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Z. P. Lu[a]; C. B. Ching[a]
[a] CHEMICAL DEPARTMENT, NATIONAL UNIVERSITY OF SINGAPORE KENT RIDGE, SINGAPORE

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Dynamics of Simulated Moving-Bed Adsorption Separation Processes

Z. P. LU and C. B. CHING*
CHEMICAL DEPARTMENT
NATIONAL UNIVERSITY OF SINGAPORE
KENT RIDGE, SINGAPORE 119260

ABSTRACT

Two mathematical models, namely the continuous moving-bed model (steady-state model) and the intermittent moving-bed model (transient model), have been used to describe simulated moving-bed adsorption separation processes. Four-column and 12-column simulated moving-bed systems for the separation of optical isomers with nonlinear adsorption isotherms were studied with the two models, respectively. The model equations were solved by using the numerical method of orthogonal collocation in finite elements. For the 4-column simulated moving bed, the differences between the simulation results from the two mathematical models are very obvious. Process dynamics, i.e., evolution of the species concentrations in the extract and raffinate and the axial profiles at different times, of the above systems in one switching period at the cyclic steady state are presented and discussed. They were numerically simulated with the intermittent moving bed model. The computations in a Cray J916 computer were very time consuming for the 12-column system.

Key Words. Separation; Simulated moving bed; Modeling; Numerical simulation

INTRODUCTION

Simulated moving-bed (SMB) separation technology has been extensively used for the large-scale fractionation of sugars and xylene isomers

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* To whom correspondence should be addressed.

for more than 30 years (2). Recently, this technology has been brought into the field of fine chemistry, pharmaceutical, and agricultural research and production (3). It is very clear that simulated moving-bed separation leads to a great saving of eluent and a significant improvement of adsorbent efficiency when compared with preparative elution chromatography (1). However, there are some limitations in the use of simulated moving-bed separation processes as pointed out by Nicoud et al. (4). A simulated moving bed is basically a binary separator. For a multicomponent system, a simulated moving bed can be used without technical modifications if the product to be recovered is the first or the last eluted one in a multicomponent mixture. The main drawback of a simulated moving bed stems from its lack of versatility. Therefore, a simulated moving bed is normally designed for long-term productions.

A sketch of a continuous moving bed is shown in Fig. 1(a). In this configuration the liquid goes up and solid goes down in each zone, and then countercurrent contact between solid and liquid occurs, leading to

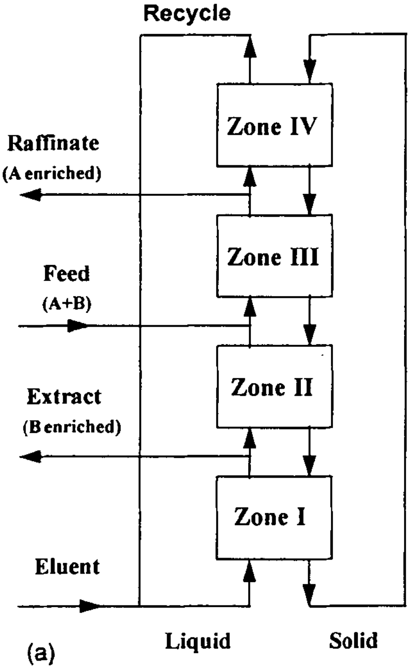

FIG. 1 Sketch of the operating schemes. (a) Continuous moving bed. (b) 12-column simulated moving bed.

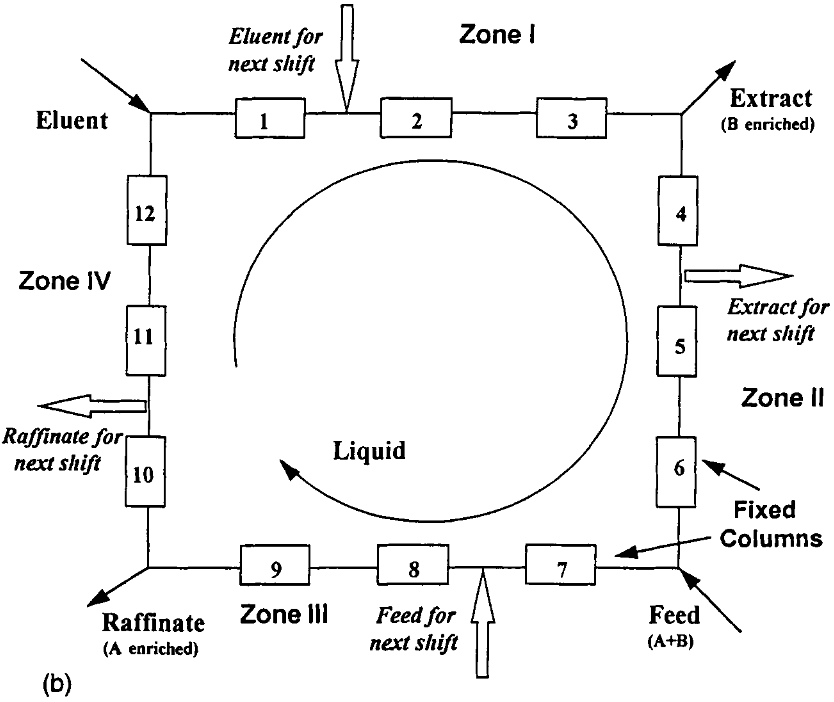

FIG. 1 Continued

a high mass transfer driving force. Provided that the adsorption affinities of species A and B on the adsorbent are different, it is possible to choose the right flow rates of the solid and the liquid to force A to move upward and B to move downward, thus leading to a spatial separation. This system requires two inlet lines (one for the feed and one for the eluent) and two outlet lines (one for the raffinate and one for the extract). Unfortunately, the concept cannot really be implemented since the movement of solid is extremely difficult to handle. This is the main reason why a simulated moving bed is preferred. In the configuration of a simulated moving bed as shown in Figure 1(b), the adsorbent is kept fixed but the inlet and outlet lines are moved step by step between a given number of fixed columns (a simulated moving bed is normally made up of 4 to 24 columns). When the number of columns used increases and the length of the column decreases, i.e., as the switching time decreases, the simulated moving bed approaches the continuous moving-bed system. The movement of adsorbent is only simulated by shifting the inlet and outlet lines. Therefore, the simulated solid flow rate is directly related to the switching time. A simulated moving bed normally consists of four zones (less or more for some particular cases) (5, 6) which is divided by the inlet and outlet lines as shown in Fig. 1(b). If the recycle flow rate is defined as the flow rate in the columns between the eluent and the extract lines and in Zone I, then columns between extract and feed lines are in Zone II, columns between feed and raffinate lines are in Zone III, and columns between raffinate and eluent lines are in Zone IV. The flow rates in each zone must kept constant.

Modeling and simulation of the simulated moving-bed separation processes have gained increasing attention because they could lead to significant savings in materials (particular for expensive materials) and time as the operating parameters could be determined during the technology development stage itself. The design of a simulated moving bed mainly relies on the appropriate choice of different flow rates: recycle, feed, eluant, extract, raffinate, and solid (equivalent to the switching time). The design guideline for linear systems has been stated by Ruthven and Ching (7). However, for nonlinear systems the estimation of flow rates is extremely difficult and has a significant effect on the separation results. Hashimoto et al. (8) developed the model equations for simulated moving-bed reactors and continuous moving-bed reactors and solved them by using the finite difference method. Although the configurations were made of three zones, the reaction was considered in the processes. They stated that the simulation methods can be applied to both linear and nonlinear systems, but this was not substantiated by simulation results for the nonlinear system. Computer software for the design of a simulated moving bed was developed by Nicoud et al. (4). The main principle of the software relies on the estimation of different flow rates which allows the dispersion or compression (owing to the steep isotherm) to stabilize in the right zones. Storti et al. (9) proposed a method to design optimal operating conditions for simulated moving-bed adsorption separation process based on the equilibrium theory but which neglected the mass transfer resistances and axial dispersion. Separation of enantiomers with simulated moving-bed technology was also recently studied by Rodrigues et al. (10) with the continuous moving bed model by a steady-state mathematical model. However, a simulated moving bed is operated at the cyclic steady state, and the operation between two switchings of the input and output lines is in a transient regime. Hence, the question raised is: What are the limitations for using the steady-state mathematical model to describe transient operation for simulated moving-bed operations. In 1988, Storti et al. (11). studied xylene isomer separation with the simulated moving-bed technology. A steady-state countercurrent column model and a simulated moving-bed column model were developed, numerically solved, and compared. They mainly focused on the process separation performance difference of the two separation processes, countercurrent moving bed, and simulated moving bed.

The objective of this paper is to study the process dynamics of the simulated moving bed and compare the simulation on-column concentration profiles from the transient mathematical model and the steady-state mathematical model.

PROCESS DESCRIPTION AND MATHEMATICAL MODEL

The separation system to be studied in this work is the enantiopurification of the (±)-1a,2,7,7a-tetrahydro-3-methoxy-naphth(2,3-b)-oxirane on microcrystalline cellulose triacetate (C.T.A.) with pure methanol as the eluent (1). The simulated moving beds were made of 4 and 12 Superformance columns packed with C.T.A. (dp > 40 μm), the working temperature was set to 25°C, and the other parameters used are listed in Table 1. For simplification, the (+) isomer is called species A and the (−) isomer is called species B, where species B is more adsorbable and the eluant is nonadsorbable.

The mathematical models for the two configurations shown in Figs. 1(a) and 1(b) are based on the following assumptions:

1. The adsorbent is homogeneous.
2. The flow pattern inside columns or sections can be described by axial dispersed plug flow.
3. The "dead" volumes at both ends of the packed adsorbents are negligible.
4. The mass transfer between fluid and particle can be described by the Linear Driving Force model (12).

TABLE 1
Values Used in the Simulations

- Superformance column:
  - Column number $m = 4$ and 12
  - Column length $L = 11$ cm
  - Bed porosity $\epsilon = 0.4$
- Adsorption isotherms:
  - $K_A = K_B = 1.57$ mg/mL of beads
  - $q_m = 5.8$ mg/mL of beads
  - $b_A = 0.045$, $b_B = 0.127$ mL/mg
- Mass transfer:
  - $k_A = k_B = 0.1$ s^{-1}
- Operating parameters:
  - $C_{fA} = C_{fB} = 5$ mg/mL
  - $V_{ra} = 205$ mL/min, $V_{fe} = 152$ mL/min
  - $V_{ex} = 400$ mL/min, $V_d = 4.63$ mL/min
  - $V_{re} = 2037$ mL/min, $t_s = 433$ min

5. The nonlinear multicomponent adsorption isotherms for species A and B follows the extended Langmuir expressions (13).

Continuous Moving-Bed Model (steady-state mathematical model)

Introducing the dimensionless variable, $x = z/L_j$, we can get:

- Mass balances inside the sections and mass transfer between the fluid and the adsorbent:

$$\frac{1}{\mathrm{Pe}_i}\frac{d^2c_{ij}}{dx^2} - \frac{dc_{ij}}{dx} - \frac{(1-\epsilon)}{\epsilon}\xi_j\frac{dq_{ij}}{dx} = 0 \tag{1}$$

$$\alpha_i\frac{dq_{ij}}{dx} = f(c_{ij}) - q_{ij} \tag{2}$$

- Boundary conditions for the four sections:

$$x = 0, \qquad c_{ij} - \frac{1}{\mathrm{Pe}_j}\frac{\partial c_{ij}}{\partial_x} = c_{ij} \qquad \frac{\partial q_{ij}}{\partial x} = 0 \tag{3a}$$

$$x = 1, \qquad \frac{\partial c_{ij}}{\partial x} = 0, \qquad q_{ij} = q_{ij+1}|_{x=0} \tag{3b}$$

- Multicomponent Langmuir adsorption isotherms (3):

$$f(c_{ij}) = K_i c_{ij} + \frac{q_m b_i c_{ij}}{1} + \sum_{i=1}^{n} b_i c_{ij} \tag{4}$$

- Overall mass balances at the nodes of the sections:

$$\begin{aligned} V_1 &= V_{\mathrm{re}} + V_{\mathrm{el}}, \qquad V_2 = V_{\mathrm{el}} + V_{\mathrm{re}} - V_{\mathrm{ex}}, \\ V_3 &= V_{\mathrm{re}} + V_{\mathrm{ra}}, \qquad V_4 = V_{\mathrm{re}} \end{aligned} \tag{5}$$

- Species mass balances at the nodes of sections:

$$c_{fij} = c_{ij-1}|_{x=1} \qquad \text{for } j = 2 \text{ and } 4 \tag{6}$$

$$c_{fi1} = \frac{V_4}{V_1}c_{i4}|_{x=1}, \qquad c_{fi3} = \frac{V_2 c_{i2}|_{x=1} + V_{fe}c_{ij}}{V_3} \tag{7}$$

The model parameters are: (a) Axial Peclet number:

$$\mathrm{Pe}_j = \frac{(v_j + u_s)L_j}{D_{L_j}} \tag{8a}$$

(b) Ratio of the flow rate between solid and liquid:

$$\xi_j = \frac{u_s}{v_j} \tag{8b}$$

(c) Reciprocal of mass transfer unit:

$$\alpha_{ij} = \frac{1 u_s}{k_i L_j} \tag{8c}$$

where i = A, B refers to the species, $j = 1, 2, \ldots$, refers to the number of sections in the continuous moving bed, L_j is the length of the section, v_j is the interstitial liquid velocity, D_{Lj} is the axial dispersive coefficient, k_i is the lumped mass transfer coefficient of the species i between the fluid and the adsorbent, and u_s is the equivalent interstitial solid velocity in the process for which $u_s = L/t_s$ for the simulated moving bed, where L is the length of the column and t_s is the switching time.

Intermittent Moving-Bed Model (transient mathematical model)

Introducing the dimensionless variables $x = z/L$ and $\tau = t/t_\iota$, we can get:

- Mass balances inside the columns and mass transfer between the fluid and the adsorbent:

$$\frac{1}{\mathrm{Pe}}\frac{\partial^2 c_{ij}}{\partial x^2} - \gamma_j \frac{\partial c_{ij}}{\partial_x} = \frac{\partial c_{ij}}{\partial \tau} + \frac{(1-\epsilon)}{\epsilon}\frac{\partial q_{ij}}{\partial \epsilon} \tag{9}$$

$$\alpha_i \frac{\partial q_{ij}}{\partial \tau} = f(c_{ij}) - q_{ij} \tag{10}$$

where $f(c_{ij})$ is stated in Eq. (4).

- Boundary and initial conditions for the columns:

$$x = 0, \qquad c_{ij} - \frac{1}{\gamma_j \mathrm{Pe}}\frac{\partial c_{ij}}{\partial x} = c_{ifj} \tag{11a}$$

$$x = 1, \qquad \frac{\partial c_{ij}}{\partial x} = 0 \tag{11b}$$

$$\tau = 0, \qquad c_{ij} = c_{ij0}, \quad \forall x \tag{11c}$$

- Mass balances at the nodes of the columns:

$$c_{fij} = c_{ij-1}|_{x=1} \tag{12a}$$

Except:

$$c_{fij} = \frac{V_{j-1}}{V_j} c_{ij-1}\big|_{x=1} \tag{12b}$$

for the column where the eluant is introduced

$$c_{fij} = \frac{V_{j-1}\big|_{x=1} + V_f c_{fi}}{V_j} \tag{12c}$$

for the column where the feed is introduced

The model parameters are: (a) Axial Peclet number:

$$\text{Pe} = \frac{v_1 L}{D_L} \tag{13a}$$

(b) Ratio of the liquid flow rate between bed j and bed 1:

$$\gamma_j = \frac{v_j}{v_1} \tag{13b}$$

(c) Reference reciprocal of mass transfer unit:

$$\alpha_i = \frac{1}{k_i} \frac{v_1}{L} \tag{13c}$$

where i = A, B refers to the species, $j = 1, 2 \ldots$ refers to the number of the column, $t_1 = L/v_1$ is the reference space time, and v_1 is the interstitial liquid velocity in column 1.

Process Performance Parameters

1) Purity of the products in their enriched streams:

a) For the continuous moving-bed model:

$$y_A = \frac{c_A}{c_A + c_B} \text{ (in the raffinate)}; \qquad y_B = \frac{c_B}{c_A + c_B} \text{ (in the extract)} \tag{14a}$$

b) For the intermittent moving-bed model:

$$y_A = \frac{\int_0^s c_A d\tau}{\int_0^s (c_A + c_B) d\tau} \text{ (in the raffinate)};$$

$$y_B = \frac{\int_0^s c_B d\tau}{\int_0^s (c_A + c_B) d\tau} \text{ (in the extract)} \tag{14b}$$

2) Recovery of the products in their enriched streams:

a) For the continuous moving-bed model:

$$R_A = \frac{V_{ra}c_A}{V_{fe}c_{fA}} \text{ (in the raffinate)}; \qquad R_B = \frac{V_{ex}c_B}{V_{fe}c_{fB}} \text{ (in the extract)} \tag{15a}$$

b) For the intermittent moving-bed model:

$$R_A = \frac{V_{ra}\int_0^s c_A d\tau}{\tau_s V_{fe} c_{fA}} \text{ (in the raffinate)}; \qquad R_B = \frac{V_{ex}\int_0^s c_B d\tau}{\tau_s V_{fe} c_{fB}} \text{ (in the extract)} \tag{15b}$$

where τ_s is the dimensionless switching time.

SIMULATION RESULTS AND DISCUSSIONS

In the above model equations the boundary conditions are related between the sections or columns and they vary with time in the intermittent moving bed model, so the equations for all sections and columns could be solved simultaneously. The method of orthogonal collocation in finite elements was used to obtain the numerical simulation results [PDECOL package by Madsen and Sincovec (14)]. Fifteen elements were normally used in each section or each column, and only minor numerical oscillations in axial concentration profiles were found (Figs. 2b and 5). Very obvious numerical oscillations were found when the number of the elements used was reduced. The details of simulating the transitions of the boundary conditions while switching the input and output lines can be found elsewhere (15). For the continuous moving-bed model, each calculation took 15 minutes of CPU time in a Cray J916 computer. However, the numerical calculations for the intermittent moving-bed model were very time consuming. Normally, 9 to 10 cycles were needed from the clean column initial conditions to reach the cyclic steady state, which means 2 hours and 90 hours of CPU times in the Cray J916 computer for the 4-column and 12-column systems, respectively. When the number of elements used is reduced in each column, the CPU times will be greatly reduced but the accuracy of the simulation results is limited, as mentioned before. Because the boundary conditions at the inlet of each column vary with time, integration of the model equations was very time consuming, and this took the major part of CPU time (15).

Continuous Moving-Bed Model

In previous work (10) a simulated moving bed for the separation system specified above was studied with the continuous moving-bed model, and the performance parameters purity, recovery, solvent consumption, and productivity were defined. The effect of operation parameters on the performance of the simulated moving bed measured by these parameters was also studied. However, a simulated moving bed is actually operated under cyclic steady state. The real operation in the period between two shiftings of the input and output lines is a transient operation since the species concentrations in the output streams are not constants but functions of time. Therefore, for better understanding of the dynamics of the simulated moving bed, a transient mathematical model is essential. Before starting to study the intermittent moving-bed model, we first have to review the continuous moving-bed model. The numerical simulation results found by using the continuous moving-bed model are shown in Figs. 2(a) and 2(b) for the 4- and 12-column systems, respectively. A Peclet number of 1000 was assumed in each section in the simulations. Actually, the effect of the Peclet number on the performance of the processes was studied. When the Peclet number is larger than 500 in each section, the axial profiles are almost the same. The difference in the modeling between the 12-column system and the 4-column system is only the value of the parameter, α_{ij}, the reciprocal of mass transfer unit, i.e., $(\alpha_{ij})_{3\text{-column}} = 3(\alpha_{ij})_{12\text{-column}}$, and which means that the number of the mass transfer unit for the 12-column system is 3 times of that for the 4-column system. The purities of the species A and B in the raffinate and the extract streams are 97.9 and 97.3% for the 12-column system, 84.3 and 78.4% for the 4-column system, respectively. The recoveries are 97.2 and 97.9% for the 12-column system, 76.3 and 85.7% for the 4-column system.

Intermittent Moving-Bed Model

The evolution of the concentrations for species A and B in the extract and the raffinate for one switching period at the cyclic steady state is shown in Figs. 3(a) and 3(b) for the 4- and 12-column systems, respectively. The concentrations of species A and B increase in the raffinate and decrease in the extract with the time. This is because that concentra-

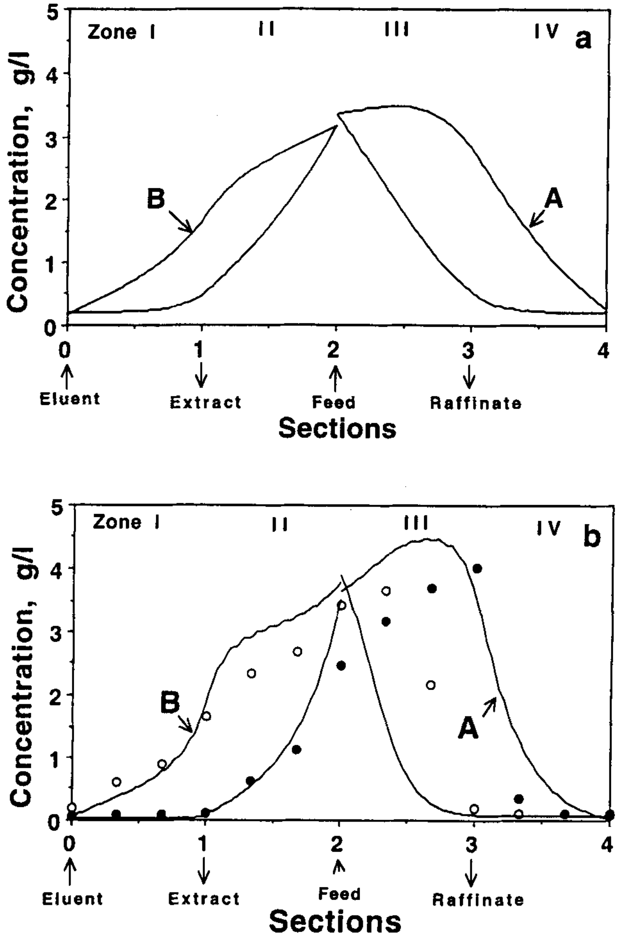

FIG. 2 Axial concentration profiles simulated with the continuous moving-bed model. (a) 4-column system. (b) 12-column system.

tion peaks locate in Zones II and III and move in the same direction as the recycle liquid with time. The decreases and increases of the concentrations are not linear, which means their average values are different from those at the middle of the switching period. The variations of species concentrations are very significant. Concentrations more than 2 times higher or lower between the beginning and the end in a switching period is found for both systems. The purity of species A and B, defined in Eq.

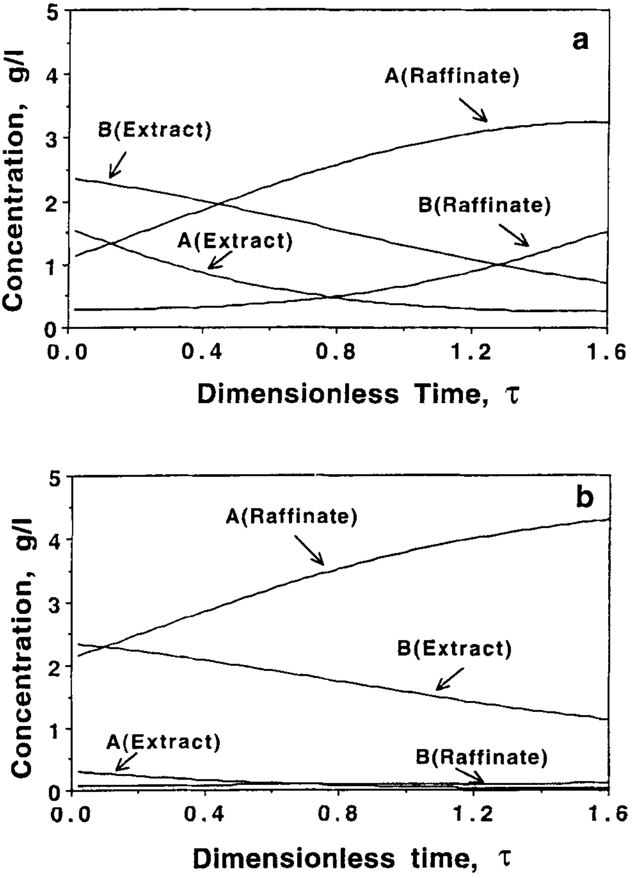

FIG. 3 Elution of concentrations of species A and B in the extract and the raffinate for a switching period at the cyclic steady-state simulated with the intermittent moving-bed model. (a) 4-column system. (b) 12-column system.

(14b), in the raffinate and the extract are 79.3 and 71.6% for the 4-column system, 97.6 and 95% for the 12-column system, respectively. The recoveries for species A and B, defined in Eq. (15b), are 67.5 and 82.4% for the 4-column system, 94.8 and 97.6% for the 12-column system, respectively. Compared with the results from the continuous moving-bed model, the separation performance of a continuous moving bed is certainly better than that of a simulated moving bed. The separation performance of the 12-column simulated moving bed approaches that of the continuous moving bed, but for the 4-column simulated moving bed the difference is very obvious. Cross points of concentration evolution of species A and B in

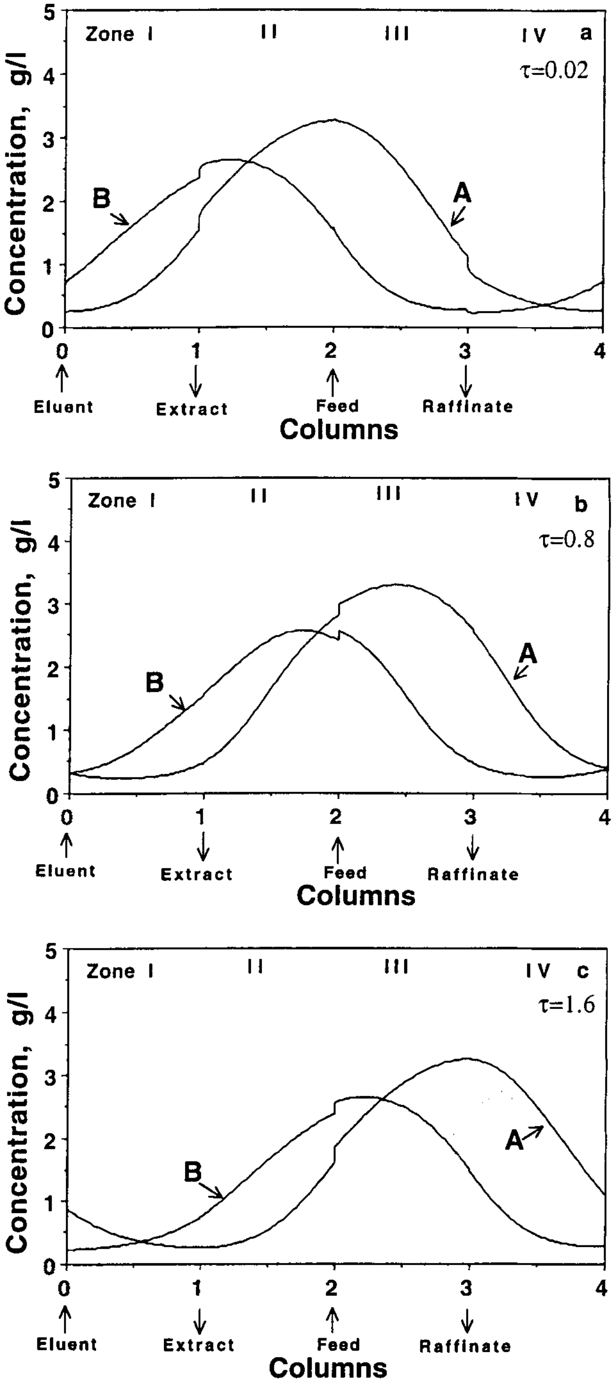

FIG. 4 Axial concentration profiles for the different dimensionless times at the cyclic steady-state of the 4-column system simulated with the intermittent moving model. (a) $\tau = 0.02$. (b) $\tau = 0.8$. (c) $\tau = 1.6$.

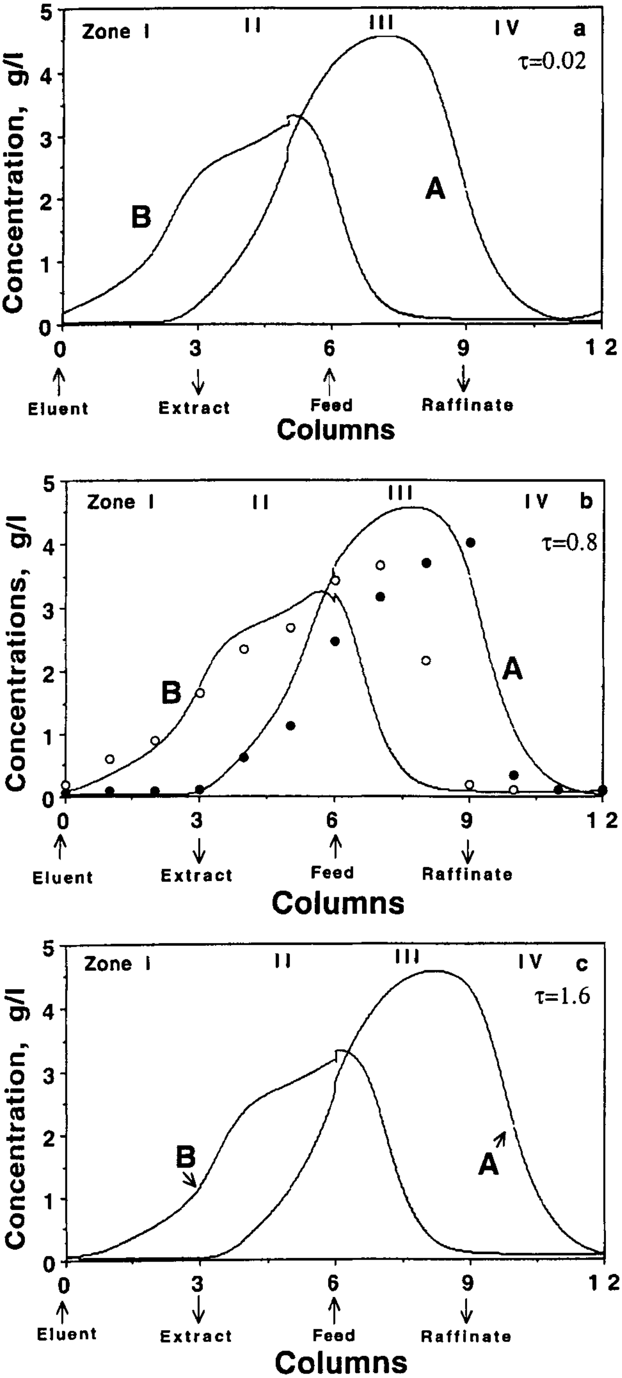

FIG. 5 Axial concentration profiles for the different dimensionless times at the cyclic steady-state of the 12-column system simulated with the intermittent moving model. (a) $\tau = 0.02$. (b) $\tau = 0.8$. (c) $\tau = 1.6$.

the extract and the raffinate can be seen in the Fig. 3(a), which means that in the some operation regime the concentrations of the species to be separated are even lower in their enriched streams than in their by-product streams. However, the decision of how many columns should be used in a simulated moving-bed separation process for a good result is strongly related to the adsorption isotherms and mass transfer rates of the separation system used. It cannot be extended to other cases with justification.

The axial concentration profiles at different dimensionless times in a switching period of the cyclic steady state for the 4- and 12-column systems are shown in Figs. 4 and 5, respectively. Again the concentration peaks of species A and B travel from left to right, i.e., the same direction as the movement of the recycle liquid, with time in one switching period. This is similar to what is observed in elution chromatography. In elution chromatography the peak of the less adsorbed species moves faster along the column than that of the more adsorbed species, which leads to spatial separation since it is a batch process. However, more or less the same traveling speed of the two species peaks should be obtained with the right choice of liquid flow rates in each zone, the switching time in a simulated moving bed for the desired separation, and simulated steady-state operation. Two concentration jumping positions can be seen at the nodes where the feed and the eluent lines are introduced. Axial concentration profiles from the continuous moving-bed model are shaped very similarly to those from the intermittent moving-bed model in the middle of a switching period although some differences are also very obvious, particularly for the 4-column system. Because of the simple and less time needed for computation of the continuous moving-bed model, it is acceptable for predicting the separation performance of simulated moving-bed separation processes in the early stages, particularly for systems with more columns. However, the intermittent moving-bed model is still necessary in order to gain the complete operating picture of the simulated moving-bed processes.

Finally, the experimental results of Ref. 1 are plotted in Figs. 2(b) and 5(b). Although the separation performance, i.e., species purities and recoveries in the extract and raffinate streams, is predicted well by both models, the fronts of the concentration peaks in zone III are quite different between the model predictions and the experimental results. The reasons may be that the "dead volume" at both ends of the columns is assumed to be negligible (16), the Linear Driving Force mass transfer model (12) is used, and high species concentrations occur in this zone.

CONCLUSIONS

Two mathematical models, a continuous moving-bed model and a intermittent moving-bed model, have been used to analyze the simulated moving-bed separation process. The models consist of mass balances of species, lumped mass transfer coefficients, and extended Langmuir adsorption isotherms. Danckwerts boundary conditions were used at both ends of the columns or sections. Model equations were numerically solved by using the method of orthogonal collocation in finite elements. Four-column and 12-column simulated moving-bed systems for the separation of optical isomers (1) were studied with the two models and compared. The transition of boundary conditions during shifting of the input and output lines was simulated with a exponential function for the intermittent moving-bed model (16).

Simulation results again showed that a continuous moving bed has better separation performance than a simulated moving bed. The more columns a simulated moving bed has, the better its separation performance as it approaches that of a continuous moving bed. Since the species concentrations in the extract and the raffinate do not increase or decrease linearly with time during a switching period, the axial concentration profiles of the system in the middle of the switching period cannot be used to represent the process performance of a simulated moving bed. We conclude from the simulation results that the continuous moving-bed model is acceptable for general separation performance studies of a simulated moving bed, but the intermittent moving-bed model is necessary for better understanding of the process dynamics. The experimental separation results for the above-mentioned system were well predicted by both models. However, obvious deviations of the axial concentration profiles were found between the experimental and the simulation results. These could be caused by the omission of the "dead volumes" at both ends of the columns and use of the Linear Driving Force mass transfer model.

NOTATIONS

b_i	the extended multicomponent Langmuir isotherm parameter (l/g)
c_{ij}	liquid phase concentration of species *i* in the section or the column *j* (g/L)
c_{fi}	species concentration in the feed or at the inlet (g/L)
D_{Lj}	axial dispersive coefficient in the section or the column *j* (m^2/S)
k_i	lump mass transfer coefficient of the species *i* between fluid and solid phases (l/s)
K	linear adsorption isotherm coefficient
L_j	length of the section *j* (m)
Pe	Peclet number in the bulk fluid
q_{ij}	solid phase concentration of species *i* in the section or the column *j* (g/L)

q_m	maximum adsorption capacity in the Langmuir isotherm (g/L)
R	recovery of the species in its enriched stream
t	time (min)
t_s	switch time (min)
u_s	equivalent interstitial solid velocity in the process (m/min)
v_j	interstitial fluid velocity in the section or the column j (m/min)
V_{el}	eluent flow rate (mL/min)
V_{ex}	extract flow rate (mL/min)
V_{fe}	feed flow rate (mL/min)
V_j	liquid flow rate in the section or the column f (mL/min)
V_{ra}	raffinate flow rate (mL/min)
V_{re}	recycle flow rate (mL/min)
x	dimensionless axial coordinate in the section or the column
y	mole fraction of the species in their enriched streams

Greek Letters

α_i	reciprocal of mass transfer unit stated in Eqs. (8c) and (13c)
ϵ	bed porosity
τ	dimensionless time
τ_s	dimensionless switch time
γ_j	ratio of the fluid velocities stated in Eq. (13b)
ξ_j	ratio of velocities between solid and fluid stated in Eq. (8b)

Subscripts

i	species
j	section or column

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