

Simulation of the Influence of Parameters on Simulated Moving Bed

Chao-Fan Xie, Huang-Chu Huang, Yu-Ju Chen, and Rey-Chue Hwang

Abstract—Chromatographic separation by simulated moving bed (SMB) is an important skill for the modern material separation process. It is widely used in chemical and medical pharmaceutical industries. It has been recognized as a clean and green technology in the chromatographic application. In order to achieve a precision control for SMB, the influence and the effect of parameters to the final axial separation is an important study for realizing the behaviors of SMB. However, such kind of study is hardly to implement in the real SMB system due to the high experimental cost and the sensitivity of parameters. Thus, the computer simulation for studying the influence parameters to the final axial separation was implemented and presented in this paper. From the simulation results shown, the whole study is quite consistent with the actual behavior of SMB. It indeed has a great help for the future's development of precision control of SMB.

Index Terms—Simulated moving bed, chromatographic separation, adsorption.

I. INTRODUCTION

In year 1946, Universal Oil Products (UOP) company developed a countercurrent continuous circulation moving bed (TMB) for the separation of hydrocarbons with small molecular weight. The separation of components is based on the stationary phase (12-60 activated carbon) having the difference of adsorption capacity of each component in the system. In the separation process, the stationary phase moves from the top to the bottom due to gravity, and sequentially passes through the cooling zone, the adsorption zone, the rectification zone, and the desorption zone. Once reaching the bottom, the activated carbon is then lifted on the top by gas for reuse and the mobile phase (water vapor) moves from the bottom to the top. This method actually has been commercialized into the industrial application in 1960s [1]-[4]. However, in the liquid chromatography, due to the flow rate of stationary phase in the system is very difficult to be controlled, this method did not be widely used and had no further development.

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In the early 1970s, UOP improved its chromatographic technology, which made a great progress for SMB separation. But, to the application of pharmaceutical and fine chemical fields, the technology of SMB development was quite slow. The main reason is the lacks of SMB processing model, effective numerical calculation method and high speed computer. In 1980s, due to the development of SMB's theoretical framework, the emergence of simulation programs and the new hardware of liquid chromatography, SMB was widely reused in the field of chromatographic separation [5]-[9].

Basically, the whole process of SMB is shown in Fig. 1. The Zone I of SMB is located between the inlet of eluent and the outlet of extraction. In this zone, the desorption of component B will be proceeded. Usually, the stationary phase should be cleaned so that component B cannot be brought into Zone IV. Thus, the Zone I flow rate (Q_1) should be faster than the speed of component B moving downward with the stationary phase. In Fig. 1, the direction of arrow represents the upward direction.

The Zone II of SMB is located between the outlet of extraction liquid and the inlet of feed, which acts as a distillation column to make the adsorbed component B be adsorbed, desorbed and concentrated repeatedly. In order to get pure component B at the outlet of the extraction, the Zone II flow rate (Q_2) is within the moving speeds of component A and component B so that the component A can move up and component B can move down.

The Zone III of SMB is located between the feed inlet and the outlet of raffinate. Its function is to adsorb component A on the stationary phase as much as possible. In Zone III, the flow rate (Q_3) should be controlled appropriately such that component A could move upward and component B could move down, the pure component A then can be obtained at the outlet of raffinate. The Zone IV of SMB is located between the eluent inlet and the raffinate outlet. On the one hand, component A in the liquid phase is adsorbed by the stationary phase, and the eluent enters Zone I with the fresh eluent to achieve the purpose of recycling. On the other hand, in order to prevent the component A in the residual liquid from entering the Zone I and contaminating the extract, the Zone III and Zone I are separated. It can have a certain buffering effect. Therefore, the flow rate (Q_4) in the Zone IV should be less than the downward movement of component A, so that the liquid in the loop has no component A and the contamination will not be happened in Zone I [10], [11].

As mentioned above, SMB is a complex and nonlinear system. For achieving a precision control for SMB, its characters must be studied and analyzed. Therefore, a computer simulation for investigating the influence of adsorption parameters to the final axial separation of SMB is

implemented in this research.

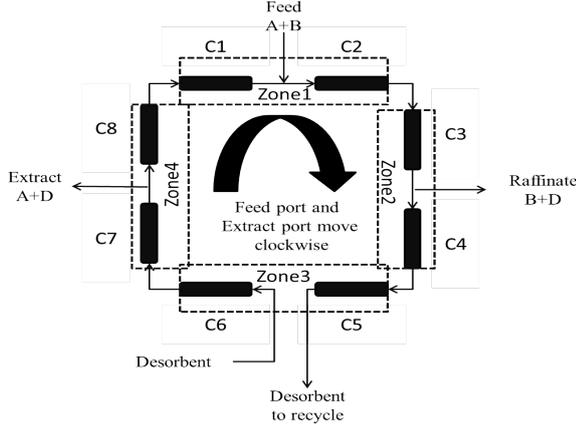


Fig. 1. Simulated moving bed (SMB) operation process.

II. MATHEMATICAL MODEL OF SMB

It is known that the traditional SMB dynamic mathematical model is deduced by using TMB mathematical model. Here, an overview of SMB dynamic model is described as follows [12].

For TMB, the mass balance of bulk phase is:

$$\frac{\partial C_{i,j}}{\partial t} = D_i \frac{\partial^2 C_{i,j}}{\partial x^2} - v_j^* \frac{\partial C_{i,j}}{\partial x} - \frac{1-\varepsilon}{\varepsilon} k_i (q_{ij}^* - q_{ij}) \quad (1)$$

$$\frac{\partial q_{i,j}}{\partial t} = \frac{\partial}{\partial x} u_s q_{ij} + k_i (q_{ij}^* - q_{ij}) \quad (2)$$

x : the moving direction and distance

k_i : the comprehensive mass transfer constant

v_j : the velocity of liquid phase in section j

u_s : the solid flow rate

$C_{i,j}$: the fluid phase concentration of component i in section j

i, j are omitted below.

$q_{i,j}$: the solid phase concentration of component

$q_{i,j}^*$: the solid phase concentration at equilibrium

between solid phase and liquid phase

v_j^* : the velocity of liquid phase in section j

Q_j^* : the flow rate

H_i : Henry coefficient of the adsorption isotherm

TMB and SMB can be converted to each other as follows:

$$\frac{\partial C_{i,j}}{\partial t} = D_i \frac{\partial^2 C_{i,j}}{\partial x^2} - v_j^* \frac{\partial C_{i,j}}{\partial x} - \frac{1-\varepsilon}{\varepsilon} \frac{\partial q_{i,j}}{\partial t} \quad (3)$$

The adsorption equilibrium for both enantiomers is represented by linear isotherms (4) or nonlinear Langmuir isotherms (5):

$$q_{i,j} = H_i C_{i,j} \quad (4)$$

$$q_{i,j} = \frac{GK_i C_{i,j}}{1 + K_i C_{i,j} + K_2 C_{i,j}^2} \quad (5)$$

Boundary conditions are:

$$C_{i,j}(x, 0) = C_{0,i,j}(x) \quad (6)$$

$$\frac{\partial C_{i,j}(x, t)}{\partial x} \Big|_{x=l_k} = 0 \quad (7)$$

$$D \frac{\partial C_{i,j}(x, t)}{\partial x} \Big|_{x=0} = v_j [C_{i,j}(0, t) - \bar{C}_{i,j}^{sect}(t)] \quad (8)$$

$C_{0,i,j}$: initial concentration; $\bar{C}_{i,j}^{sect}$: the column inlet concentration in sect=I, II, III, IV; K_i : the adsorption constant; G : the saturation concentration.

III. MATH SIMULATION

In our simulation, the related parameters are listed in Table I.

TABLE I: THE RELATED INITIAL PARAMETERS FOR SMB SEPARATION OF LINEAR ISOTHERMS

Parameter	Value	Parameter	Value
$L(cm)$	23	$C_{f,i}(gL^{-1})$	5
$d(cm)$	0.55	$\theta(\min)$	3
$H_A(gL^{-1})$	0.05	$Q_I(cm^3 \min^{-1})$	6.082
$H_B(gL^{-1})$	0.35	$Q_{II}(cm^3 \min^{-1})$	5.607
$D_A(cm^2 \min^{-1})$	0.2	$Q_{III}(cm^3 \min^{-1})$	6.516
$D_B(cm^2 \min^{-1})$	1.265	$Q_{IV}(cm^3 \min^{-1})$	3.529
ε	0.8		

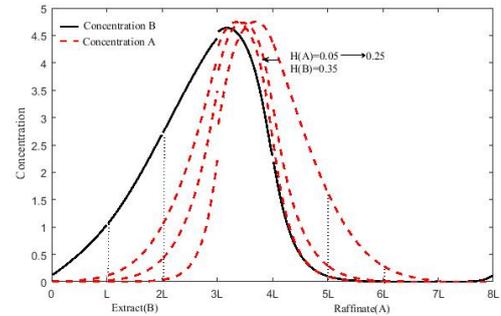
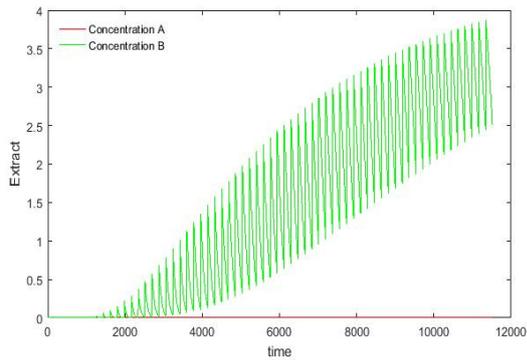


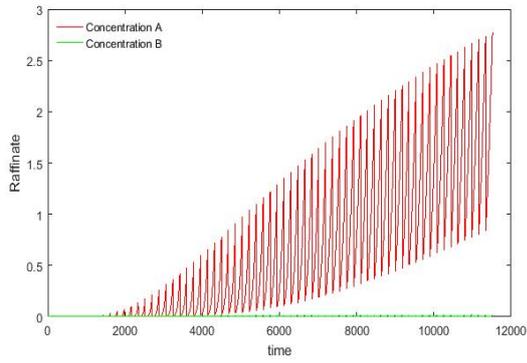
Fig. 2. The variations of concentrations versus adsorption rates (H_A).

Fig. 2 shows the variations of concentrations versus adsorption rates. Fig. 3 and Fig. 4 display the concentration separation results of two materials at extract and raffinate outlets with different H_A values. It can be found that the separation effect of two materials at the outlet is getting worse while the adsorption rates of two materials are approached gradually. From the viewpoint of the axial concentration change, the curve of concentration A move towards to curve of concentration B, two concentration curves of the axial separation will be closer and closer, and the separation of two materials cannot be achieved finally. In Fig. 2, the graph shows that the material A concentration curve only has the parallel displacements, and its concentration pattern does not change. Therefore, for the case of linear isotherm, the most important factor for the

separation of two substances is to find a good adsorbent to make A and B substances have the obvious adsorption differences.

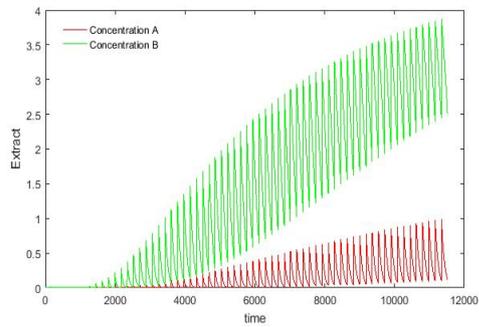


(a)

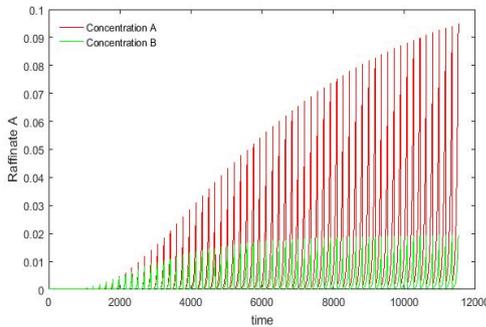


(b)

Fig. 3. Concentration separation results of extract and raffinate ($H_A = 0.05$).



(a)



(b)

Fig. 4. Concentration separation results of extract and raffinate ($H_A = 0.25$).

Next, the effects of the concentration in feed port and switching time to the separation condition are studied and observed. Fig. 5 shows the concentration variations of A and B at different feed port concentrations. Fig. 6 and Fig. 7 show

the concentration separation results of two materials at extract and raffinate outlets. In Fig. 5, the results show that the influence of the feed port concentration has a great influence on the shape of the axial separation curve. The curve shows a left tilt situation. The higher feed port concentration has the higher peak value. The two separation curves are actually closer.

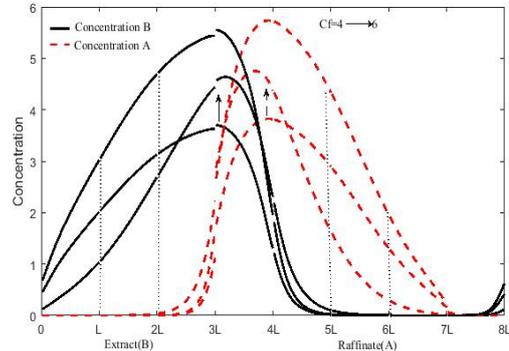
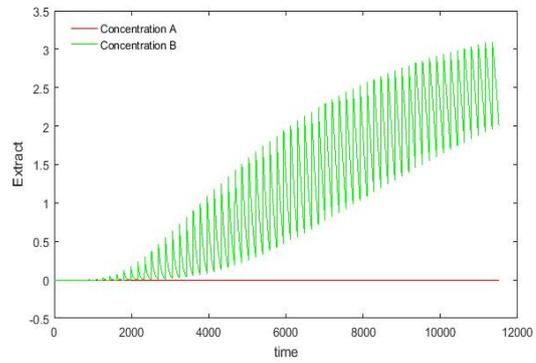
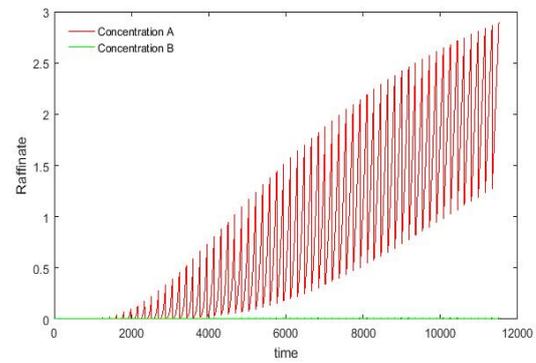


Fig. 5. The concentration variations of A and B versus different feed port concentrations (C_f).

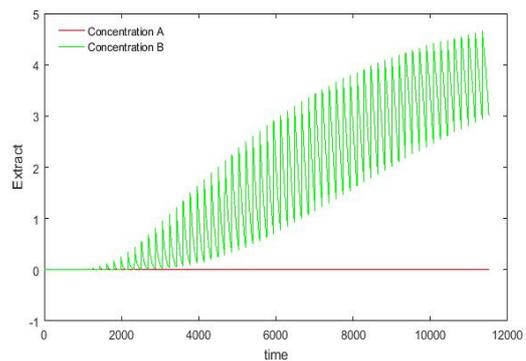


(a)



(b)

Fig. 6. Concentration separation results of extract and raffinate ($C_f = 4$).



(a)

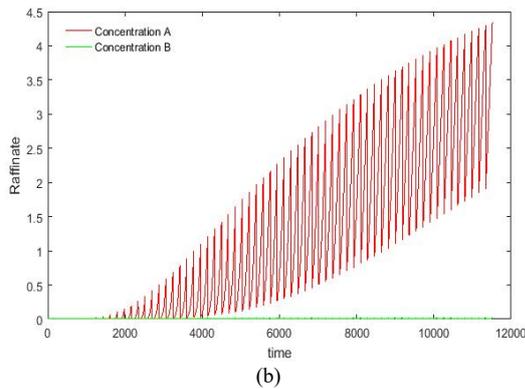


Fig. 7. Concentration separation results of extract and raffinate ($C_f = 6$).

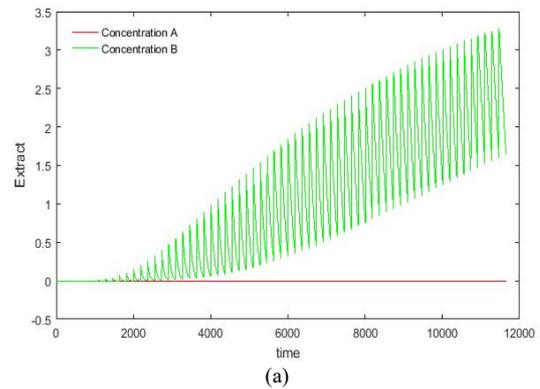


Fig. 8 to Fig. 10 display the separation effects caused by switching time. It is found that the switching time indeed plays an important factor on the separation results of SMB. In fact, the behavior of SMB is quite sensitive to the switching time.

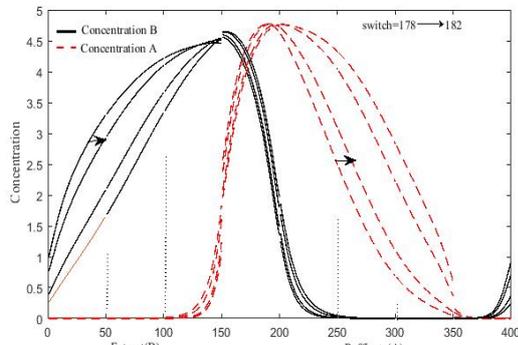


Fig. 8. The separation effects caused by different switching time (θ).

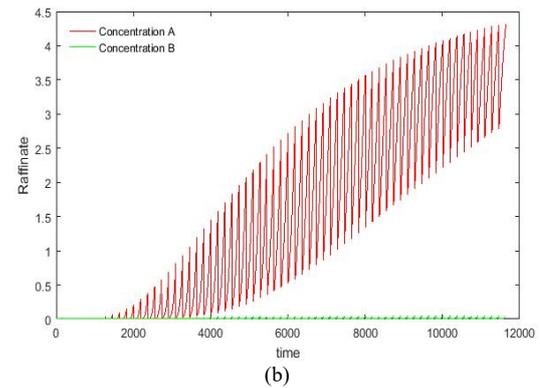


Fig. 10. Concentration separation results of extract and raffinate ($\theta = 182$).

The separation results show that while the switching time is increased, then the final separated concentration is decreased. In the absence of pathological conditions, a shorter switching time means that the separation of substances can be achieved more quickly, so the concentration will also be higher.

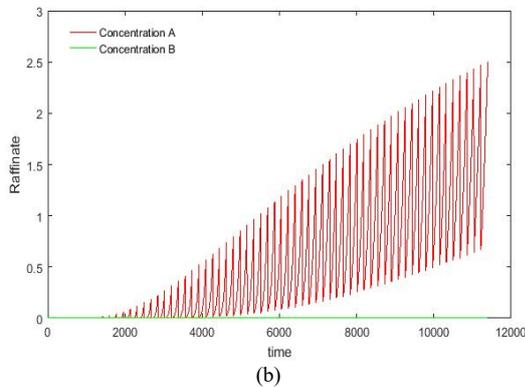
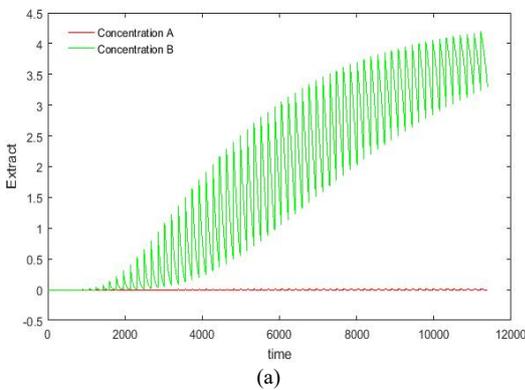


Fig. 9. Concentration separation results of extract and raffinate ($\theta = 178$).

IV. CONCLUSION

In this paper, the computer simulation of SMB system was carried out for observing the influence of parameters on the separation effect. The purpose of simulation is to explore and realize the behavior of the real SMB system. In our studies, the influences caused by three parameters, including the adsorbent, switching time and feed port concentration, are studied and analyzed. From the simulation results shown, the most influential parameters are adsorbent and switching time. If the adsorbent has a good adsorption effect on the substances, then a spatial separation effect can be formed. It can be concluded as the first prerequisite for a successful separation process. The switching time ensures the separation process is able to be operated continuously and it is also highly related to the final concentration value of the separation. The whole study results are quite consistent with the actual behavior of SMB. It indeed has a great help for the future's development of precision control of SMB.

CONFLICT OF INTEREST

The authors declare no conflict of interest.

AUTHOR CONTRIBUTIONS

Chao-Fan Xie performed the analytic calculations and the

numerical simulations; Both Huang-Chu Huang and Yu-Ju Chen contributed to the writing of the manuscript; Rey-Chue Hwang conducted and supervised the whole research; all authors had approved the final version.

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