



Evaluation of center-cut separations applying simulated moving bed chromatography with 8 zones



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ABSTRACT

Different multi-column options to perform continuous chromatographic separations of ternary mixtures have been proposed in order to overcome limitations of batch chromatography. One attractive option is given by simulated moving bed chromatography (SMB) with 8 zones, a process that offers uninterrupted production, and, potentially, improved economy. As in other established ternary separation processes, the separation sequence is crucial for the performance of the process. This problem is addressed here by computing and comparing optimal performances of the two possibilities assuming linear adsorption isotherms. The conclusions are presented in a decision tree which can be used to guide the selection of system configuration and operation.

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1. Introduction

1.1. Simulated moving bed

Simulated moving bed chromatography (SMB) was first patented by Broughton et al. in 1961 for application in the petrochemical industry [1]. It is based on the principle of the true moving bed (TMB), which is itself based on the concept of a continuous countercurrent extractor, as the notation commonly used for its description suggests. The idea behind this process is to maximize the separation driving force by moving the adsorbent and the solvent in opposite directions. However, in practice, moving the adsorbent is not a trivial task, since it is usually composed of small particles and pumping it implies in back-mixing of the solvent, which reduces resolving power. One practical solution found for this problem was to divide the adsorbent into columns and instead of moving the adsorbent in a continuous way, to move the columns upstream in discrete intervals (or by changing the valve connections, effectively changing the relative positions of the columns in the system), thus creating the SMB [2].

In recent years the application of the SMB concept has been mostly studied for the separation of petrochemical derivatives, sugars, biotechnological products, plant extracts and chiral molecules. These separations are typically done using chromatography due to the need to separate solutes with very similar physicochemical properties. Furthermore these separations are also characterized by small differences in adsorption isotherms and/or large scale production and/or relatively expensive mobile phases, a combination of factors typically best dealt with by SMB in comparison to batch chromatography [3,4].

1.2. Center-cut separations

A major shortcoming of the classical SMB is that the solute being isolated must either be the one with the highest or the one with the lowest affinity to the adsorbent [5–7]. This restricts its application to more specific cases, usually simpler mixtures.

Taking as an example a mixture composed of 3 components eluting in sequence A, B and C, the most straightforward approach to employ the SMB process to isolate the intermediary eluting solute B is to use two SMBs in sequence in such a way that the first unit separates the solute in the elution series that stands between the intermediary eluting solute B and one of the extremes of the elution series. The feed entering the second unit then contains the intermediary eluting solute in either the first or the last position of

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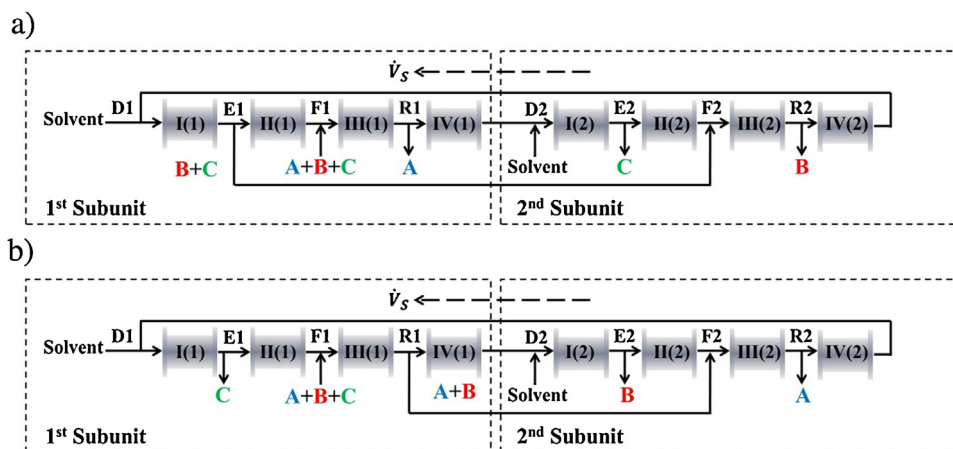


Fig. 1. (a) 8 zone SMB with extract recycle. The first subunit splits the feed into two fractions, A and B+C, the second subunit splits the recycled stream into the two solutes B and C. (b) 8 zone SMB with raffinate recycle. The first subunit separates the feed into a stream containing solute C, that is recovered in the extract, and one stream containing A and B that is recycled through the raffinate to the second subunit that separates it into the solutes A and B. The continuous lines show the solvent flow and the dashed lines represent the direction of the adsorber movement in the system.

the elution series, making it possible to separate it from the other solute. It is possible to merge these two SMB units into a larger integrated SMB unit with 8 zones [4,5,8–11]. There are two ways of doing this coupling, either by recycling the extract from the first subunit into the second subunit (Fig. 1a) or the raffinate (Fig. 1b)). The difference being which side of the elution series (the least or the most retained solute, respectively) is separated first [9,11].

Many different SMB configurations have been developed for the separation of ternary mixtures. Nicolaos et al. [10] compared different options of cascades with 4 and 5 zone SMB units in the frame of the equilibrium theory, other authors have used dynamic calculations and optimization algorithms for more realistic comparisons between different SMB column arrangements [5,6,9,12,13]. Furthermore, many promising semi-continuous configurations, such as the JO (Japan Organo Corp.) and the MCSGP (Multicolumn Countercurrent Solvent Gradient Purification) processes have also been proposed and thoroughly analyzed for performing center-cut separations [9,14].

An 8 zone SMB works, essentially, as a cascade of two SMBs [11], but it is one pump and one multi-port valve simpler and consumes less solvent [5]. Its main weakness is caused by the fact that all columns must be switched with the same period, limiting the maximal achievable recovery yield [10]. This limitation complicates the optimization process, since it creates a trade off between productivity and recovery yield, causing the optimal separation sequence in a SMB cascade to be different than that of an 8 zone SMB.

The purpose of this work is to use the TMB analogy with the SMB [15–17] to provide tools for the choice between its two configuration options (extract or raffinate recycle, shown in Fig. 1) and for the definition of optimal flow rates in each zone. This will be done in the three following steps:

First, the operating regions in the parameter space allowing recovery of pure intermediary eluting solute will be defined using the equilibrium theory [18,19] and cross-validated using the stage model of TMB [8,20,21].

Second, a novel strategy for the calculation of ideal 8 zone TMB performance is presented and used, together with the economic description of the process components, to optimize the flow rates. The analytical optimization of 8 zone TMB operating conditions has not yet been done, since this system does not allow complete separation of three fractions, which makes a straightforward solute mass balance impossible [8,10]. Also because of the maximal recovery yield limitation, the optimization of 8 zone TMB operating conditions is more complex than that of a cascade of 4 zone TMBs

and cannot be done solely based on physicochemical data. It also requires economic information about the components involved in the process. This problem has often been dealt with using objective functions [5,6,9]. Here the objective function is defined as the profit of the process in order to compare the two configuration options on an economical basis.

Third, the comparison of the optimized performances of each configuration is used to derive explicit criteria for the choice between them, that is, which separation should be done in the first subunit [8–10], a problem also encountered in the field of continuous distillation [22,23].

2. Theory

2.1. Optimization

We assume that the purpose of optimizing the operating conditions is to maximize the profit of the production process while respecting purity constraints. A definition for the profit (P) is:

$$P = \frac{(\text{money earned} - \text{money invested})}{\text{time interval}} \quad (1)$$

According to Kawajiri and Biegler [24], the profit can be expressed as a function of various performance indicators as shown in Eq. (2):

$$P = \dot{V}_{S\text{Feed}} \frac{\varepsilon_{\text{Total}}}{1 - \varepsilon_{\text{Total}}} \times Pr \times PSP - SC \times SCo - \dot{V}_{\text{Outlet}} \times SRCo - C_{\text{Feed}} \dot{V}_{\text{Feed}} \times FCo \quad (2)$$

where SC is the total solvent consumption, and, PSP , SCo , $SRCo$, and, FCo are the coefficients defined in Table 1. In this work, a term representing the cost of removing solvent from the product stream is added to account for product dilution. The profit is defined in this way because, as long as the purity requirements are met, the performances of 8 zone SMB with extract or raffinate recycle differ only in terms of productivity, product recovery, product concentration, and, solvent consumption.

The dimensionless productivity (Pr) is defined as:

$$Pr = \frac{\dot{V}_{\text{Outlet}} (1 - \varepsilon_{\text{Total}}) C_{\text{Product}}}{\dot{V}_S \varepsilon_{\text{Total}} C_{\text{Feed}}} \quad (3)$$

Each of the profit function coefficients is a non-exhaustive list of costs belonging to each of the categories shown in Table 1.

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