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Large scale optimization strategies for zone configuration of simulated moving beds

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Abstract

Simulated moving bed (SMB) processes are widely used in sugar, petrochemical, and pharmaceutical industries. However, systematic optimization of SMB, especially finding the optimal zone configuration including the standard and modified non-standard configurations, is still a challenging problem. This paper proposes a simultaneous, fully discretized approach with an SMB superstructure using an interior-point solver. To find the optimal structure, two superstructures are analyzed to develop standard and non-standard configurations. In case studies of the linear and bi-Langmuir isotherms, optimal zone configurations have been successfully obtained without introducing discrete variables. Finally, the effect of the number of columns on the optimal throughput is investigated.

Keywords: Simulated moving bed; SMB; Zone configuration; Dynamic optimization; Interior-point method; Superstructure

1. Introduction

The simulated moving bed (SMB) chromatographic process, originally developed and commercialized by UOP (Broughton & Gerhold, 1961), performs a continuous and pseudo-countercurrent operation. SMB has been gaining more attention in food, sugar, and petrochemical industries. In recent years, SMB has been widely used as an enantiomeric separation technique in the pharmaceutical industry.

An SMB system consists of multiple columns connected to each other in a circle, as shown in Fig. 1. The feed and desorbent are supplied continuously, and simultaneously the raffinate and extract products are withdrawn also continuously. Here, instead of actual movement of the adsorbent, the countercurrent operation is "simulated" by intermittently switching the four streams, desorbent, extract, feed, and raffinate, in the direction of the liquid flow. Because of this rotational operation, SMB does not reach a steady state but *Cyclic Steady State* (CSS). The operation of an SMB system is uniquely determined by the switching interval (step time) and the four velocities of the four zones, I, II, III, and IV. Furthermore, in SMB processes with more than four columns, the relative positions of the four streams are not unique. Fig. 2(a–c) shows configurations of $(N_{\text{I}}, N_{\text{II}}, N_{\text{III}}, N_{\text{IV}}) = (2, 2, 2, 2)$, $(1, 3, 3, 1)$, and $(1, 1, 5, 1)$, respectively, where N_m is the number of columns in Zone m. This creates a large number of different zone configurations. In addition to the standard zone configurations, there have been a number of non-standard configurations proposed to improve the performance. Fig. 3(a) shows the *Three-zone* configuration (Ching, Chu, Hidajat, & Uddin, 1992; Ruthven & Ching, 1989), where the circulation from the right end to the left is cut and all liquid is withdrawn as the raffinate stream. Fig. 3(b) shows the *Three-zone configuration with purging*, where the column at the left end is isolated and the components in the column is purged into the extract stream. Therefore, we need to deal with quite a large number of choices in designing SMB systems.

Optimization approaches of periodic adsorption processes, which are characterized by CSS, can be classified into three classes: the first is the nested approach, where the mathematical model described by partial differential algebraic equations (PDAEs) is discretized only in the spatial domain, and integrated until it reaches the CSS. Applications of this approach include SMBs and SMB reactors (Dünnebier, Fricke, & Klatt, 2000; Toumi, Hanisch, & Engell, 2002). The second approach, tailored with a single discretization, discretizes the PDAE model only in the spatial domain, but the CSS profiles are

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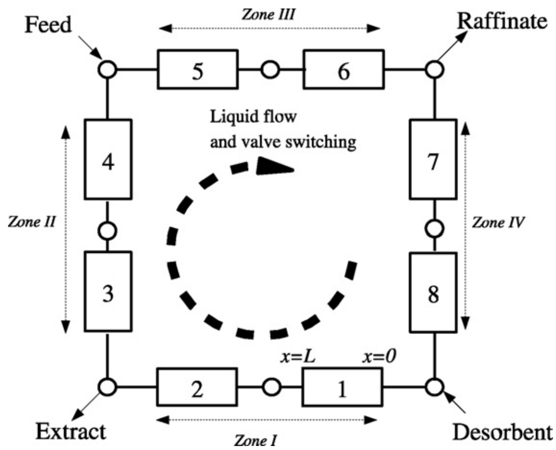

Fig. 1. Schematic diagram of eight column SMB.

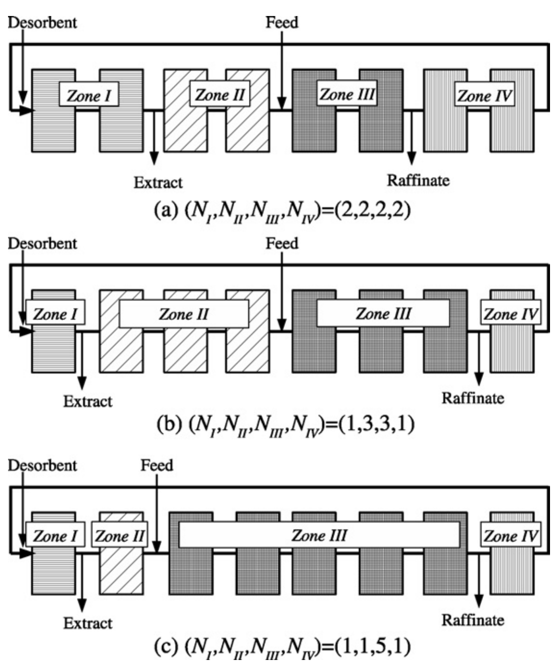

Fig. 2. Examples of standard SMB zone configurations: eight column SMB.

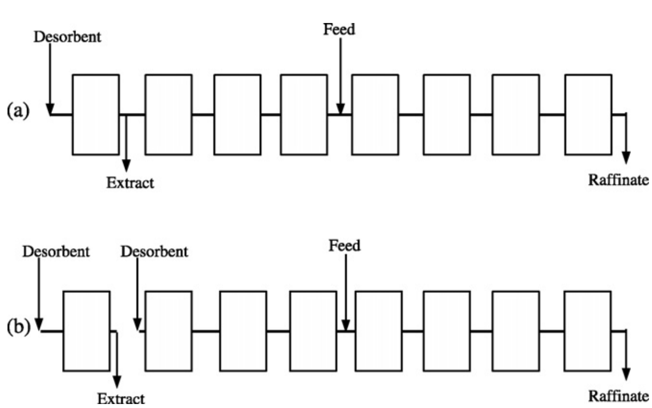

Fig. 3. Examples of non-standard configurations: (a) Three-zone configuration, (b) Three-zone configuration with purging.

obtained by enforcing equality constraints, which reduces the integration cost significantly (Jiang, Biegler, & Fox, 2003). The final approach is full-discretization, where the PDAE model is fully discretized both in the spatial and temporal domain, producing a large number of algebraic constraints (Ko, Siriwardane, & Biegler, 2003; Nilchan, 1997). In our previous study, we reported successful results of the full-discretization approach for SMB processes (Kawajiri & Biegler, 2006b).

Although several optimization approaches have been applied to SMBs, the SMB zone configuration problem has seen little investigation, particularly for a large number of columns. Zhang, Hidajat, Ray, and Morbidelli (2002) reported the multi-objective optimization of SMB and VARICOL processes of up to six columns, while finding optimal zone configurations. They employed a genetic algorithm to explore every possible zone configuration. In addition, superstructure formulations have been considered in Karlsson (2001) and Emet and Westerlund (2004), where a two column system was optimized, and Toumi (2005), where a relaxed nonlinear programming (NLP) formulation was developed for SMB. We previously reported an optimization approach using an SMB superstructure for standard zone configurations (Kawajiri & Biegler, 2006d). Nevertheless, the open problem of optimal zone configuration still remains especially for a large number of columns and non-standard configurations.

In this work, we develop an optimization approach for both the standard and non-standard configurations by using a superstructure of SMB alternative systems. We apply a full discretization formulation, where a central finite difference formula is used for the spatial discretization and Radau collocation on finite elements is used for the temporal discretization (Kawajiri & Biegler, 2006b). The discretized equations are incorporated within a large-scale nonlinear programming (NLP) problem, which is solved using an interior-point solver, IPOPT (Wächter & Biegler, 2005). In this extended paper, the superstructure for the standard SMB optimization (Kawajiri & Biegler, 2006d) is compared with a more extensive superstructure to consider non-standard configurations. The discussion of the mathematical model and the two superstructures are given in Section 2. The reliability and efficiency of our superstructure approach are demonstrated with several case studies in Sections 3 and 4. Finally the effect of the number of columns on the optimal throughput is discussed in Section 5.

2. Mathematical modeling and problem formulation

2.1. Modeling of chromatographic column

For the modeling of each chromatographic column, we use the same mathematical model as in our previous work (Kawajiri & Biegler, 2006b). Here both axial dispersion and diffusion into adsorbent particles, which cause band broadening, are lumped into a mass transfer coefficient (Dünnebier & Klatt, 2000; Golshan-Shirazi & Guiochon, 2003; van Deemter, Zuiderweg, & Klinkenberg, 1956). The mass balance in the liquid phase is