

Chapter 1

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, is still a challenging problem. This paper proposes a simultaneous, fully discretized approach with an SMB superstructure using an interior-point solver. In case studies of the linear and bi-Langmuir isotherms, optimal zone configurations have been successfully obtained without introducing discrete variables.

Keywords: Simulated Moving Bed, zone configuration, dynamic optimization, interior-point method, superstructure

1. Introduction

Simulated Moving Bed (SMB) chromatographic process, originally developed and commercialized by UOP, 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 The feed and desorbent are supplied continuously, and simultaneously the raffinate and extract products are withdrawn also continuously.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. 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 4 columns, the relative positions of the four streams are not unique, as shown in Fig. 2. This creates a large number of different zone configurations. As a consequence, we need to deal with quite a large number of choices in designing SMB systems.

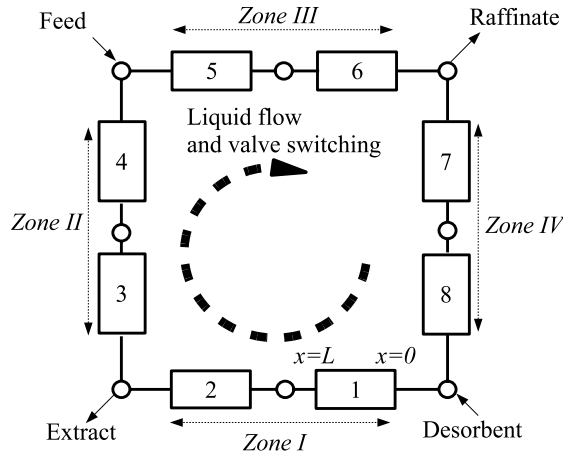


Figure 1. Schematic diagram of SMB: 8 column type with $(N_I, N_{II}, N_{III}, N_{IV}) = (2, 2, 2, 2)$

Some optimization techniques have been found to be useful in finding successful designs of SMB systems. Newton-based nonlinear programming approaches as well as meta-heuristic optimization approaches have been applied to SMB systems. In our previous work [1], we reported advantages of optimization with a spatial and temporal discretization using interior-point methods for SMB and PowerFeed processes, but did not consider optimal configuration of zones. Zhang et al. [2] reported the multi-objective optimization of SMB and VARICOL processes of up to 6 columns with finding optimal zone configurations. They employed a genetic algorithm to explore every possible zone configuration. In addition, superstructure formulations have been considered in Karlsson [3], where system of up to three columns system were optimized, and Toumi [4], where a relaxed Nonlinear Programming (NLP) formulation was developed for SMB and VARICOL. Nevertheless, the general problem of optimal zone configuration, determined for multiple columns with a fast NLP algorithm, still remains. In this work, we develop such an optimization approach for zone configuration by using a superstructure of SMB alternative systems. We apply a full discretization formulation, where a central finite difference is used for the spatial discretization and Radau collocation on finite elements is used for the temporal discretization [1]. The discretized equations are incorporated within a large-scale NLP problem, which is solved using an interior-point solver, IPOPT [5]. The reliability and efficiency of our approach are demonstrated with several case studies in Section 4.

2. Mathematical model

We employ the following model:

Mass balance in the liquid:

$$\varepsilon_b \frac{\partial C_{n,i}(x,t)}{\partial t} + (1 - \varepsilon_b) \frac{\partial q_{n,i}(x,t)}{\partial t} + u_m \frac{\partial C_{n,i}(x,t)}{\partial x} = 0 \quad (1)$$

Mass balance in the adsorbent:

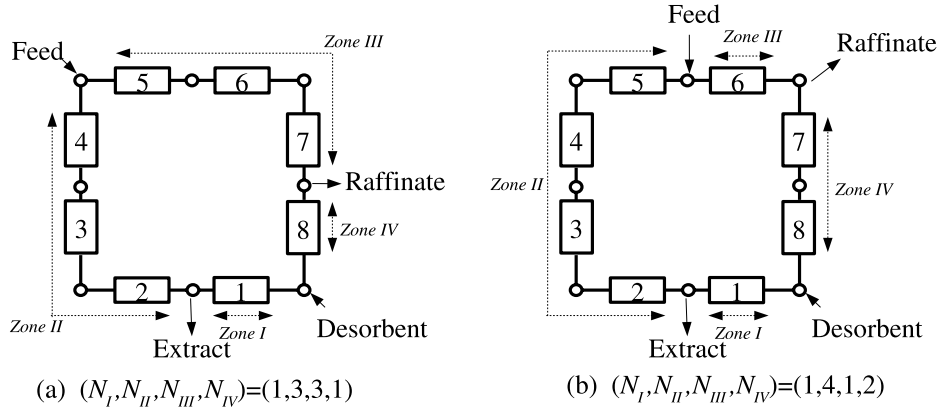


Figure 2. Examples of different zone configurations; with 8 columns, there are 35 configurations.

$$\text{liquid phase based: } (1 - \varepsilon_b) \frac{\partial q_{n,i}(x, t)}{\partial t} = K_{appl,i} (C_{n,i}(x, t) - C_{n,i}^{eq}(x, t)) \quad (2)$$

$$\text{or solid phase based: } \frac{\partial q_{n,i}(x, t)}{\partial t} = K_{apps,i} (q_{n,i}^{eq}(x, t) - q_{n,i}(x, t)) \quad (3)$$

Isotherm:

$$\text{Liquid phase based: } f(C_{n,i}^{eq}(x, t), q_{n,i}(x, t)) = 0 \quad (4)$$

$$\text{or solid phase based: } f(C_{n,i}(x, t), q_{n,i}^{eq}(x, t)) = 0 \quad (5)$$

where ε_b is the void fraction, $C_{n,i}(x, t)$ is the concentration in the liquid phase of component i in column n , $q_{n,i}(x, t)$ is the concentration in the solid phase, u_m is the superficial liquid velocity in Zone m , $C_{n,i}^{eq}(x, t)$ is the equilibrium concentration in the liquid phase, $q_{n,i}^{eq}(x, t)$ is the equilibrium concentration in the solid phase, $K_{apps,i}$ and $K_{appl,i}$ are the solid-phase based and liquid-phase based mass transfer coefficient, respectively. The subscripts i correspond to chemical components, n the index of columns, and m the zone number, I , II , III , and IV , as shown in Fig. 1. N_{column} is the number of columns, N_m is the number of columns in Zone m with $N_I + N_{II} + N_{III} + N_{IV} = N_{column}$. The cyclic steady state is given by:

$$C_{n,i}(x, 0) = C_{n+1,i}(x, t_{step}) \quad n = 1, \dots, N_{column} - 1, \quad C_{N_{column},i}(x, 0) = C_{1,i}(x, t_{step}) \quad (6)$$

$$q_{n,i}(x, 0) = q_{n+1,i}(x, t_{step}) \quad n = 1, \dots, N_{column} - 1, \quad q_{N_{column},i}(x, 0) = q_{1,i}(x, t_{step}) \quad (7)$$

Also continuity constraints of concentrations and velocities between columns are enforced. For further details of the modeling, refer [1].

3. Problem formulation

We construct a superstructure of SMB that covers all possible zone configurations with the assumption that there is at least one column in each zone (Fig. 3). Then the following optimization problem is considered:

$$\text{minimize} \quad F(u_D, u_{Dj}, u_{Ej}, u_{Fj}, u_{Rj}, u_m, C_{n,i}(x, t_{step}), q_{n,i}(x, t_{step})) \quad (8)$$

$$\text{(Extract Product Purity)} = \frac{\sum_{j=1}^{N_{Column}-3} \int_0^{t_{step}} u_{Ej}(t) C_{Ej,k}(t) dt}{\sum_{j=1}^{N_{Column}-3} \sum_{i=1}^{N_C} \int_0^{t_{step}} u_{Ej}(t) C_{Ej,i}(t) dt} \geq Pur_{min} \quad (9)$$

$$\text{(Extract Product Recovery)} = \frac{\sum_{j=1}^{N_{Column}-3} \int_0^{t_{step}} u_{Ej}(t) C_{Ej,k}(t) dt}{\sum_{j=1}^{N_{Column}-3} \int_0^{t_{step}} u_{Fj}(t) C_{F,k} dt} \geq Rec_{min} \quad (10)$$

$$u_l \leq u_j(t) \leq u_u, \quad j = 1 \dots N_{Column} \quad (11)$$

where t_{step} is the valve switching interval, or step time, Pur_{min} and Rec_{min} are the purity and recovery requirements of the desired product which should be recovered in the extract stream respectively. The desired product is denoted by the index k . $C_{F,k}$ is feed concentration of component k , and $C_{Ej,k}(t)$ is concentrations of component k in the j -th extract stream. u_u and u_l are the upper and lower bounds on the zone velocities, respectively. The variables are constrained by the model equations discussed in Section 1. We now extend the approach in [1] to the more extensive problem stated above and shown in Fig. 3.

4. Case studies

As the first case study, we consider the separation of fructose and glucose, which is typically modeled by the linear isotherm [6]:

$$q_{n,i}(x, t) = K_i C_{n,i}^{eq}(x, t) \quad (12)$$

In this example, the total length of columns $N_{Column} \times L$ is set to 8 m, and we choose $u_l = 0$ m/h, $u_u = 8$ m/h, $Pur_{Min} = 0.9$, and $Rec_{Min} = 0.8$. Also, as a more challenging example, we consider the bi-Langmuir isotherm which is suitable for modeling of enantiomer separations [7]:

$$q_{n,i}^{eq}(x, t) = \frac{H_{1,i} C_{n,i}(x, t)}{1 + K_{11} C_{n,1}(x, t) + K_{12} C_{n,2}(x, t)} + \frac{H_{2,i} C_{n,i}(x, t)}{1 + K_{21} C_{n,1}(x, t) + K_{22} C_{n,2}(x, t)} \quad (13)$$

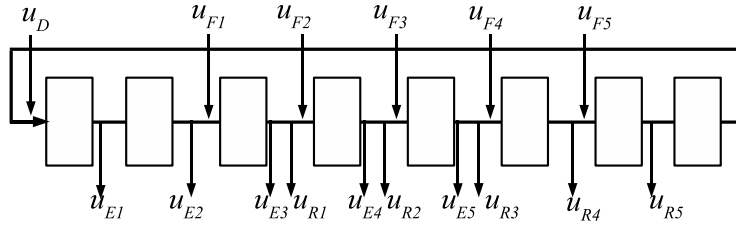


Figure 3. 8 column superstructure for optimal zone configuration problem.

Table1. Feed velocity maximization of 1,1'-bi-2 naphthol enantiomeric separation (bi-Langmuir isotherm) for 12 columns with different feed compositions. For u_{Fj} , only the dominant flow is shown in each case. The discretized NLP formulation has 27139 variables and 27110 equalities.

Feed composition (fructose:glucose)	80:20 %	50:50 %	20:80 %
u_{Fj} [m/h]	$u_{F6}=1.9008$	$u_{F6}=1.2366$	$u_{F6}=0.8712$
$(N_b, N_{II}, N_{III}, N_{IV})$	(3,4,4,1)	(2,5,4,1)	(2,5,4,1)
Number of iterations	61	74	115
CPU time [min]	3.28	3.80	6.92

with $N_{Column} \times L = 0.84 m$, $u_l=0 m/h$, $u_u=6.424 m/h$, $Pur_{Min}=0.97$, and $Rec_{Min}=0.8$.

After discretization, we implement the above optimization problems within the AMPL modeling environment. The optimization problem is solved using IPOPT. All computations are carried out on a 3.2 GHz Xeon processor.

As our first case study, we consider maximizing the sum of all feed streams, $\sum_j u_{Fj}$.

The results of the nonlinear isotherm with different feed compositions are tabulated in Table 1. As can be seen in the table, the optimal zone configuration is dependent on the feed composition. It is interesting that only one stream of each kind (u_{Fj} , u_{Ej} , and u_{Rj}) has a dominant nonzero flow and the rest have negligible values, typically less than 0.01% of the dominant flow. This is observed throughout our case studies, as long as appropriate tolerance and scaling are chosen. Therefore we are able to obtain the optimal zone configuration with an NLP formulation and without the addition of logic constraints or integer variables. This follows because streams of different types should be placed as far away as possible from each other to prevent contamination; the optimizer successfully finds such configurations.

We also investigate how the objective function influences the optimal solution. (Table 2). As the minimization of the desorbent velocity is introduced in the objective function, N_{IV} increases. This is because reducing the desorbent velocity requires a corresponding increase of the recycle stream, which could lead to elimination of the faster component at the downstream end of Zone IV that would contaminate the extract. To compensate, the optimizer also increases N_{IV} to prevent the elimination of the faster component. Again, only one stream of each kind is dominant and the rest are negligible.

Table 2. Optimization of fructose and glucose separation (linear isotherm) for 8 columns with different objective functions. For u_{Fj} , only the dominant flow is shown in each case. The discretized NLP formulation has 34731 variables and 34714 equalities.

Objective function F	$-\sum_j u_{Fj}$	$-\sum_j u_{Fj} + 0.5u_D$	u_D^*
u_{Fj} [m/h]	$u_{F3}=1.1584$	$u_{F3}=0.6233$	$u_{F3}=0.5000$
u_D [m/h]	3.50 (fixed)	0.6878	0.4773
$(N_b, N_{II}, N_{III}, N_{IV})$	(1,3,3,1)	(2,2,2,2)	(2,2,2,2)
CPU time [min]	1.73	2.81	4.00
Number of iterations	57	88	113

(* constrained with $\sum_j u_{Fj} = 0.5$)

5. Conclusions and future work

A fully-discretized NLP formulation with an SMB superstructure and interior-point solver has been found to be efficient and reliable for the optimal zone configuration problem. Moreover, discrete variables seem not to be required. In our future work, multi-component separations and more complex operations will be investigated.

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