

Modeling on a Modified Feeding Mode of Simulated Moving Bed for Improving Productivity^{*}

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Abstract A new feeding mode for a simulated moving bed (SMB) is proposed. The outlet stream from zone II is collected at regular intervals. The concentration of the solution is increased by dissolving raw materials and then fed to zone III as the feed stream during the next collection interval. In this feeding mode, the concentration of the stream fed to zone III is identical to that of original feed, while in a conventional SMB, the feed is diluted by mixing with the outlet stream of zone II before feeding to zone III. The new feeding mode increases the inlet concentration of zone III. A modeling investigation shows that higher inlet concentration of zone III increases the height of concentration band in SMB, improving the separation performance significantly. In comparison with the traditional feeding mode, the new feeding mode increases the productivity by 23.52% and decreases the solvent consumption by 22.56%, so as to increase the raffinate and extract concentrations by 53.17% and 20.38%, respectively. The collection interval for the outlet stream from zone II has no effect on the separation performance after reaching the steady state, so that the collection interval can be increased to make the operation more convenient.

Keywords simulated moving bed, feeding mode, modified operation, simulation

1 INTRODUCTION

The simulated moving bed (SMB), developed by Universal Oil Products [1], is a powerful technique for difficult separations. It has been successfully applied to the areas of biotechnology, fine chemicals and pharmaceuticals since 1990s [2–7]. The periodic switches of the feed, desorbent, raffinate and extract ports give the simulated counter-current movement of stationary phase against mobile phase, so that the SMB has the advantage over batch chromatography in terms of the productivity and solvent consumption for binary separations [8].

As shown in Fig. 1 (a), the feed stream is mixed with the outlet stream from zone II of SMB and then enters zone III, which is a process of dilution as the outlet concentration of zone II is normally lower than the feed concentration. The dilution should be suppressed as much as possible to improve the separation processes [9]. Recently, some modifications on the feeding mode were proposed, such as periodical change of feed concentration (ModiCon [10, 11]) or feed flow rate (PowerFeed [10, 12]) during each switch interval, which improve the SMB separation process. However, the dilution of feed stream by the outlet stream from zone II was not avoided.

Wei and Zhao [13] have developed a modified feeding mode, where the outlet stream of zone II flows into a tank to dissolve the solid raw materials and is then pumped into zone III. The inlet concentration of zone III is increased and the solvent consumption is reduced significantly. However, the continuous addition of solid raw materials is a little difficult. And it is

hard to keep a constant dissolution rate of solid materials, so that the inlet concentration of zone III may change randomly, leading to an unsuccessful separation in the case of nonlinear adsorption.

To address the above problem, the operation is further modified as shown in Fig. 1 (b). Zone II does not connect with zone III through any tube or vessel. The stream out of zone II, containing some unseparated solutes, is collected at regular intervals to dissolve fresh raw materials. The solution is then fed back as the feed stream to zone III during the next collection interval. Evidently, the feed concentration in Fig. 1 (b) is higher than that in Fig. 1 (a), potentially improving the productivity. This work will investigate the modified SMB (MF-SMB). A model will be established to compare the MF-SMB with traditional SMB (Tr-SMB).

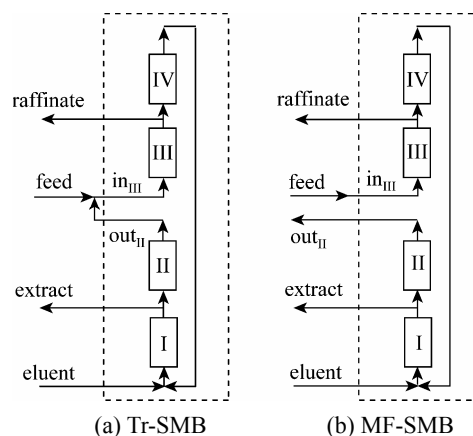


Figure 1 Scheme of traditional SMB and modified SMB

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2 MF-SMB MODEL

The SMB model [7, 13, 14] with the periodic switches of four ports is adopted. During each switch interval, the change of component i in the column k is described by the following transport-dispersive equations.

$$\frac{\partial C_{i,j}}{\partial t} + \frac{1-\varepsilon}{\varepsilon} \cdot \frac{\partial q_{i,j}}{\partial t} = -u_j \cdot \frac{\partial C_{i,j}}{\partial Z} + D_{L,i} \cdot \frac{\partial^2 C_{i,j}}{\partial Z^2} \quad (1)$$

$$\frac{\partial q_{i,j}}{\partial t} = k_{f,i} \cdot (q_{i,j}^* - q_{i,j}) \quad (2)$$

where q^* is the solid concentration in equilibrium with the liquid concentration C , and j is the serial number of column started from the first column in zone I. Adsorption equilibrium follows the Langmuir isotherm:

$$q_i^* = \frac{H_i \cdot C_i}{1 + K_A \cdot C_A + K_B \cdot C_B}, \quad (i = A, B) \quad (3)$$

where H_i and K_i are the Henry constant and adsorption equilibrium constant of the i th component, respectively.

There are three types of cycle in MF-SMB. The first is represented by the switch interval, the period between two successive switches of the inlet and outlet ports. The second is that the columns have completed a full revolution and are "back" to their original positions. The third is the time interval between two successive collections, in which the solution out of zone II is collected in an out-line container, added with the raw materials and the mobile phase and then pumped into zone III completely during the next collection interval. Consequently, the inlet concentration of the first column in zone III remains unchanged during the k th collection interval as follows:

$$C_{i,j,k} = \frac{\bar{C}_{i,II,k-1} \cdot F_{II} \cdot T_{\text{coll}} + n_{k-1} \cdot x_i}{F_{III} \cdot T_{\text{coll}}} \quad (4)$$

where $\bar{C}_{i,II,k-1}$ is the average concentration of i th component in the outlet solution of zone II collected during the $(k-1)$ th collection interval, T_{coll} is the time interval for collecting the solution out of zone II, n_{k-1} is the amount of raw materials added into the solution collected during the $(k-1)$ th collection interval, and x_i is the fraction of i th component in the raw materials.

Except for the inlet condition of zone III, the initial conditions and other boundary conditions are identical to those in Tr-SMB. The inlet concentration of the first column in zone I is

$$C_{i,1}(t, 0) = \frac{C_{i,N}(t, L) F_{IV}}{F_I} \quad (5)$$

The inlet concentration of the other column is

$$C_{i,j}(t, 0) = C_{i,j-1}(t, L) \quad (6)$$

At the outlet of each column,

$$\frac{\partial C_{i,j}(t, L)}{\partial Z} = 0 \quad (7)$$

After each switch interval t^* , the inlet and outlet ports are moved by one column in the direction of the fluid flow. So the concentration profile in the $(j+1)$ th column at the end of the $(n-1)$ th switch interval is identical to the initial condition in the j th column at the beginning of the n th switch interval, that is

$$C_{i,j}(t_k = 0, Z) = C_{i,j+1}(t_{k-1} = t^*, Z) \quad (8)$$

$$q_{i,j}(t_k = 0, Z) = q_{i,j+1}(t_{k-1} = t^*, Z) \quad (9)$$

where t_k is the time during the k th switch interval t^* .

The above model is discrete to ordinary differential equations (ODEs) with the method in Ref. [15]. The convective terms are approximated using five-point biased upwind finite difference schemes, and the dispersion items are approximated with five-point centered schemes. The ODEs are solved by the ODE15s solvers in Matlab.

The purities (p), productivities (P) and solvent consumptions (S) of the weak retained component A and the strong retained component B are calculated with the average concentrations in the extract and raffinate streams as follows:

$$p_A = \frac{\bar{C}_{A,\text{Raff}}}{\bar{C}_{A,\text{Raff}} + \bar{C}_{B,\text{Raff}}} \quad (10)$$

$$p_B = \frac{\bar{C}_{B,\text{Extr}}}{\bar{C}_{A,\text{Extr}} + \bar{C}_{B,\text{Extr}}} \quad (11)$$

$$P_A = \frac{\bar{C}_{A,\text{Raff}} \cdot F_{\text{Raff}}}{V_{\text{col}} \cdot N} \quad (12)$$

$$P_B = \frac{\bar{C}_{B,\text{Extr}} \cdot F_{\text{Extr}}}{V_{\text{col}} \cdot N} \quad (13)$$

$$S_A = \frac{F_{\text{Eluent}} + (F_{\text{III}} - F_{\text{II}})}{\bar{C}_{A,\text{Raff}} \cdot F_{\text{Raff}}} \quad (14)$$

$$S_B = \frac{F_{\text{Eluent}} + (F_{\text{III}} - F_{\text{II}})}{\bar{C}_{B,\text{Extr}} \cdot F_{\text{Extr}}} \quad (15)$$

3 RESULTS AND DISCUSSION

The SMB operation can be well simulated by a proper model [7, 8, 13, 14, 16–21] if the mass transfer coefficients, axial dispersion coefficients and adsorption isotherms are appropriately estimated in advance. This work adopts the model used by several authors [7, 13, 14]. The adsorption isotherm given by Morbidelli *et al.* [22, 23] is used, and its parameters as well as the other model parameters are listed in Table 1.

3.1 Study on separations by Tr-SMB

Triangle theory [22, 23] is widely used to design

Table 1 Model Parameters

ε	L/cm	d/cm	N	$C_{\text{Feed,A}} (= C_{\text{Feed,B}})$ / $\text{g}\cdot\text{L}^{-1}$	$x_A (= x_B)$	H_A	H_B	K_A / $\text{L}\cdot\text{g}^{-1}$	K_B / $\text{L}\cdot\text{g}^{-1}$	$k_{f,1} (= k_{f,2})$ / min^{-1}	$D_{L,1} (= D_{L,2})$ / $\text{cm}^2\cdot\text{min}^{-1}$
0.75	10	1.0	8	5	0.5	3.85	5.30	0.0175	0.0321	60.0	0.002

SMB operations. It lumps the flow rates and the switch time into four dimensionless numbers m_j , with $j = \text{I to IV}$,

$$m_j = \frac{F_j \cdot t^* - V_{\text{col}} \cdot \varepsilon}{V_{\text{col}} \cdot (1 - \varepsilon)} \quad (16)$$

In the ideal case, there are some constraints on m_j for complete separations, depending only on the adsorption equilibrium of the components to be separated. These constraints define a complete separation region in the four dimensional space spanned by the four coordinates m_{I} , m_{II} , m_{III} and m_{IV} . As illustrated by Fig. 2, the complete separation region in the plane of $m_{\text{II}}-m_{\text{III}}$ is a deformed triangle. However, the operating conditions given by triangle theory needs to be tuned through simulations or experiments in the presence of non-ideal factors. In this work, the optimum operation, Run 1, is obtained through simulation using a trial and error procedure. As shown in Fig. 3 (a), the rears of the two components hardly move out of the first column in zones I and II at the end of a switch, respectively, whereas their fronts hardly move out of the last column in zones III and IV, respectively. The corresponding operating conditions and separation results are listed in the second column in Table 2.

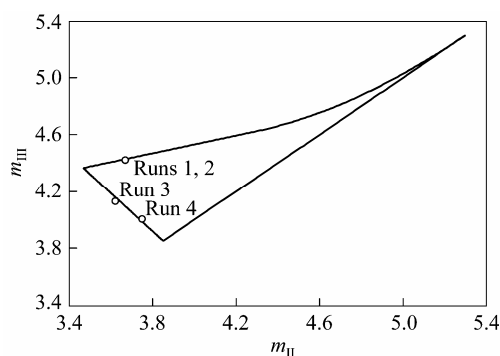


Figure 2 Operational points of Runs 1 to 4 in triangle separation region

3.2 Study on separations by MF-SMB

To compare MF-SMB and Tr-SMB, the feed concentration in MF-SMB is identical to that in Tr-SMB, $10 \text{ g}\cdot\text{L}^{-1}$. This requirement can be fulfilled by controlling the suitable addition amount of raw materials, n_{k-1} , from Eq. (4).

The optimum operating conditions of Tr-SMB, such as the flow rates and the switch interval, are first applied to MF-SMB without any change (see Run 2 in Table 2). The height of solute band in MF-SMB increases as shown in Fig. 3 (b), improving the product

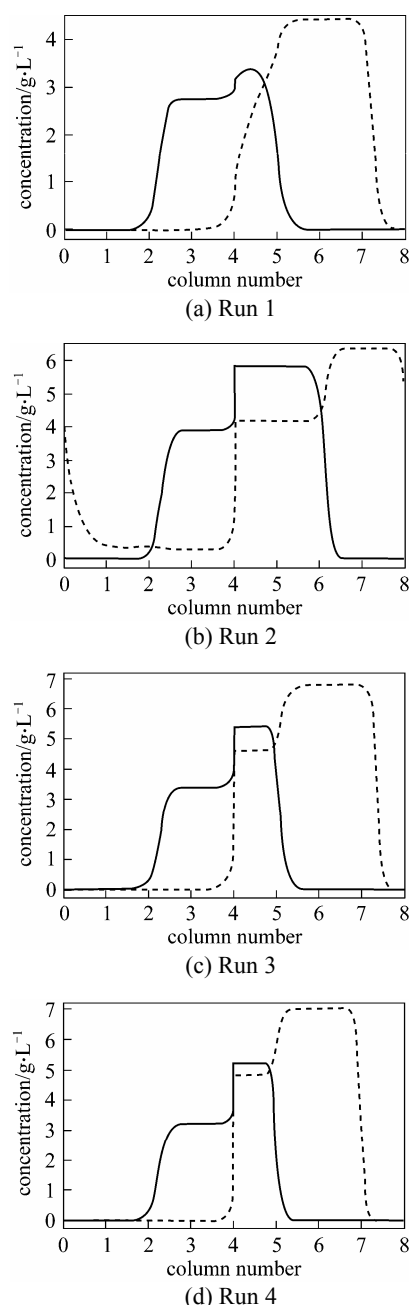


Figure 3 The concentration profiles of the strong (solid line) and weak (dotted line) retained solute in SMB at the end of a switch after reaching steady state

concentration and productivity. The movement of the band boundary is also accelerated, however, so that the two fronts cross their respective borderlines to reduce the purities of the raffinate and extract products.

Table 2 Operating conditions and corresponding simulation results of Tr-SMB and MF-SMB

	Operating conditions						Raffinate product				Extract product			
	F_I /ml·min ⁻¹	F_{II} /ml·min ⁻¹	F_{III} /ml·min ⁻¹	F_{IV} /ml·min ⁻¹	t^* /min	T_{coll} /min	$\bar{C}_{A,Raff}$ /g·L ⁻¹	p_A /%	P_A /g·L ⁻¹ ·h ⁻¹	S_A /L·g ⁻¹	$\bar{C}_{B,Extr}$ /g·L ⁻¹	p_B /%	P_B /g·L ⁻¹ ·h ⁻¹	S_B /L·g ⁻¹
Run 1 Tr-SMB	6.692	5.238	5.830	5.158	2.5	—	4.405	100	2.827	0.718	2.036	100	2.827	0.718
Run 2 MF-SMB	6.692	5.238	5.830	5.158	2.5	5.0	5.931	86.26	3.806	0.533	2.621	89.23	3.639	0.558
Run 3 MF-SMB	6.692	5.200	5.600	5.058	2.5	5.0	6.747	100	3.492	0.556	2.451	100	3.492	0.556
Run 4 MF-SMB	6.692	5.300	5.500	5.030	2.5	5.0	6.735	100	3.023	0.588	2.274	100	3.022	0.588

The flow rates in zones II to IV therefore need to be lowered simultaneously to enhance the purity as illustrated by Run 3. The results show that MF-SMB is superior to Tr-SMB (see columns 2 and 4 in Table 2). The productivity is increased by 23.52%, while the solvent consumption is reduced by 22.56%. Accordingly, the raffinate and extract concentrations are increased by 53.17% and 20.38%, respectively. It is interesting that the operational point of Run 3 is beyond the triangle complete separation region in the plane of m_{II} - m_{III} (Fig. 2), which should be also mainly ascribed to increasing the band height as shown in Fig. 3 (c), equivalent to Tr-SMB operation at a feed concentration higher than 10 g·L⁻¹.

The operation will be more robust when the operating conditions deviate from the optimum point. For instance, increasing the flow rate in zone II and decreasing the flow rate in zone III in Run 4 make both the front of strong retained solute and the rear of weak retained solute far from their respective borderlines. Accordingly, the allowable fluctuations of flow rates in Run 4 is less rigorous. Moreover, the separation performance given by Run 4 is much better than that by Run 1, the optimum operation of Tr-SMB, though it is worse than that by Run 3.

There are three tasks to be accomplished during each collection interval: collect the solution out of zone II in a container, add the raw materials and solvent to the container, and convert the solution in this container to the inlet solution of zone III at the end of collection interval. Obviously, longer collection interval will reduce the tedious repetitions for the procedure, making the operation more convenient and friendly. Thus, the effect of collection interval is investigated. As shown in Fig. 4, the average concentrations of the two products with different collection intervals approach an identical value, though at different rates. The results indicate that the collection interval has no effect on the separation after reaching the steady state.

4 CONCLUSIONS

A new feeding mode of SMB is proposed. The raw materials and solvent are added to the solution

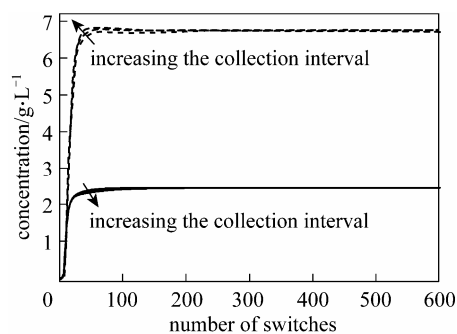


Figure 4 The change of raffinate (dotted line) and extract (solid line) concentrations during switch interval of 5, 10 and 15 min under the operating conditions for Run 3

periodically collected at the outlet of zone II to give a feed solution with a fixed concentration. The feed solution then completely flows into zone III during the next collection interval. The simulation results show that this feeding mode can be applied to binary separations. In comparison with a traditional feeding mode, the feed solution is in relatively higher concentration, so that the height of concentration band in SMB increases, improving the separation performance significantly. The new feeding mode increases the productivity, the raffinate and extract concentrations by 23.52%, 53.17% and 20.38%, respectively, while decreases the solvent consumption by 22.56%. The collection interval has no effect on the separation performance, and thus one can increase the collection interval to facilitate the operation.

NOMENCLATURE

C	liquid concentration, g·L ⁻¹
$\bar{C}$	average liquid concentration, g·L ⁻¹
D_L	axial dispersion coefficient, cm ² ·min ⁻¹
d	diameter of chromatographic column, cm
F	flow rate, ml·min ⁻¹
H	Henry constant
K	adsorption equilibrium constant, L·g ⁻¹
k_f	overall mass-transfer coefficient, min ⁻¹
L	length of chromatographic column, cm
m	flow-rate ratio in triangle theory

N	number of columns in SMB
n	amount of raw materials added to the collected solution during a collection interval, g
P	productivity, $\text{g}\cdot\text{L}^{-1}\cdot\text{h}^{-1}$
p	purity, %
q	solid concentration, $\text{g}\cdot\text{L}^{-1}$
q^*	solid concentration in equilibrium with C , $\text{g}\cdot\text{L}^{-1}$
S	solvent consumption, $\text{L}\cdot\text{g}^{-1}$
T_{coll}	collection interval, min
t	time, min
t^*	switch interval, min
u	flow velocity, $\text{cm}\cdot\text{min}^{-1}$
V_{col}	column volume, ml
x	composition of raw materials
Z	axial coordinate of column, cm
ε	column voidage

Subscripts

Extr	extract stream
Eluent	eluent stream
Feed	feed stream
I, ..., IV	zone of SMB
i	component A, B
j	column number
k	collection number
n	switch number
Raff	raffinate stream

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