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High-performance strategy of a simulated moving bed chromatography by simultaneous control of product and feed streams under maximum allowable pressure drop

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ABSTRACT

In this study, a novel operating strategy was developed to improve the separation performance of simulated moving bed (SMB) chromatography by the simultaneous control of product outlet streams and feed inlet stream (SimCon). The SimCon operation can achieve a high separation performance without exceeding the maximum allowable pressure drop in an SMB system. The SimCon operation consisted of three steps within a single switching period: the initial, middle, and last steps. The extract port and feed-inlet port were closed at the initial step, but the raffinate port was closed at the last step. Therefore, in the SimCon strategy, we introduce two additional operating variables in a switching period, namely the middle time and middle length. In the SimCon operation, the middle step is a key factor to achieving a good separation performance because concentration profiles can be well controlled by two new middle-step variables. The SimCon operation showed outstanding results compared with those of the corresponding conventional SMB and other stream-control strategies in terms of purity, recovery, productivity, and eluent consumption. Because the SimCon operation can be operated with smaller flow and pressure fluctuations than other flow-rate-control strategies and improves the column efficiency, it is expected that the strategy can be practically adapted to real SMB processes with a good separation performance.

1. Introduction

The simulated moving bed (SMB) chromatography process, which is a multicolumn chromatography process, has been applied to various industrial fields, such as foods, petrochemicals, fine chemicals, and pharmaceuticals. The countercurrent movement of the adsorbent bed is simulated by periodically shifting the inlet and outlet nodes to the direction of the flow during each switching period [1]. Therefore, the SMB process can achieve high productivity and low solvent consumption.

The SMB process can be applied to a wide variety of systems because of its powerful separation capability. In order to enhance the separation performance of the SMB process, many operating strategies have been introduced. Modulating operation parameters between two consecutive switches have been proposed [2–5]. In addition to the modulation, some of the product was recycled to the SMB configuration for further improvement of product purity [6–8]. An alternating collection of products, which is done by controlling product streams, has also been developed for the SMB operation [9–11]. As another operating strategy, a short chromatographic column was added in front of the SMB system, providing partially separated peaks to the SMB system [12,13].

As an alternative, because two inlet streams and two outlet streams are continuous in the conventional SMB process, product streams or a feed-inlet stream can be controlled to improve the separation performance. The impurity profile at each product node is shifted by controlling the feed flow rate or product flow rate. In the partial-feed (PF) strategy, the impurity was successfully decreased by varying the feed flow rate during each switching period [9]. In the outlet streams swing (OSS) operation, the purity can be improved by decreasing the product flow rate as the propagation of contaminated profiles was delayed from the product node [10]. Open and close control of a product port or the partial feeding/partial closing of a product port could lead to improving the SMB performance [14–16]. The concept of changing the flow rate at the product node was also proposed; this is called three-port operation in a three-zone SMB (TT-SMB) [11]. Because the TT-SMB requires only a three-zone and generated products with high purity

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and recovery, its separation performances, especially the productivity and eluent consumption, were significantly improved over those of conventional SMB processes.

However, the operating strategies that control only the product streams can lead to an excessive flow rate inside the columns during SMB operations if the maximum flow rate is not fixed. Therefore, such a flow fluctuation can cause a significant pressure drop, while harsh flow conditions can lead to deteriorating adsorbents and columns. If the bed porosity is changed or adsorbents are contaminated, the separation performance of the SMB is considerably worsened because of malfunctional columns [13]. Therefore, the SMB operations using the flow-rate control can be limited by the applicable pressure and flow rate at each zone even though the separation performance is theoretically high.

The SMB operational strategy using flow-rate control has to be developed under the constraints of the maximum allowable pressure or flow rate. If the control of the feed stream is incorporated with the control of product streams, flow fluctuation inside the columns can be reduced. In this study, a novel operating strategy (SimCon) was developed for a four-zone SMB, which simultaneously controlled the raffinate and extract outlet streams, and feed inlet stream. The results of the SimCon operation were compared with those of a conventional SMB and other product-stream control strategies in terms of four performance parameters: purity, recovery, productivity, and eluent consumption. Because the SimCon strategy could be operated under the allowable pressure and flow-rate conditions in the SMB processes, it was expected that it could be applicable for practical SMB operations.

2. Principles of simultaneous control of product streams and feed stream in SMB process

In the study, one column per zone SMB system (1-1-1-1 configuration) was selected as a representative model system for conventional SMB and SimCon operations. The conventional SMB consists of four zones in a closed loop for the separation of a mixture, as shown in Fig. 1(a). The separation of two components mainly occurs in the separation zone (zones II and III), and the regeneration of adsorbent and desorbent mainly occurs in the regeneration zone (zones I and IV), respectively.

The schematic of the SimCon operation is shown in Fig. 1(b). In the SimCon operation, the switching period is divided into the initial, middle, and last steps. During the initial step, the raffinate port is opened, but the feed and extract ports are closed. On the other hand, during the last step, the control of the product ports is opposite, but the feed is supplied. We note that the operation during the middle step is the same as the conventional SMB operation in Fig. 1(a). In the middle step, two additional operating variables for the middle length (middle-step duration) and middle time (middle-step position) in a switching period were introduced, as shown in Fig. 2. The middle length referred to the time duration of the middle step, and the middle time implied the location of the center of the middle step during a switching period. In the study, these two variables were expressed as a fraction (%) of the switching period. For example, the middle time of 50% implied the center of the time position in a switching period. For the SimCon operation, the special case was that the middle length was set to 0%. This case became the same as the combined OSS operation with PF operation (OSS-PF) [17], and the switching period was divided into two sub-intervals.

In the SimCon operation in Fig. 2, the raffinate product was withdrawn in the initial and middle steps, and the raffinate port was closed in the last step. On the other hand, the extract port was closed in the initial step, while the production occurred in the middle and last steps. This product port-control method was determined from an understanding of the product concentration profiles of both products in a conventional SMB because a relatively smaller amount of impurity was being collected at each product node [5,17]. However, the close and open control of only product ports could lead to significant pressure and flow-rate fluctuations inside columns.

To reduce such fluctuations, feed was also injected intermittently, which was similar to the control of product outlet streams. No feed was supplied to the system during the initial step because the internal flow rate was increased by closing the outlet flow at the extract port. During the middle and last steps, the decreased internal flow rate was balanced by supplying feed to the system. As explained above, the flow rates in the SimCon operation varied during the operation, but the weight-averaged flow rates in all zones over a switching period were the same as in a conventional SMB operation. Furthermore, the total flow-rate fluctuation was significantly reduced; this will be discussed in detail later.

One of the key parameters that should be considered in the design of the chromatographic process is the pressure-drop limitation in a column [2]. Therefore, the design of operating conditions is required to adhere to the limit of the maximum allowable pressure drop. The Ergun equation (Eq. (1)) has been widely used to calculate the pressure drop in a packed bed [18,19], and the results suggested the maximum allowable flow rate for a given system condition.

$$\frac{\Delta P_j}{L} = 150\frac{\mu u_j}{{D_p}^2}\left(\frac{1-\varepsilon_e}{\varepsilon_e}\right)^2 + \frac{7}{4}\frac{\rho {u_j}^2}{D_p}\left(\frac{1-\varepsilon_e}{\varepsilon_e}\right) \tag{1}$$

$$\Delta P_{total} = \sum_{j=I}^{IV} \Delta P_j \tag{2}$$

In the above equations, ΔP_j is the pressure drop in zone j (j = I, II, III, and IV), μ is the fluid viscosity, D_p is the average adsorbent particle size, ρ is the fluid density, and u_j is the interstitial fluid velocity in zone j. L is the column length, and ε_e is the inter-particle porosity. The total pressure drop, ΔP_{total}, is calculated from Eq. (2) as a summation of the pressure drops in all zones.

The flow rate in zone I in the SimCon operation was fixed as a maximum allowable flow rate in a column because the flow rate in zone I generally has a maximum value of among all zones in the conventional SMB [20]. A more detailed explanation is provided in Section 3.

3. Modeling of conventional SMB and SimCon operations

3.1. Mathematical models

The transport-dispersive model was applied to conventional SMB and SimCon operations to predict the internal concentration profiles and performance parameters (purity, recovery, productivity, and eluent consumption). In the column model, it was assumed that the rate of the adsorption-desorption was fast when compared with the rate of mass transfer [1,21,22]. The linear driving-force model was used to describe the mass-transfer rate of the solute to the surface of the adsorbent [1].

The differential mass-balance equation of the transport-dispersive model is given by

$$\frac{\partial C_i}{\partial t} + u_j\frac{\partial C_i}{\partial z} + \frac{1-\varepsilon_t}{\varepsilon_t}\frac{\partial q_i}{\partial t} = D_L\frac{\partial^2 C_i}{\partial z^2} \quad D_L = \frac{u L}{2 N_{disp}} \tag{3}$$

using the following linear driving-force model:

$$\frac{\partial q_i}{\partial t} = k_i({q_i}^* - q_i) \tag{4}$$

The following initial and boundary conditions were used:

$$\text{at t} = 0 \quad C_i(0, z) = 0 \quad q_i(0, z) = 0 \tag{5}$$