

Scaling and Intensification Procedures for Simulated Moving-Bed Systems

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Scaling rules and intensification procedures developed for single adsorption or chromatographic columns are extended for both linear and nonlinear isotherms to simulated moving-bed (SMB) systems. The effects of particle diameter, column length, column diameter, switching time, flow rates, mass transfer, axial dispersion, and dead volume are studied in order to design a new SMB. Changes in the pressure drop, separation, and throughput can be changed as desired. Once an original design has been developed, the scaling procedure requires only algebraic manipulation. Simulations done by Aspen Chromatography showed that the new designs were remarkably good at producing the same product purities and pressure drops as the original design. Intensification is predicted when particle diameter is decreased. The limitations of the technique are that the number of columns per zone cannot be changed, the relative velocities in each zone are fixed, and for nonlinear systems the results apply only for the same feed concentration.

Introduction

Simulated moving-bed (SMB) systems have been used commercially for the separation of liquid mixtures since their commercialization by UOP (Universal Oil Products) in the 1960s. The SMB process is attracting considerable attention in the pharmaceutical industry, for the purification of chemicals used as drugs and especially for the separation of enantiomers (Juza et al., 2000; Nicoud, 2000). A typical four-zone SMB with two columns per zone used for binary separation is shown in Figure 1. The four-zone system is highly efficient for binary separations and minimizes desorbent usage. The design of SMB systems for binary separations has been extensively studied by many groups and is now well understood (Gentilini et al., 1998; Mazzoti et al., 1997; Migliorini et al., 1998, 1999a,b, 2000; Pais et al., 1997; Ruthven and Ching, 1989; Wankat, 1986; Zhong and Guiochon, 1997). The methods available range from the simple, but qualitative local equilibrium theory to very detailed simulations. The “triangle” theory (Gentilini et al., 1998; Mazzoti et al., 1997; Migliorini et al., 1998, 1999a,b, 2000) has been widely adopted. The scaling rules, which are simple methods for predicting mass transfer and pressure-drop effects without detailed simulations, complement the triangle theory. The

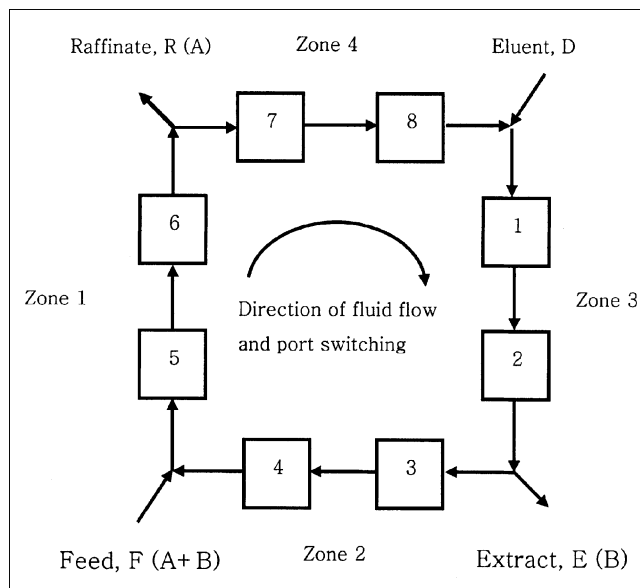


Figure 1. The four-section SMB.

objective of this article is to extend scaling rules developed for single chromatographic and adsorption columns (Mohammad et al., 1992; Rota and Wankat, 1990; Snyder, Wankat,

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1986, 1990, 1992; Wankat and Koo, 1988) to an SMB system with linear and nonlinear isotherms. We will then explore the effects of scaling several variables in an attempt to improve separation or intensify the system.

Basic Scaling Concept

The method for scaling columns for sorption processes assumes that an “old” design based on experiments or detailed simulations exists. By comparing the “new” design to the old design the effects of changes in the column length and diameter, particle diameter, and cycle time on the pressure drop, separation, and throughput can be predicted. This method has been applied for both linear and nonlinear isotherms and other situations (pore diffusion controls or does not control, laminar or turbulent flow). The scaling rules apply to both linear and nonlinear elution chromatography with independent solutes (Wankat and Koo, 1988) and to coupled solutes, gradient elution, and displacement chromatography (Wankat, 1992). If smaller diameter particles with high mass-transfer rates are used, the system is intensified, that is, a smaller system can process the same amount of material with the same purities and pressure drops. The scaling rules are particularly simple when pore diffusion controls.

Dispersion or zone spreading in SMB systems is caused by a combination of mass-transfer resistances, external mixing and dispersion, axial dispersion due to eddy and molecular diffusivities (the $\partial^2 c / \partial z^2$ term in the mass balance), and in nonlinear systems the diffuse wave caused by the isotherm. The previous scaling and intensification procedures all assumed that axial dispersion due to eddy and molecular diffusivities is negligible. Migliorini et al. (1999a) explored dispersion effects in SMBs using a linearized model. The dispersive resistances from axial dispersion and mass transfer were summed up to give the number of theoretical stages, $N_{p,i}$ (their Eq. 7)

$$\frac{1}{N_{p,i}} = \frac{1}{N_{\text{mix},i}} + \frac{2}{N_{\text{mt},i}} \left(\frac{(1-\epsilon)H_i}{\epsilon + (1-\epsilon)H_i} \right)^2$$

where $N_{\text{mix},i}$ is the number of mixing stages from axial dispersion, $N_{\text{mt},i}$ is the number of mass-transfer stages, and H_i is the Henry's law constant. For their nonlinear example for the separation of enantiomers the values are 4.208 and 2.788, $N_{\text{mix}} = 1,000$, and $N_{\text{mt}} = 45$. By averaging the predictions for $N_{p,i}$, they obtained $N_p = 32$. If we ignore the axial dispersion term, we obtain $N_{p,\text{w/o axial dispersion}} = 33$, which is a 3% error. Thus, ignoring axial dispersion but retaining mass transfer appears to be justified. As further evidence that the second-order axial dispersion term can be neglected in liquid-phase SMBs, a number of detailed simulations were done. These simulations, which are discussed in detail later, show that axial dispersion coefficients in the expected range have a very small effect on product purities.

In this section, we will extend scaling rules for single chromatographic columns to SMB systems with linear and nonlinear isotherms. All columns in the SMB are assumed to be

identical. The scaling factors are

$$\begin{aligned} a &= \frac{d_{p,\text{new}}}{d_{p,\text{old}}}, & b &= \frac{L_{j,\text{new}}}{L_{j,\text{old}}}, & c &= \frac{D_{\text{col,new}}}{D_{\text{col,old}}} \\ g &= \frac{Q_{j,\text{new}}}{Q_{j,\text{old}}} = \text{constant} & R_p &= \frac{\Delta P_{j,\text{new}}}{\Delta P_{j,\text{old}}} \\ R_N &= \frac{(L/L_{\text{MTZ}})_{j,\text{new}}}{(L/L_{\text{MTZ}})_{j,\text{old}}} & R_V &= \frac{V_{j,\text{new}}}{V_{j,\text{old}}} \\ & & &= \frac{(\text{Adsorbent volume})_{j,\text{new}}}{(\text{Adsorbent volume})_{j,\text{old}}} \quad (1) \end{aligned}$$

where we have assumed that the ratio g is the same for every column; thus, the ratio $Q_{j,\text{new}}/Q_{j,\text{old}}$ is the same for corresponding columns in the old and new designs. We will develop the conditions necessary to keep R_p and R_N constant.

The procedure for developing the scaling equations will first be illustrated for the pressure drop. The superficial fluid velocity in the columns of each zone can be related to the volumetric flow rate, Q_j

$$v_j = \frac{4Q_j}{\pi D^2} \quad (2)$$

Then the ratio of velocities in each zone is

$$\frac{v_{j,\text{old}}}{v_{j,\text{new}}} = \frac{Q_{j,\text{old}}}{Q_{j,\text{new}}} \left(\frac{D_{\text{col,new}}}{D_{\text{col,old}}} \right)^2 = \frac{c^2}{g} \quad (3)$$

Note that the ratio of velocities is the same for all columns, j . Pressure drop across each column is calculated using the Carman-Kozeny equation, which is valid for laminar flow

$$\Delta P_j = \frac{-1.5 \cdot 10^{-3} \mu (1-\epsilon)^2 v_j L}{4 \psi^2 d_p^2 \epsilon^3} \quad (4)$$

where we have assumed that the v^2 term is negligible. Equation 4 is written for both the old and the new designs, and the ratio of pressure drops is determined

$$\frac{1}{R_p} = \frac{\Delta P_{j,\text{old}}}{\Delta P_{j,\text{new}}} = \left(\frac{v_{j,\text{old}}}{v_{j,\text{new}}} \right) \left(\frac{L_{j,\text{old}}}{L_{j,\text{new}}} \right) \left(\frac{d_{p,\text{new}}}{d_{p,\text{old}}} \right)^2 \quad (5)$$

Since $(v_{j,\text{old}}/v_{j,\text{new}})$ is the same for all columns and the columns are identical, R_p is a constant. We have assumed that the porosity, ϵ , and fluid properties are constant. The assumption of constant porosity requires first that the particles are rigid [this assumption can be relaxed (Mohammad et al., 1992)], that the ratio D_{col}/d_p remains large enough in both designs (~ 30), and that the particles are close to spherical. The assumption of constant fluid properties is not needed when $R_N = 1$. If $R_p = 1$, the pressure drop will be the same for the two designs.

Although product purity does not lend itself to a simple equation, a surrogate, the fractional bed use in an adsorption column, is related to the ratio of bed length to length of the mass-transfer zone. For nonlinear systems, the value for L_{MTZ} is readily determined (Wankat, 1990). By taking the ratio of the fractional bed use in the old and new designs, R_N is

$$\frac{1}{R_N} = \frac{(L/L_{MTZ})_{j,old}}{(L/L_{MTZ})_{j,new}} = \left(\frac{v_{j,new}}{v_{j,old}} \right) \left(\frac{L_{j,old}}{L_{j,new}} \right) \left(\frac{k_m a_{p,old}}{k_m a_{p,new}} \right) \quad (6)$$

To develop Eq. 6 the isotherms are assumed to be identical in the two designs, which requires identical chemistry for the sorbent as the particle diameter changes. When $R_N = 1$, the fractional bed use will be constant in the two designs and the product purities will be identical. In linear systems R_N can also be related to the ratio of plate counts, N , in the chromatographic columns (Wankat and Koo, 1988). If $R_N = 1$, the two columns have an identical value of N , and the product purities are identical. If pore or surface diffusion controls, Eq. 6 simplifies to

$$\frac{1}{R_N} = \frac{(L/L_{MTZ})_{j,old}}{(L/L_{MTZ})_{j,new}} = \left(\frac{v_{j,new}}{v_{j,old}} \right) \left(\frac{L_{j,old}}{L_{j,new}} \right) \left(\frac{d_{p,new}}{d_{p,old}} \right)^2 \quad (7)$$

Note that R_N is a constant for corresponding columns in the two designs. Since pore-diffusion control is very common in liquid SMB systems, Eq. 7 will be used in the remainder of this article.

Inserting Eq. 3 into Eqs. 5 and 7, $1/R_P$ and $1/R_N$ become

$$\frac{1}{R_P} = \left(\frac{Q_{j,old}}{Q_{j,new}} \right) \left(\frac{D_{col,new}}{D_{col,old}} \right)^2 \left(\frac{L_{j,old}}{L_{j,new}} \right) \left(\frac{d_{p,new}}{d_{p,old}} \right)^2 = \frac{a^2 c^2}{bg} \quad (8)$$

$$\frac{1}{R_N} = \left(\frac{Q_{j,new}}{Q_{j,old}} \right) \left(\frac{D_{col,old}}{D_{col,new}} \right)^2 \left(\frac{L_{j,old}}{L_{j,new}} \right) \left(\frac{d_{p,new}}{d_{p,old}} \right)^2 = \frac{a^2 g}{bc^2} \quad (9)$$

The ratio of volumes of adsorbent in the new and the old systems is

$$R_V = \frac{(\text{Adsorbent volume})_{new}}{(\text{Adsorbent volume})_{old}} = \left(\frac{D_{col,new}}{D_{col,old}} \right)^2 \left(\frac{L_{j,new}}{L_{j,old}} \right) = bc^2 \quad (10)$$

The switching time in the SMB needs to be scaled to keep the relative movements of the solute waves the same. Since the average velocity of solute i is related to the superficial velocity, v_j , in each zone

$$u_{ij} = (\text{constant}_i) v_j = C_i v_j \quad (11)$$

the fractional penetration of solute wave i into the column is

$$\frac{u_{ij} t_{sw}}{L} = \frac{C_i v_j t_{sw}}{L} \quad (12)$$

Taking the ratio of the old and new designs, we obtain the ratio of fractional penetrations

$$R_{pen} = \frac{(C_i v_j t_{sw}/L_j)_{new}}{(C_i v_j t_{sw}/L_j)_{old}} = \frac{(v_j t_{sw}/L_j)_{new}}{(v_j t_{sw}/L_j)_{old}} \quad (13)$$

where R_{pen} is a constant for all corresponding columns in the two designs. Setting $R_{pen} = 1$ and simplifying, we obtain

$$\frac{t_{sw,new}}{t_{sw,old}} = \frac{(L_j/v_j)_{new}}{(L_j/v_j)_{old}} = \frac{(L_j D_{col}^2)_{new}}{(L_j D_{col}^2)_{old}} \frac{Q_{j,old}}{Q_{j,new}} = \frac{bc^2}{g} = \frac{R_V}{g} \quad (14)$$

If the adsorbent volumes are the same in the two designs, Eq. 14 becomes

$$\frac{t_{sw,new}}{t_{sw,old}} = \frac{Q_{j,old}}{Q_{j,new}} = \frac{1}{g} \quad (15)$$

The effect of extra-column dead volume or “dead” volume is well known to be important in SMB processes (Beste et al., 2000; Migliorini et al., 1999b). If the dead volume is modeled as a stirred tank, the important variable is the volume of fluid processed between switching intervals divided by the dead volume (Rota and Wankat, 1990)

$$R_D = \frac{(Q_j t_{sw}/V_D)_{new}}{(Q_j t_{sw}/V_D)_{old}} = \left(\frac{Q_{j,new}}{Q_{j,old}} \right) \left(\frac{t_{sw,new}}{t_{sw,old}} \right) \left(\frac{V_{D,old}}{V_{D,new}} \right) \quad (16)$$

where V_D is the dead volume and R_D is a constant for all corresponding columns in the two designs. To have identical product purities, set $R_D = 1$. If pore diffusion controls, we obtain ($R_D = 1$)

$$V_{D,new}/V_{D,old} = (Q_{j,new}/Q_{j,old})(t_{sw,new}/t_{sw,old}) = R_V \quad (17)$$

The dead volume needs to be scaled in the same way as the adsorbent volume. During intensification of the SMB, reducing the dead volume proportionally can be difficult.

Intensification Example

These rules can be used to estimate the changing operating conditions. For example, consider the following case with pore diffusion controlling. The same product purities are desired, $R_N = 1$; the ratio of flow rate in each zone is the same, $g = 1$; the particle diameter is cut in half, $a = 1/2$; and the pressure drop is cut in half, $R_P = 1/2$. How should the column be scaled?

Multiplying Eqs. 8 and 9 and solving for b , we obtain

$$b = (R_P R_N a^4)^{1/2} \quad (18)$$

Table 1. Base Conditions for Simulations

Configuration: SMB4: 1,1,1,1; SMB8: 2,2,2,2; SMB12: 3,3,3,3	Recycle flow rate, Q_{recycle} (mL/min): 35.38
Feed concentrations, c_F (g/L): 2.9 & 10.0	Extract (B) flow rate, Q_E (mL/min): 16.00
Desorbent flow rate, Q_D (mL/min): 21.45	Raffinate (A) flow rate, Q_R (mL/min): 9.09
Feed flow rate, Q_F (mL/min): 3.64	Zone length (cm): 21.00
Column diameter (cm): 2.60	Switching time (min): 5.5, 2.75, 1.833
Particle diameter (cm): 3.2E-3	$D/F = 5.89$
Mass-transfer coefficient (1/s): 0.5	

or

$$b = L_{\text{new}}/L_{\text{old}} = \left[(1/2)(1.0)(1/2)^4 \right]^{1/2} = 0.1768$$

and dividing Eq. 8 by Eq. 9

$$c = \frac{D_{\text{col,new}}}{D_{\text{col,old}}} = g^{1/2} \left(\frac{R_N}{R_P} \right)^{1/4} \quad (19)$$

This gives $c = 1.1892$. Then the ratio of adsorbent volumes is

$$R_V = bc^2 = a^2 R_N = 1/4$$

From Eq. 14 or 17, the ratio of switching times is

$$\frac{t_{\text{sw,new}}}{t_{\text{sw,old}}} = \frac{bc^2}{g} = \frac{R_V}{g} = 1/4$$

Thus, the theory predicts that the new SMB will process the same amount of feed with the same product purities, have half the pressure drop, and use one-fourth as much adsorbent. Since the adsorbent volume and the volume of liquid in the column are one-fourth the amounts in the standard system, the intensified system will be inherently safer when hazardous chemicals are processed. In the next section, the accuracy of this prediction will be demonstrated later in Figure 3. Also, the extra-column volume needs to be reduced to one-fourth that in the old design. This might be a formidable task. The price of this intensification is that the columns are packed with smaller particles, change shape considerably, and new detailed design procedures may be required. Of course, scaling to new operating conditions can be done without intensification.

Simulations

In order to examine the validity of the scaling rules we performed simulations using Aspen Chromatography, version

10.2. Simulations of SMBs are done for three different four-zone SMBs: SMB4, with four columns, one in each zone; SMB8, with eight columns, two per zone; and SMB12, with three columns per zone. For the old or original design, the length of each fixed-bed column was chosen by keeping the total length of each zone constant. In order to test the validity of the scaling rule, the separation of the enantiomers of 1,1'-bi-2-naphthol was studied (Pais et al., 1997). The base conditions for simulations are summarized in Table 1.

Aspen Chromatography calculates flow as convection with an estimated dispersion using the Chung and Wen (1968) equation, is isothermal, and the pressure drop is calculated using the Carman-Kozeny equation. The kinetic model was a linear lumped resistance. The isotherms are correlated by the bi-Langmuir type (Pais et al., 1997)

$$q_A^* = \frac{2.69c_A}{1 + 0.0336c_A + 0.0466c_B} + \frac{0.10c_A}{1 + c_A + 3c_B} \quad (20a)$$

$$q_B^* = \frac{3.73c_B}{1 + 0.0336c_A + 0.0466c_B} + \frac{0.30c_B}{1 + c_A + 3c_B} \quad (20b)$$

where A is the less retained component. The system was simulated in both linear ($c_{A,F} = 2.9$ g/L, $c_{B,F} = 2.9$ g/L), and nonlinear ($c_{A,F} = 10$ g/L, $c_{B,F} = 10$ g/L) regions.

Axial Dispersion and Dead-Volume Effects

A number of simulations were done to check the assumption that the second-order axial dispersion term could be neglected. The axial dispersion coefficient for the base case was estimated from the Chung and Wen (1968) correlation

$$N_{pe} = 0.2 + 0.011(N_{Re})^{0.48} \quad (21)$$

Simulations were done with both a constant Peclet number [the low-velocity limit (Ruthven, 1984)] and varying Peclet numbers. This expected Peclet number was then arbitrarily

Table 2. Effects of Axial Dispersion with Zero Dead Volume for SMB8*

Conc. (g/L)	Purity (%)	Peclet Number			
		10 $N_{pe,\text{basis}}$	$N_{pe,\text{basis}} = 0.2$	0.1 $N_{pe,\text{basis}}$	0.01 $N_{pe,\text{basis}}$
2.9	Raffinate	96.6407	96.5785	95.9939	89.0474
	Extract	95.5119	95.4074	94.4524	85.0611
10	Raffinate	72.3610	72.3579	72.3159	70.7213
	Extract	99.2622	99.2172	98.6840	89.8678

*Other conditions in Table 1.

Table 3. Effects of Column Dead Volume and Peclet Number, $N_{pe,basis} = 0.2$ and $c_F = 2.9$ g/L (linear range) for SMB8*

N_{pe}	Purity (%)	Dead Volume (V_D)				
		0%	5%	10%	15%	20%
$10N_{pe,basis}$	Raffinate	96.6407	95.8853	94.7500	93.0019	89.7888
	Extract	95.5119	91.8718	86.5143	79.6526	71.8035
$N_{pe,basis}$	Raffinate	96.5785	95.8282	94.6948	92.9420	89.7102
	Extract	95.4074	91.7458	86.3776	79.5205	71.6893
$0.1N_{pe,basis}$	Raffinate	95.9939	95.3044	94.1890	92.3985	89.0105
	Extract	94.4524	90.6277	85.1845	78.3760	70.7120
$0.01N_{pe,basis}$	Raffinate	89.0474	89.1784	88.5645	86.8599	83.2568
	Extract	85.0611	81.3601	76.4845	70.8828	65.1151

*Other conditions in Table 1.

multiplied by 10, 0.1, or 0.01 to study the sensitivity of the simulations to the Peclet number.

Table 2 shows the effect of different Peclet numbers for the base case listed in Table 1 for a 4-zone SMB with two columns per zone (SMB8) with constant Peclet numbers. Multiplying the base-case Peclet number by a factor of 10 (smaller axial dispersion coefficient) has almost no effect ($\sim 0.1\%$ change) on the product purities. Multiplying the base-case Peclet number by 0.1 (large axial dispersion coefficient) has a very modest effect ($\sim 1\%$ change) on the product purities, while multiplying the base-case Peclet number by 0.01 has a significant effect (up to 10% change). Thus, within the normal range of the Peclet number axial dispersion has a very small effect on the product purities of SMB systems. These results are for a 32- μm particle. For larger particles (shown later in Tables 15 and 16), axial dispersion effects are even less important. Therefore, ignoring axial dispersion in the development of the scaling rules is a reasonable approximation.

Dead volume (or extra-column dead volume), on the other hand, clearly has a significant effect on product purities (Tables 3 and 4). Dead volume has an effect on spreading the concentration profiles in the SMB unit due to additional back mixing in the dead volume itself and on increasing the residence time in the module made of the dead volume and the chromatographic column. It is generally recognized that the dead volume yields extra-column band broadening of chromatographic peaks, thus hindering column efficiency and

separation performance. However, dead volume has another, more important effect, which is the introduced lag time (Birelli et al., 2000; Migliorini et al., 1999b; Peddeferri et al., 1999).

Tables 3 and 4 show the effect of the dead volume with the variation of the Peclet number in the linear and nonlinear regions. In the linear region (Table 3), the purities for raffinate and extract product are about 97% and 95% when the Peclet number is 0.2 and the dead volume is zero (basis case). The results of the simulations show that with constant dead volume the purities decrease with a decreasing Peclet number. The purities decrease with increasing dead volume when the Peclet number is constant. Increasing the feed composition from $c_F = 2.9$ g/L to $c_F = 10$ g/L makes the system nonlinear. The purities for the raffinate and extract product are about 72% and 99% when the Peclet number is 0.2 and the dead volume is zero (basis case). At constant dead volume purities again decrease with decreasing Peclet number. Now with a constant Peclet number increasing, the dead volume causes an increase in raffinate purity (Table 4). Migliorini et al. (1999b) use the triangle theory to explain this effect. The lag time caused by the dead volume moves the separation into the complete separation region.

To check this argument, we adjusted only the raffinate and extract flow rates for an SMB8 with zero dead volume under the conditions that D/F , feed flow rate, and flow rates in zone 4 and zone 3 (Figure 1) are constant. Then, the sum of raffinate and extract flow rates is constant. The results with

Table 4. Effects of Column Dead Volume and Peclet Number, $N_{pe,basis} = 0.2$ and $c_F = 10$ g/L (nonlinear range) for SMB8*

N_{pe}	Purity (%)	Dead Volume (V_D)				
		0%	5%	10%	15%	20%
$10N_{pe,basis}$	Raffinate	72.3610	76.3873	82.3186	90.2480	93.6575
	Extract	99.2622	99.3511	99.1002	98.5487	97.2818
$N_{pe,basis}$	Raffinate	72.3579	76.3849	82.3012	90.1416	93.5640
	Extract	99.2172	99.3206	99.0676	98.5059	97.2232
$0.1N_{pe,basis}$	Raffinate	72.3159	76.3459	82.0835	89.1250	92.6165
	Extract	98.6840	98.9687	98.7095	98.0501	96.6179
$0.01N_{pe,basis}$	Raffinate	70.7213	74.1617	77.9798	81.7069	84.5447
	Extract	89.8678	91.9681	92.4290	91.6145	89.6613

*Other conditions in Table 1.

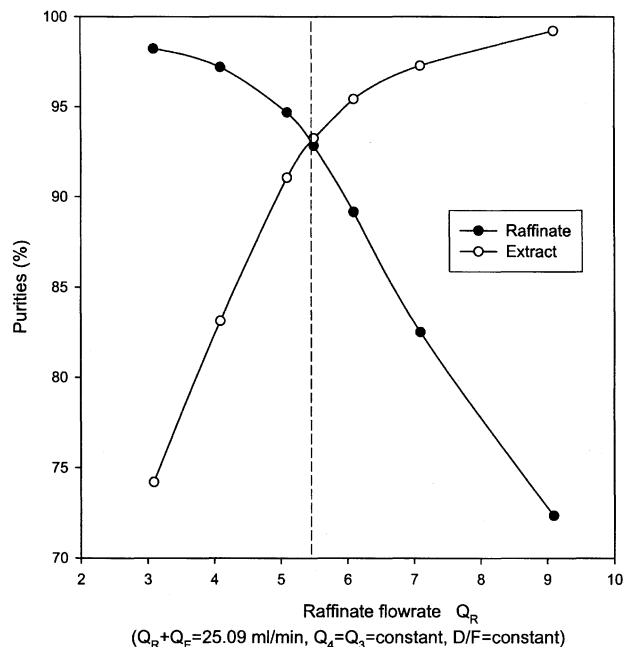


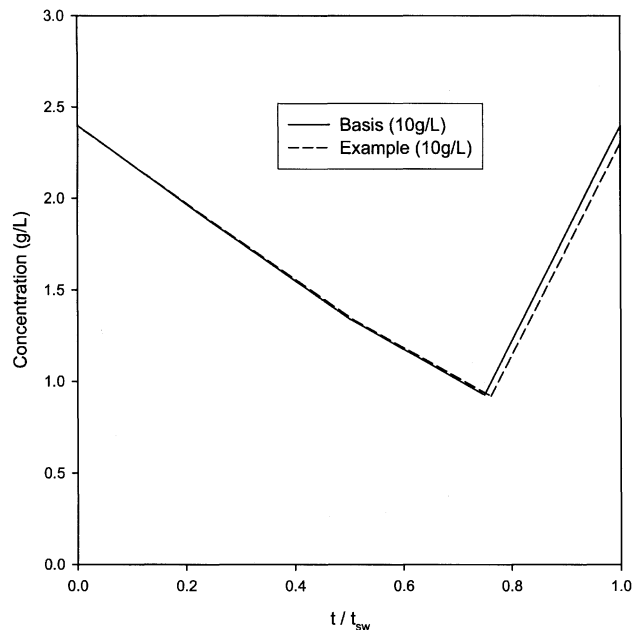
Figure 2. Influence of raffinate and extract flow rates for SMB8 with zero dead volume in nonlinear range ($C_F = 10.0$ g/L).

zero dead volume are shown in Figure 2. The raffinate purity is increased and the extract purity is decreased with decreasing raffinate flow rate.

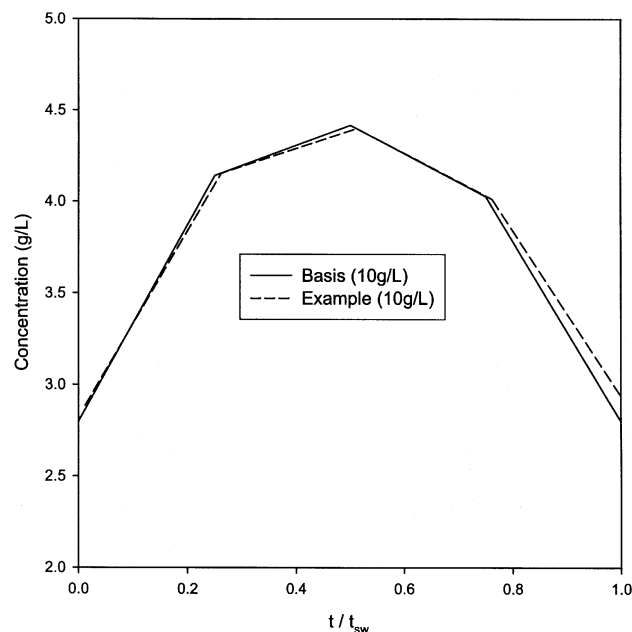
Simulation Results for Scaling

Figure 3 shows the outlet concentration profiles in extract and raffinate of an SMB8 for feeds in the nonlinear range for the simulation conditions described in Table 1 and the example ($R_N = 1$, $g = 1$, $a = 1/2$, and $R_P = 1/2$) after the tenth cycle. Figure 3 shows that the agreement between the base and scale-up profiles is quite good, but not perfect. Thus, the resulting product purities are very close. With $R_N = 1$, the concentrations are mapped between the old and new designs so that concentrations are identical at the same values of dimensionless distance, z/L , and dimensionless time within a cycle, t/t_{sw} . Thus, for $R_N = 1$ fluid properties can depend on concentration or temperature and the scaling procedure still works.

The scaling rules were used to predict new conditions with specified changes in purity, feed rate, or pressure drop. Then simulations were done to check these predictions. The results obtained from the simulation for SMB4, SMB8, and SMB12 are given in Tables 5 to 20 and are shown in Figures 4–6. The influence of the numbers of column per zone with a constant amount of adsorbent is shown in Figure 4 and Tables 5 to 7. Increasing the number of columns per zone increases the purity. Figure 4 also shows the effect of feed concentration. The separation is easier in the linear range, and raffinate purities in particular are higher. Higher raffinate purities can be obtained by changing the distribution of flows (Figure 2). Tables 5 to 7 show that the scaling procedures are accurate with $R_N = 1$ in the nonlinear range, since product



(a)



(b)

Figure 3. Purity profiles for scaling shown in the Example ($g = 1$, $a = 1/2$, $R_N = 1$, $R_P = 1/2$) at the end of the 10th period.

SMB8 (2,2,2,2). Base case shown in Table 1. N_{pe} calculated by Eq. 21. (a) Extract profiles; (b) raffinate profiles.

purities are almost identical. Table 8 shows that the scaling procedure also works in the linear range.

Figure 5 and Tables 6 and 8 for SMB8 show the influence of pressure drop for the two designs when the fractional bed use of the two designs is the same, $R_N = 1$, and volumetric flow rates are the same, $g = 1$. This figure and these tables

Table 5. Scaled Design for SMB4 (1,1,1,1) Constituted by Four Columns, One per Zone When $R_N = 1$, $D/F = 5.89$, and $c_F = 10$ g/L (nonlinear region)*

	Scaled Design					
	Basis	1	2	3	4	5
$a = d_{p,new}/d_{p,old}$	1	1	1	1	0.9535	2
$b = L_{new}/L_{old}$	1	0.707	0.5	0.354	1	4
$c = D_{col,new}/D_{col,old}$	1	1.189	1.414	1.682	1	1
$g = Q_{new}/Q_{old}$	1	1	1	1	1.1	1
R_p	1	1/2	1/4	1/8	1.21	1
$t_{sw,new}/t_{sw,old}$	1	1	1	1	0.9091	4
Purity (%) in raffinate	71.6206	71.6156	71.6025	71.6416	71.6143	71.6317
Purity (%) in extract	90.6502	90.6007	90.5265	90.4634	90.6496	90.7136

* N_{pe} calculated by Eq. 21. Other conditions in Table 1.

show that the purities are kept very close to constant when $R_N = 1$. Tables 9 and 10 show the effects of R_p when Peclet numbers are varied. Only the lowest Peclet number (outside the normal range) shows a significant change in purities.

Figure 6 and Tables 11 and 12 show the influence of changing the ratio of the fractional bed use (R_N) in SMB8 when the pressure drop for the two designs is the same ($R_p = 1$) and feed rates are constant ($g = 1$). The designs with increasing R_N (Tables 11 and 12) can achieve somewhat higher purity, particularly in the linear region, with the same throughput of feed. However, purity depends on R_N in a very nonlinear fashion. Large increases in the raffinate purity for the 10-g/L feed will require adjusting the velocities in the column (Figure 2). Similar trends were observed for SMBs with 4 and 12 columns. Since $R_N = R_V = bc^2$ when $a = g = 1$, Figure 6 also shows the change of purity vs. the ratio of adsorbent volumes. By increasing the adsorbent volumes, the purity can be increased.

Tables 13 and 14 show the influence of increasing the ratio of the flow rates, g , in the SMB8 when pressure drop for the two designs is the same ($R_p = 1$) and the fractional bed use of the two designs is the same ($R_N = 1$). With constant D/F , increases in g require corresponding increases in F , D , raffinate, and extract flow rates between the old and new designs. Thus, g is also the scale-up parameter

$$g = \frac{F_{new}}{F_{old}} = \frac{D_{new}}{D_{old}} \quad (22)$$

Table 6. Scaled Design for SMB8 (2,2,2,2) when $R_N = 1$, $g = 1$, $a = 1$, $D/F = 5.89$ and $c_F = 10$ g/L (nonlinear region)*

	Scaled Design					
	1	2	Basis	3	4	5
$a = d_{p,new}/d_{p,old}$	1	1	1	1	1	1
$b = L_{new}/L_{old}$	2	1.414	1	0.707	0.5	0.354
$c = D_{col,new}/D_{col,old}$	0.707	0.841	1	1.189	1.414	1.682
$g = Q_{new}/Q_{old}$	1	1	1	1	1	1
R_p	4	2	1	1/2	1/4	1/8
Purity (%) in raffinate	72.3021	72.3769	72.3577	72.3735	72.3586	72.4154
Purity (%)	99.2374	99.2343	99.2180	99.1987	99.1671	99.1296

* N_{pe} calculated by Eq. 21. Other conditions in Table 1.

Table 7. Scaled Design for SMB12 (3,3,3,3) Constituted by Twelve Columns, Three per Zone When $R_N = 1$, $D/F = 5.89$, and $c_F = 10$ g/L (nonlinear region)*

	Scaled Design					
	Basis	1	2	3	4	5
$a = d_{p,new}/d_{p,old}$	1	1	1	1	0.9535	2
$b = L_{new}/L_{old}$	1	0.707	0.5	0.354	1	4
$c = D_{col,new}/D_{col,old}$	1	1.189	1.414	1.682	1	1
$g = Q_{new}/Q_{old}$	1	1	1	1	1.1	1
R_p	1	1/2	1/4	1/8	1.21	1
$t_{sw,new}/t_{sw,old}$	1	1	1	1	0.9091	4
Purity (%) in raffinate	72.4666	72.4638	72.4742	72.4970	72.5650	72.4406
Purity (%) in extract	99.8062	99.7983	99.7870	99.7704	99.7437	99.8157

* N_{pe} calculated by Eq. 21. Other conditions in Table 1.

Tables 13 and 14 show that purities are kept constant regardless of the feed rate if $R_N = 1$.

Tables 15 and 16 show the scaled design results in the linear and nonlinear regions when the particle diameters are varied and Peclet numbers are constant. Since $R_N = 1$, the purities are essentially constant. These results illustrate *intensification*. As the particle diameter is decreased, essentially the same separation is obtained with the same pressure drop, but with a significantly shorter column and, therefore, less adsorbent. Note that for larger particle diameters (larger a) the purities at the two Peclet numbers are closer than for the base case ($d_p = 32$ μ m). Thus, the second-order axial dispersion term is less important with larger particles.

Tables 17 and 18 show the effects of R_p when Peclet numbers are constant and dead volumes are always 10% of the column volume. Only the lowest Peclet number (outside the normal range) shows a significant change in purities. Tables 19 and 20 show the scaled design results in the linear and nonlinear regions when the particle diameters are varied and Peclet numbers are constant and the dead volumes are always 10% of the column volume. Since $R_N = 1$, the purities are essentially constant. These results illustrate *intensification* when dead volume is present.

Discussion and Conclusions

The scaling procedures developed in this article are effective for simulated moving beds with linear and nonlinear

Table 8. Scaled Design for SMB8 (2,2,2,2) Constituted by Eight Columns, Two per Zone When $R_N = 1$, $g = 1$, $a = 1$, $D/F = 5.89$, and $c_F = 2.9$ g/L (linear region)*

	Scaled Design					
	1	2	Basis	3	4	5
$a = d_{p,new}/d_{p,old}$	1	1	1	1	1	1
$b = L_{new}/L_{old}$	2	1.414	1	0.707	0.5	0.354
$c = D_{col,new}/D_{col,old}$	0.707	0.841	1	1.189	1.414	1.682
$g = Q_{new}/Q_{old}$	1	1	1	1	1	1
R_p	4	2	1	1/2	1/4	1/8
Purity (%) in raffinate	96.6194	96.5947	96.5796	96.5512	96.5166	96.4551
Purity (%) in extract	95.4982	95.4272	95.4091	95.3654	95.3020	95.1749

* N_{pe} calculated by Eq. 21. Other conditions in Table 1.

Table 9. Effect of Changing R_p for SMB8*

		Scaled Design					
		1	2	Basis	3	4	5
$a = d_{p,new}/d_{p,old}$		1	1	1	1	1	1
$b = L_{new}/L_{old}$		2	1.414	1	0.707	0.5	0.354
$c = D_{col,new}/D_{col,old}$		0.707	0.841	1	1.189	1.414	1.682
$g = Q_{new}/Q_{old}$		1	1	1	1	1	1
R_p		4	2	1	1/2	1/4	1/8
$10N_{pe,basis}$	Raffinate (%)	96.6467	96.6334	96.6407	96.6469	96.6374	96.6623
	Extract (%)	95.5441	95.4926	95.5119	95.5589	95.5285	95.6444
$N_{pe,basis}$	Raffinate (%)	96.6187	96.5939	96.5785	96.5674	96.5246	96.5012
	Extract (%)	95.4937	95.4261	95.4074	95.4265	95.3406	95.3809
$0.1N_{pe,basis}$	Raffinate (%)	96.3327	96.1860	95.9939	95.7240	95.3061	94.7171
	Extract (%)	95.0250	94.7530	94.4524	94.0747	93.4132	92.6527

*Results of scaled design when $R_N = 1$, $N_{pe,basis} = 0.2$, and $c_F = 2.9$ g/L (linear region). Other conditions in Table 1.

Table 10. Effect of Changing R_p for SMB8*

		Scaled Design					
		1	2	Basis	3	4	5
$a = d_{p,new}/d_{p,old}$		1	1	1	1	1	1
$b = L_{new}/L_{old}$		2	1.414	1	0.707	0.5	0.354
$c = D_{col,new}/D_{col,old}$		0.707	0.841	1	1.189	1.414	1.682
$g = Q_{new}/Q_{old}$		1	1	1	1	1	1
R_p		4	2	1	1/2	1/4	1/8
$10N_{pe,basis}$	Raffinate (%)	72.3038	72.3793	72.3610	72.2660	72.3033	72.1102
	Extract (%)	99.2594	99.2653	99.2622	99.2513	99.2520	99.2284
$N_{pe,basis}$	Raffinate (%)	72.3023	72.3770	72.3579	72.2616	72.2769	72.1012
	Extract (%)	99.2370	99.2338	99.2172	99.1862	99.1593	99.0908
$0.1N_{pe,basis}$	Raffinate (%)	72.2845	72.3498	72.3159	72.1955	72.1871	71.9161
	Extract (%)	98.9910	98.8762	98.6840	98.3706	97.9176	97.1200

*Results of scaled design when $R_N = 1$, $N_{pe,basis} = 0.2$, and $c_F = 10$ g/L (nonlinear region). Other conditions in Table 1.

isotherms. Once a base or old design is available, the scaling procedure calculates changes in the column length, column diameter, particle diameter and flow rate so that pressure drop, product purities, and throughput change in a predictable fashion. The same product purities will be obtained if $R_N = 1$. If $R_N > 1$, the separation will be improved. If particle diameters are decreased, the operation will be intensified, resulting in a smaller and probably less expensive sys-

tem. The need to decrease dead volumes, cycle faster, and effectively pack small-diameter particles will ultimately limit intensification. However, since many SMB systems use particles with diameters significantly greater than the 32- μ m dia. used for the base case here, there is significant room for intensification of SMB processes. The bed can also be scaled without changing the particle diameter.

Table 11. Effect of Changing R_N *

		Scaled Design					
		1	2	Basis	3	4	5
$a = d_{p,new}/d_{p,old}$		1	1	1	1	1	1
$b = L_{new}/L_{old}$		0.5	0.7071	1	1.4142	2	2.8284
$c = D_{col,new}/D_{col,old}$		0.7071	0.8409	1	1.1892	1.4142	1.6818
$g = Q_{new}/Q_{old}$		1	1	1	1	1	1
R_N		1/4	1/2	1	2	4	8
bc^2		1/4	1/2	1	2	4	8
$t_{sw,new}/t_{sw,old}$		1/4	1/2	1	2	4	8
Purity (%) in raffinate		82.5059	92.1116	96.5796	98.3631	98.9135	99.2039
Purity (%) in raffinate		80.4199	90.5245	95.4091	97.4921	98.4480	98.8626

*Results of scaled design for SMB8 (2,2,2,2) when $R_p = 1$, $g = 1$, $a = 1$, $D/F = 5.89$, and $c_F = 2.9$ g/L (linear region). N_{pe} calculated by Eq. 21. Other conditions in Table 1.

Table 12. Effect of Changing R_N *

		Scale Design					
		1	2	Basis	3	4	5
$a = d_{p,new}/d_{p,old}$		1	1	1	1	1	1
$b = L_{new}/L_{old}$		0.5	0.7071	1	1.4142	2	2.8284
$c = D_{col,new}/D_{col,old}$		0.7071	0.8409	1	1.1892	1.4142	1.6818
$g = Q_{new}/Q_{old}$		1	1	1	1	1	1
R_N		1/4	1/2	1	2	4	8
bc^2		1/4	1/2	1	2	4	8
$t_{sw,new}/t_{sw,old}$		1/4	1/2	1	2	4	8
Purity (%) in raffinate		68.9379	71.6154	72.3577	72.5847	72.6518	72.7038
Purity (%) in extract		86.3019	95.7905	99.2180	99.8673	99.9677	99.9875

*Results of scaled design for SMB8 (2,2,2,2) when $R_p = 1$, $g = 1$, $a = 1$, $D/F = 5.89$, and $c_F = 10$ g/L (nonlinear region). N_{pe} calculated by Eq. 21. Other conditions in Table 1.

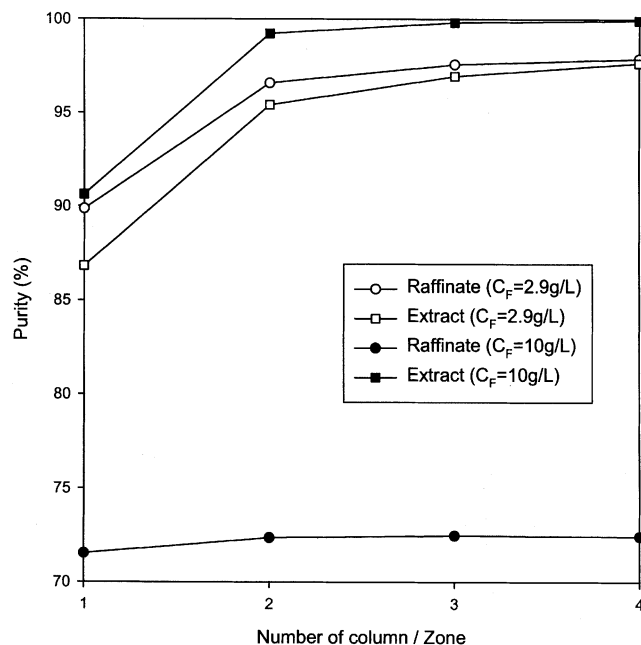


Figure 4. Influence of number of columns per zone with constant amount of adsorbent.
Simulations of base cases listed in Table 1; N_{pe} calculated by Eq. 21.

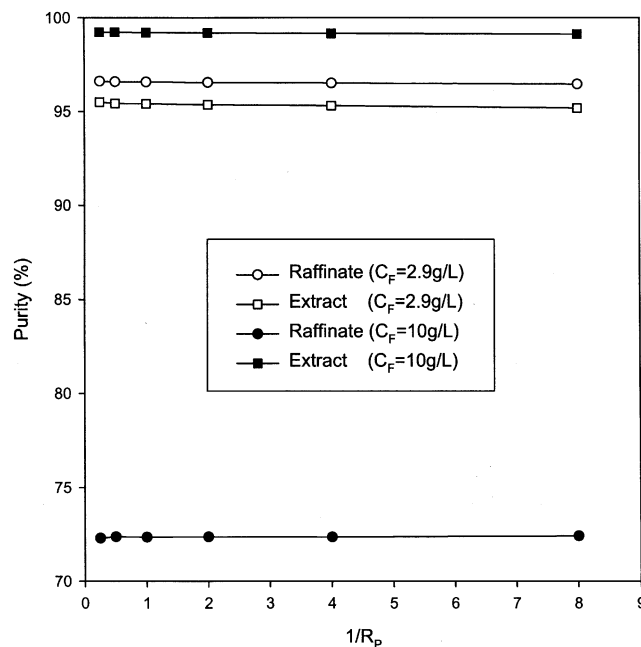


Figure 5. Influence of R_p for (2,2,2,2) SMB8 when $R_N = 1$, $g = 1$, $a = 1$, $D/F = 5.89$.
 N_{pe} calculated by Eq. 21. Base case listed in Table 1.

Identical scaling rules can be developed by ignoring the second-order axial dispersion terms in the mass and energy balances, and then nondimensionalizing the equilibrium equations, mass balances, energy balances, transfer equations, and boundary conditions (Wankat, 1992). Equation 14

Table 13. Scale-up by Increasing Flow Rates for SMB8 (2,2,2,2) when $R_p = 1$, $R_N = 1$, $a = 1$, $b = 1$, $D/F = 5.89$, and $c_F = 2.9$ g/L (linear region)*

	Scaled Design				
	Basis	1	2	3	4
$g = Q_{new}/Q_{old}$	1	2	5	10	100
$c = D_{col,new}/D_{col,old}$	1	1.4142	2.2361	3.1623	10
$t_{sw,new}/t_{sw,old}$	1	1	1	1	1
Purity (%) raffinate	96.5796	96.5786	96.5791	96.5795	96.5794
Purity (%) in extract	95.4091	95.4057	95.4078	95.4094	95.4088

* N_{pe} calculated by Eq. 21. Other conditions in Table 1.

Table 14. Scale-Up by Increasing Flow Rates for SMB8 (2,2,2,2) when $R_p = 1$, $R_N = 1$, $a = 1$, $b = 1$, $D/F = 5.89$, and $c_F = 10$ g/L (nonlinear region)*

	Scaled Design				
	Basis	1	2	3	4
$g = Q_{new}/Q_{old}$	1	2	5	10	100
$c = D_{col,new}/D_{col,old}$	1	1.4142	2.2361	3.1623	10
$t_{sw,new}/t_{sw,old}$	1	1	1	1	1
Purity (%) in raffinate	72.3577	72.3645	72.3614	72.3588	72.3577
Purity (%) in extract	99.2180	99.2184	99.2181	99.2178	99.2179

* N_{pe} calculated by Eq. 21. Other conditions in Table 1.

Table 15. Effect of Changing Particle Diameter for SMB8*

	Scaled Design				
	1	2	Basis	3	4
$a = d_{p,new}/d_{p,old}$	0.6	0.75	1	2	4
$b = L_{new}/L_{old}$	0.36	0.563	1	4	16
$t_{sw,new}/t_{sw,old}$	0.36	0.563	1	4	16
$g = Q_{new}/Q_{old}$	1	1	1	1	1
$N_{pe,basis}$ Raffinate (%)	96.5377	96.5670	96.5785	96.6097	96.6252
Extract (%)	95.3444	95.3881	94.4074	95.4597	95.4858
$0.1N_{pe,basis}$ Raffinate (%)	95.5359	95.7778	95.9939	96.3240	96.4841
Extract (%)	93.7407	94.1114	94.4524	94.9859	95.2499

*Results of scaled design when $R_N = 1$, $N_{pe,basis} = 0.2$, and $c_F = 2.9$ g/L (linear region). Other conditions in Table 1.

Table 16. Effect of Changing Particle Diameter for SMB8*

	Scaled Design				
	1	2	Basis	3	4
$a = d_{p,new}/d_{p,old}$	0.6	0.75	1	2	4
$b = L_{new}/L_{old}$	0.36	0.563	1	4	16
$t_{sw,new}/t_{sw,old}$	0.36	0.563	1	4	16
$g = Q_{new}/Q_{old}$	1	1	1	1	1
$N_{pe,basis}$ Raffinate (%)	72.3279	72.3357	72.3579	72.3596	72.3605
Extract (%)	99.1834	99.2039	99.2172	99.2424	99.2548
$0.1N_{pe,basis}$ Raffinate (%)	72.2458	72.2753	72.3159	72.3417	72.3522
Extract (%)	98.2002	98.4560	98.6840	98.9986	99.1388

*Results of scaled design when $R_N = 1$, $N_{pe,basis} = 0.2$, and $c_F = 10$ g/L (nonlinear region). Other conditions in Table 1.

arises naturally from the dimensionless form of the boundary conditions. With this approach it is easy to show that the scaling procedure is applicable to competitive nonlinear

Table 17. Effect of Changing R_p for SMB8*

		Scaled Design					
		1	2	Basis	3	4	5
$a = d_{p,new}/d_{p,old}$		1	1	1	1	1	1
$b = L_{new}/L_{old}$		2	1.414	1	0.707	0.5	0.354
$c = D_{col,new}/D_{col,old}$		0.707	0.841	1	1.189	1.414	1.682
$g = Q_{new}/Q_{old}$		1	1	1	1	1	1
R_p		4	2	1	1/2	1/4	1/8
$10N_{pe,basis}$	Raffinate (%)	94.7680	94.6130	94.7500	94.7765	94.7598	94.8245
	Extract (%)	86.5885	85.9912	86.5143	86.6287	86.5679	86.8277
$N_{pe,basis}$	Raffinate (%)	94.7432	94.7044	94.6948	94.7063	94.6603	94.6836
	Extract (%)	86.5269	86.3919	86.3776	86.4551	86.3228	86.4822
$0.1N_{pe,basis}$	Raffinate (%)	94.4930	94.3487	94.1890	93.9857	93.6299	93.2044
	Extract (%)	85.9203	85.5395	85.1845	84.7926	84.0187	83.3132

*Results of scaled design when $R_N = 1$, $V_D = 0.1 V_{total}$, $N_{pe,basis} = 0.2$, and $c_F = 2.9$ g/L (linear region). Other conditions in Table 1.

Table 18. Effect of Changing R_p for SMB8*

		Scaled Design					
		1	2	Basis	3	4	5
$a = d_{p,new}/d_{p,old}$		1	1	1	1	1	1
$b = L_{new}/L_{old}$		2	1.414	1	0.707	0.5	0.354
$c = D_{col,new}/D_{col,old}$		0.707	0.841	1	1.189	1.414	1.682
$g = Q_{new}/Q_{old}$		1	1	1	1	1	1
R_p		4	2	1	1/2	1/4	1/8
$10N_{pe,basis}$	Raffinate (%)	82.2260	82.3487	82.3186	82.1634	82.2233	81.9094
	Extract (%)	99.1068	99.0997	99.1002	99.1066	99.1014	99.1142
$N_{pe,basis}$	Raffinate (%)	82.2178	82.3364	82.3012	82.1401	82.1888	81.8654
	Extract (%)	99.0906	99.0767	99.0676	99.0605	99.0357	99.0211
$0.1N_{pe,basis}$	Raffinate (%)	82.1242	82.1907	82.0835	81.8213	81.6811	81.1181
	Extract (%)	98.9409	98.8307	98.7095	98.5347	98.2488	97.8274

*Results of scaled design when $R_N = 1$, $V_D = 0.1 V_{total}$, $N_{pe,basis} = 0.2$, and $c_F = 10$ g/L (nonlinear region). Other conditions in Table 1.

Table 19. Effect of Changing Particle Diameter for SMB8*

		Scaled Design				
		1	2	Basis	3	4
$a = d_{p,new}/d_{p,old}$		0.6	0.75	1	2	4
$b = L_{new}/L_{old}$		0.36	0.563	1	4	16
$t_{sw,new}/t_{sw,old}$		0.36	0.563	1	4	16
$g = Q_{new}/Q_{old}$		1	1	1	1	1
$N_{pe,basis}$	Raffinate (%)	94.6167	94.6603	94.6948	94.8924	95.0661
	Extract (%)	86.4769	86.4963	86.3776	86.4938	86.4473
$0.1N_{pe,basis}$	Raffinate (%)	93.7638	93.7261	94.1890	94.6315	94.9384
	Extract (%)	84.5452	84.3822	85.1845	85.8931	86.1451

*Results of scaled design when $R_N = 1$, $V_D = 0.1 V_{total}$, $N_{pe,basis} = 0.2$, and $c_F = 2.9$ g/L (linear region). Other conditions in Table 1.

Table 20. Effect of Changing Particle Diameter for SMB8*

		Scaled Design				
		1	2	Basis	3	4
$a = d_{p,new}/d_{p,old}$		0.6	0.75	1	2	4
$b = L_{new}/L_{old}$		0.36	0.563	1	4	16
$t_{sw,new}/t_{sw,old}$		0.36	0.563	1	4	16
$g = Q_{new}/Q_{old}$		1	1	1	1	1
$N_{pe,basis}$	Raffinate (%)	81.2838	81.7658	82.3013	82.6126	81.7148
	Extract (%)	99.0536	98.2342	99.0676	99.0813	99.0796
$0.1N_{pe,basis}$	Raffinate (%)	80.9751	81.2184	82.0836	82.4601	81.6637
	Extract (%)	98.4270	98.5799	98.7095	98.9135	98.9976

*Results of scaled design when $R_N = 1$, $V_D = 0.1 V_{total}$, $N_{pe,basis} = 0.2$, and $c_F = 10$ g/L (nonlinear region). Other conditions in Table 1.

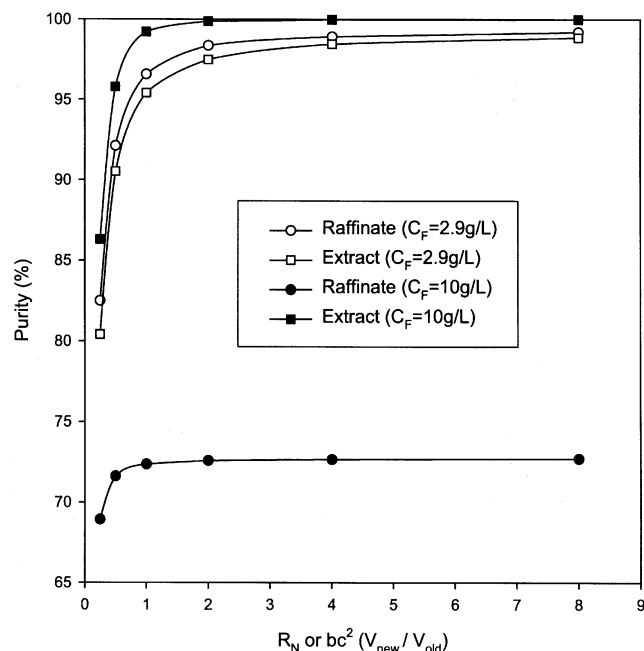


Figure 6. Influence of R_N or R_V for (2,2,2) SMB8 when $R_p = 1$, $g = 1$, $a = 1$, $D/F = 5.89$ ($R_N = R_V = bc^2$ when $a = g = 1$).

N_{pe} calculated by Eq. 21. Base case listed in Table 1.

isotherms. Although we have illustrated the scaling procedure for four-zone SMBs, they are also valid for SMB systems with different numbers of zones and for SMBs with variable flow rates. The restrictions on the boundary conditions require that the ratio of the period for each step divided by the switching time is constant. One limitation of the technique is that it cannot be used to calculate the effect of changing the number of zones or the number of columns. For example, the procedure will not calculate the conversion of a four-zone SMB into a three-zone SMB or vice versa.

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Notation

a = ratio of particle diameters in two designs, $d_{p,new}/d_{p,old}$
 b = ratio of column lengths in two designs, L_{new}/L_{old}
 c = ratio of column diameters in two designs, D_{new}/D_{old}
 c_i = concentration of component i , g/L
 c_F = feed concentration, g/L
 C_i = constant for determining solute velocity, Eq. 11
 d_p = particle diameter, cm
 D = volumetric flow rate, desorbent, mL/min
 D_{col} = column diameter, cm
 g = ratio of volumetric flow rate, $Q_{j,new}/Q_{j,old} = F_{new}/F_{old}$
 L = column length, cm
 L_{MTZ} = length of mass-transfer zone, cm
 N_{pe} = Peclet number
 N_{Re} = Reynolds number
 q^* = adsorbed concentration in equilibrium with fluid phase concentration, g/L

Q_j = volumetric flow rate in zone j , mL/min
 R_N = ratio of the fractional bed use in two designs, $(L/L_{MTZ})_{j,new}/(L/L_{MTZ})_{j,old}$
 R_p = ratio of pressure drops in two designs, $\Delta P_{j,new}/\Delta P_{j,old}$
 R_V = ratio of adsorbent volumes, $V_{j,new}/V_{j,old}$
 t_{sw} = switching time, min
 u_{ij} = velocity of solute i in zone j , cm/min
 v_j = superficial fluid velocity in zone j , cm/min
 V_D = dead volume, cm³
 V_j = adsorbent volume in zone j , cm³

Greek letters

ϵ = porosity
 μ = viscosity

Subscripts

A = less retained component
 B = more retained component

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