this SMB configuration. The Analog to a five zone SMB with one column per zone is shown in Fig. 10.

In order to evaluate the Analog of this SMB, simulations were run for a mixture of nucleosides (7) used previously for the cascade of two SMBs, replacing dT with dG (2'-deoxyguanosine). Simulations were run at three different D/F values. The operating conditions and the isotherm parameters

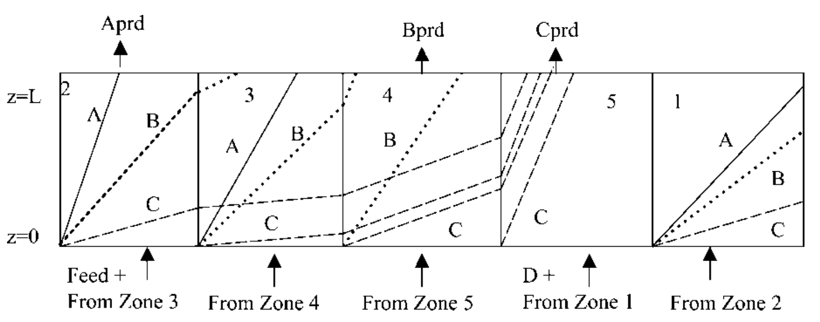

Figure 9. Local equilibrium solution for the five-zone SMB satisfying equations 6 and 7 for three nucleosides.

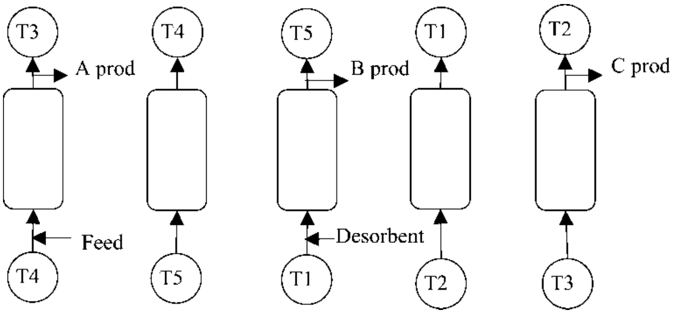

Figure 10. One column Analog to the five-zone SMB with B sidestream with one column per zone. A = dC, B = dG, C = dA.

for the five-zone SMB with one column per zone and its Analog are in Tables 10 and 11.

The Analog was first run with one tank per column of the SMB. The results from these simulations are given in Table 12. As with the binary separations, the purities achieved in the Analog were lower than those achieved in the corresponding SMBs, but these purities did increase with increasing D/F.

Table 10. Column specifications for the five-zone SMB (Figs. 8 and 11) and its analogs (Fig. 10) for nucleoside separation. Values for ε_e, ε_p, K_i, and mass transfer are from reference (7)

	Value	Unit	Description
L_{col} (5 columns)	42.03	cm	Column length
L_{col} (7 columns)	30.02	cm	Column length
d_{col}	3.75	cm	Column diameter
d_p	30	micron	Particle size
ε_e	0.4	—	External void fraction
ε_p	0.67	—	Intraparticle void fraction
K_{dA}	27.7	—	Isotherm parameter
K_{dC}	3.15	—	Isotherm parameter
K_{dG}	7.4	—	Isotherm parameter
$k_m a_{p,\ dA}$	0.1	1/s	Mass transfer coefficient
$k_m a_{p,\ dC}$	1	1/s	Mass transfer coefficient
$k_m a_{p,\ dG}$	0.5	1/s	Mass transfer coefficient
Feed flowrate	7.8125	cm^3/min	Feed flowrate
Vol_T_1	649	cm^3	Volume of Tank 1, (5col)
Vol_T_2	649	cm^3	Volume of Tank 2, (5col)
Vol_T_3	695	cm^3	Volume of Tank 3, (5col)
Vol_T_4	695	cm^3	Volume of Tank 4, (5col)
Vol_T_5	1137	cm^3	Volume of Tank 5, (5col)

Table 11. Zone velocities the five-zone SMB (Figs. 8 and 11) at the different D/F values studied

	D/F = 5.78	D/F = 7.4	D/F = 9.02
v1 (cm/min)	3.0	3.84	4.04
v2 (cm/min)	4.76	5.80	6.1
v3 (cm/min)	3.0	4.03	4.33
v4 (cm/min)	4.76	6.41	7.08
v5 (cm/min)	13.11	16.92	20.00
t_{sw} (5 columns) (min)	50	39.03	36.33
t_{sw} (7 columns) (min)	35.71	27.88	25.95

Table 12. Results for the five-zone SMBs with one column per zone (Fig. 8) and their Analogs (Fig. 10) at three different D/F values

		Purity	PI	Recovery
D/F = 5.78				
SMB	A product (%dC)	88.0	88.3	0.888
	B product (%dG)	89.0		0.827
	C product (%dA)	87.8		0.930
Analog with 5 tanks	A product (%dC)	83.1	83.4	0.831
	B product (%dG)	83.6		0.744
	C product (%dA)	83.4		0.925
Analog with 10 tanks	A product (%dC)	85.5	85.4	0.849
	B product (%dG)	86.0		0.783
	C product (%dA)	84.7		0.929
D/F = 7.4				
SMB	A product (%dC)	92.8	91.0	0.894
	B product (%dG)	90.2		0.914
	C product (%dA)	90.0		0.922
Analog with 5 tanks	A product (%dC)	87.3	85.8	0.834
	B product (%dG)	85.3		0.823
	C product (%dA)	84.9		0.916
Analog with 10 tanks	A product (%dC)	90.1	88.1	0.855
	B product (%dG)	87.7		0.868
	C product (%dA)	86.6		0.920
D/F = 9.02				
SMB	A product (%dC)	95.3	92.8	0.909
	B product (%dG)	90.7		0.944
	C product (%dA)	92.5		0.934
Analog with 5 tanks	A product (%dC)	90.1	87.8	0.844
	B product (%dG)	86.0		0.861
	C product (%dA)	87.3		0.927
Analog with 10 tanks	A product (%dC)	92.9	90.1	0.867
	B product (%dG)	88.3		0.903
	C product (%dA)	89.1		0.930

The lower purities are again a result of mixing in the tanks. Unfortunately, we were unable to design an Analog with an unmixed reservoir similar to that used for the two cascade system because there is not a set of flowrates that will satisfy the mass balances. Therefore, in order to improve the separation in the Analog, each of the tanks was split into two smaller tanks and the simulations were rerun (Table 12). As expected, the Analog purities and recoveries increased. If one needed to reach the SMB purities, the larger tanks could be divided into a larger number of small tanks or an unmixed reservoir like that proposed by Mota and Araujo (11) could be used.

In order to improve the separation in the SMB, a five-zone SMB with 7 columns in the (2, 2, 1, 1, 1) configuration was also designed (Fig. 10). Unlike the case of the four-zone SMB used for binary separations, the addition of more columns in every zone is not beneficial for the five-zone SMB. Because the B-C separation is a chromatographic separation, additional columns in zone 4 will not be helpful (8).

The SMB with seven columns was designed so that the productivity was the same as the SMB with five columns. This was achieved by reducing the column length and in turn the switching time to keep the port velocity constant for each D/F value. The new column length and new switch times are listed in Tables 10 and 11.

The results for the seven-column SMB and its Analog with one tank per column (seven tanks) are given in Table 13. When the number of columns was increased the purity indices in the SMB and the Analog increased. Comparison of Tables 12 and 13 shows that, as expected, the Analog purities were lower than the SMB purities as a result of mixing in the tanks. The Analog to the SMB with seven columns gave higher purities than the Analog to the SMB with five columns.

DISCUSSION AND CONCLUSIONS

The versatility of the Analog is illustrated since it can easily be extended to ternary separations. For the cascade of SMBs it is desirable to have the Analog for the first SMB give purities very close to those of the SMB. This leads to a better overall separation by minimizing the cumulative effect of the tank mixing. Alternatively, one could use a larger number of tanks or an unmixed reservoir in the first cascade, while using a lower number of tanks in the second cascade. The separation in the Analog with an unmixed reservoir can match the SMB if proper scaling is used (12).

Also, concentrating the BC product stream in Fig. 1 will reduce the total amount of desorbent used in the Analog or SMB. The Analog to the five-zone SMB also gives reasonably high purities for an easy separation. These purities increased when the mixed tanks were split into smaller tanks. It would be beneficial to use some kind of unmixed reservoir for this Analog as well.

Table 13. Results for the five-zone SMBs with 7 columns (Figure 11) and their Analogs

		Purity	PI	Recovery
D/F = 5.78				
SMB, 7 columns	A product (%dC)	92.9	91.1	0.928
	B product (%dG)	89.7		0.868
	C product (%dA)	90.8		0.931
Analog with 7 tanks	A product (%dC)	88.2	85.8	0.871
	B product (%dG)	84.8		0.798
	C product (%dA)	84.4		0.925
D/F = 7.4				
SMB, 7 columns	A product (%dC)	98.7	94.3	0.939
	B product (%dG)	91.0		0.963
	C product (%dA)	93.2		0.923
Analog with 7 tanks	A product (%dC)	93.7	89.2	0.877
	B product (%dG)	86.5		0.876
	C product (%dA)	87.3		0.917
D/F = 9.02				
SMB, 7 columns	A product (%dC)	99.7	95.9	0.961
	B product (%dG)	91.5		0.979
	C product (%dA)	96.5		0.929
Analog with 7 tanks	A product (%dC)	96.1	91.2	0.890
	B product (%dG)	87.1		0.912
	C product (%dA)	90.4		0.922

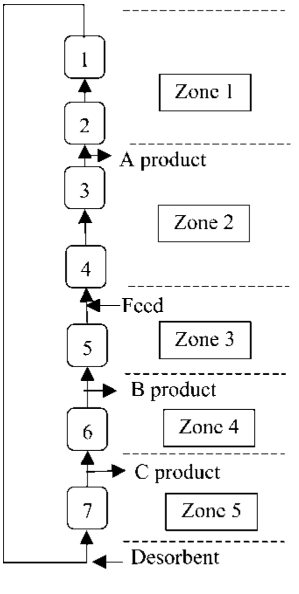

Figure 11. Five-zone SMB with B sidestream in the (2, 2, 1, 1, 1) configuration.

The cascade of SMBs and its Analog obviously require more equipment than the five-zone SMB but can separate more difficult systems. The separation in the cascade of SMBs can always be improved by increasing D/F in both trains, reducing the particle size to increase the mass transfer coefficients and/or adding more columns per zone. In this sense, the cascade of two four-zone SMBs and its Analog are robust. The five-zone SMB can obtain a relatively pure B product only when the B-C separation is easy. If this separation is not easy, increasing D/F, reducing particle size and/or adding more columns will not give a significantly purer B product. Thus, the five-zone SMB is not robust.

NOMENCLATURE

Aprd	Flowrate of A product (cm^3/min)
Bprd	Flowrate of B product (cm^3/min)
BCprd	Flowrate of BC stream (cm^3/min)
c_i	Concentration of component i (g/l)
Cprd	Flowrate of C product (cm^3/min)
D_{trn_I}	Desorbent flowrate in train I (cm^3/min)
D_{trn_II}	Desorbent flowrate in train II (cm^3/min)
K_d	Exclusion factor
K_i	Isotherm parameter, $q_i = K_i c_i$
$k_m a_p$	Lumped parameter mass transfer coefficient (1/s)
Productivity	Feed flowrate/(total volume of adsorbent)
Purity index (PI)	(%A + %B + %C)/3
q_i	Amount of solute adsorbed, kg/kg adsorbent
t_{sw}	Switch time (min)
u_i	Solute velocity (cm/min)
u_{port}	port velocity = (L_{col}/t_{sw}) (cm/min)
v	Interstitial velocity (cm/min)
ε_e	Extra-particle void fraction
ε_p	Inter-particle void fraction
ρ_s	Solid density (g/cm^3)

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