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Theoretical study of using simulated moving bed chromatography to separate intermediately eluting target compounds

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ABSTRACT

This study deals with the separation of ternary mixtures based on Simulated Moving Bed chromatography to isolate target components with intermediate adsorption strength. To overcome the limitations of conventional SMB systems, which are designed for binary separations and unable to perform center-cut separations, several modifications have been proposed. The purpose of this study was to provide a theoretical comparison of several of advanced SMB configurations capable to separate ternary mixtures. Emphasis is given to those techniques, which have already been used in practice, and to those having potential for future industrial application. SMB cascades connected in series via the extract or raffinate ports of the first unit are analyzed and compared are as well as an integrated 8-zone SMB unit with internal recycle. Additionally, the commercialized pseudo SMB process (JO process) was evaluated. The performance of these modified SMB systems was investigated based on the assumption of linear adsorption isotherms for all three components considering three separation problems characterized by different separation difficulty. Besides the influence of separation factors, the concentrations of the impurities in the feed mixture and the purity requirements for the target product were studied systematically.

1. Introduction

Simulated Moving Bed (SMB) chromatography is a well established technology for the separation of binary mixtures. In a conventional four-zone SMB a series of chromatographic columns are connected to form a circuit, which is divided into four characteristic zones by two inlet and two outlet ports. A countercurrent movement between the solid and fluid phases is simulated by switching periodically the positions of four ports along with the desorbent flow direction. Due to the ability to produce pure products with high productivity, this standard process has been employed successfully in a large number of applications.

Introduced in 1961 by Broughton [1] for hydrocarbon purification, the process has mainly been applied in large-scale petrochemical and sugar industries [2]. Since the earlier 90s many SMB processes have been developed for isolation and purification of pharmaceuticals and fine-chemicals, e.g. [3,4] as well as for bioseparations [5–7].

However, several new concepts have been proposed in order to improve the performance and extend the range of application of classical SMB technology by exploiting various additional degrees of freedom. A brief overview of the new suggestions and trends in the field of continuous countercurrent chromatography has recently been published by Blehaut and Nicoud [8], Seidel-Morgenstern et al. [9], and Gomes et al. [10].

Because of the fact that there is an increasing interest in isolating specific target component out of multicomponent feed mixtures (center-cut separations), and conventional 4-zone SMB systems are unable to produce a pure product stream if the desired component is neither the strongest nor the weakest adsorbable one, various modifications of SMB systems have been proposed. Complex multicomponent mixtures can be considered in a simplified manner as pseudo-ternary mixtures if all components which have weaker adsorption affinity than the target are considered as a weaker adsorbed impurity fraction and all compounds that are stronger bound as a stronger adsorbed impurity fraction.

The idea of separating a ternary mixture using a single SMB unit with multiple types of resins was suggested by Hashimoto et al. [11]. Application of this concept is however limited due to the difficulty in finding stationary phases that exhibit suitable binding properties for the compounds to be separated. SMB systems with different solvents [2] or with a variation of the working flow rates during the switching period [12] were also proposed.

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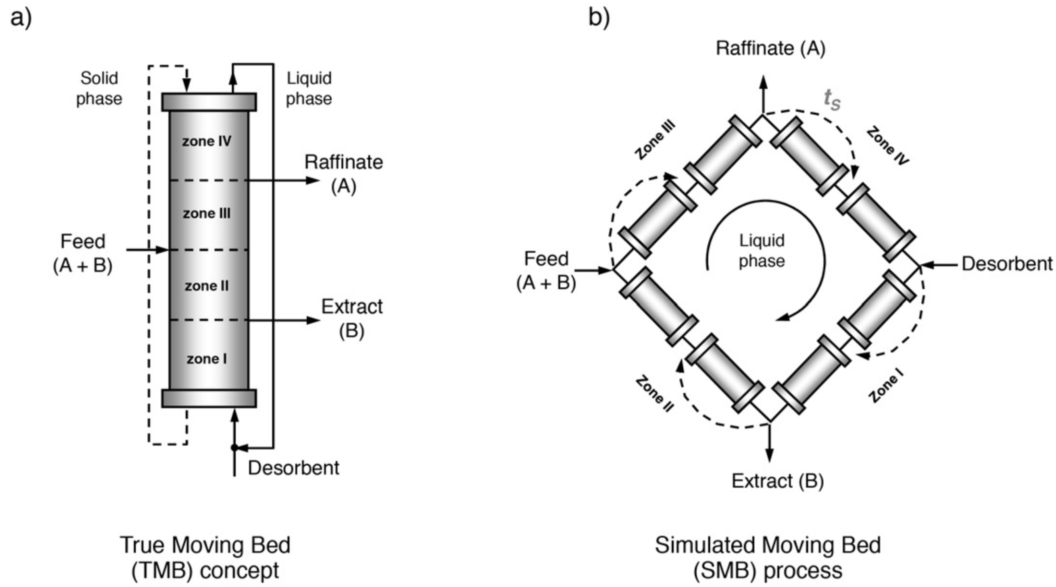

Fig. 1. The principle of binary separation based on (a) True Moving Bed (TMB) concept and (b) Simulated Moving Bed (SMB) process.

A concept based on the common knowledge that coupling two conventional SMB units can separate a ternary mixture was described by Chiang [13] and Hritzko et al. [14]. Wankat [15] suggested seven different configurations of SMB cascades and compared theoretically the minimum desorbent-feed ratio for ternary separation problems. An example of complex installation of nine integrated zones to recover glucose and xylose from a biomass hydrolyzate was suggested by Wooley et al. [16].

The performance of diverse moving bed configurations was characterized by analyzing the equivalent True Moving Bed at the low solvent consumption point by Nicolaos et al. [17] and Kessler and Seidel-Morgenstern [18] with respect to separate ternary mixtures under linear conditions.

Hur and Wankat designed a semi-continuous two-zone SMB/chromatographic hybrid system for complete ternary [19] and center-cut separations [20], which were subsequently validated experimentally for the recovery of L-phenylalanine from a ternary amino acid mixture [21]. Applications of specific five-zone systems with side streams for the collection of the component with intermediate adsorption affinity have been studied extensively [22–25].

An interesting alternative technology based on single SMB unit applied for ternary separations was introduced by Japan Organo Corp. [26] and designated as the New JO Chromatographic Separation Device. This multicomponent fractionation system combines features of both fixed-bed operation and SMB systems in a two-step continuous process.

Center-cut separations can be performed also by the GSSR process (Gradient with Steady State Recycle) [27], which comprises a multi-column, open-loop system with cyclic steady-state operation and simulates a solvent gradient moving countercurrently with respect to the solid phase. The power of solvent gradient and hybrid SMB/chromatographic modes is exploited in the MCSGP process, recently developed by Morbidelli and his co-workers [28,29].

Katsuo and Mazzotti discussed the intermittent SMB (I-SMB), an alternative multi-column chromatographic process [30], and demonstrated its performance potential for the separation of enantiomers [31–33]. This process has been extended to separate a complex mixture into three fractions [34]. Just recently, Agrawal and Kawajiri published their study [35], where they compare different isocratic 4- and 5-zone SMB schemes, introducing an efficient generalized full cycle formulation to find the best ternary separation strategy.

The objective of this work is to study theoretically different aspects of an SMB-based separation of ternary mixtures under linear conditions. Two coupled 4-zone SMB units connected in series via the extract or raffinate ports operated in continuous mode are analyzed and subsequently compared to an integrated 8-zone SMB and to the JO process. In order to evaluate the effect of separation factors on the process efficiency the performance of different arrangements is predicted using a standard SMB model for three different separation problems. Moreover, the influences of the concentrations of the impurities and the target product purity requirements are discussed.

2. Principle of standard SMB process

The principle of the countercurrent separation can be best described by introducing the hypothetical concept of True Moving Bed (TMB), which is schematically illustrated in Fig. 1(a).

The basic setup includes a chromatographic column, in which the solid and the liquid phases are moving in opposite directions. Two inlet and two outlet ports divide the system into four zones. A feed solution containing binary mixture to be separated is continuously injected into the stream of fluid phase, between zones II and III. Provided that the proper velocity of the two phases is adjusted, the less adsorbing component A travels in the direction of the liquid phase and can be continuously collected at the raffinate port, whereas the stronger adsorbing component B is transported downwards by the solid phase. Recycled liquid, along with a portion of a fresh desorbent, enters zone I making up a relatively high flow rate in this zone. As a result, the stronger adsorbed component is desorbed form the adsorbent surface and can be continuously withdrawn at the extract port. After a certain time, the process reaches stationary steady state, i.e. a stable concentration profiles within the system and constant product concentrations at the outlets.

An obvious drawback of presented above concept is the difficulty in arranging the continuous movement of the solid phase in practice [1,36]. Therefore, the Simulated Moving Bed (SMB) process was introduced [1]. In reality, instead of physically moving the stationary phase, a connection of several fixed-beds in series is used. The countercurrent movement of phases is simulated by discrete shifting the positions of all ports in the direction of the fluid phase flow, as shown in Fig. 1(b). This corresponds to moving each column