



Cycle to cycle adaptive control of simulated moving bed chromatographic separation processes



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ABSTRACT

The simulated moving bed (SMB) technology is increasingly applied in various fields, ranging from the food to the pharmaceutical sectors, for the chromatographic separation of fine (bio)chemicals. In this study, an adaptive controller acting on the fluid flow rates and commutation period is used to regulate the spatial location of the adsorption and desorption waves, and in turn the purity and productivity of the raffinate and extract effluents. This controller is based on a simple discrete-time model of the concentration fronts movement, derived from wave theory. A simple parameter adaptation scheme makes this controller robust to parameter uncertainties and drifts, and allows process start-up with minimum a priori knowledge of the separation parameters. In this study, the performance of the controller is demonstrated for two different applications: the separation of fructo-oligosaccharides (linear isotherms) and cyclopentanone–cycloheptanone (competitive Langmuir isotherms). Different plant/sensor configurations are also examined, indicating the potential of the control strategy even with reduced measurement information.

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1. Introduction

Simulated moving bed (SMB) chromatographic separation processes were first used in large scale production by Universal Oil Products (UOP) in the early 60s [1]. SMB processes (Fig. 1) allow the continuous separation of binary mixtures. Following the successful operation in hydrocarbon and sugar separation, the technology was improved and increasingly applied to the separation of fine chemicals, pharmaceuticals, forensic samples and others.

A schematic view of a typical process is presented in Fig. 1. The inputs (feed mixture and eluent) and outputs (extract and raffinate) divide the system into four zones. Each zone contains one or more chromatographic columns, depending on the separation being performed. Pumps connected at each port determine the liquid phase flow rates in each zone.

The feed mixture composed of components A and B is injected between zone 2 and 3. The adsorbent is chosen in such a way that the two components are adsorbed at different rates, allowing them to travel with different velocities. The less adsorbed component (A) is collected at the raffinate port and the more adsorbed one (B) at the extract port. The separation of the two components is performed in zones 2 and 3, whereas zones 1 and 4 are dedicated to adsorbent regeneration and eluent recycling, respectively, for total separation cases.

The liquid–solid counter-current movement is obtained by physically rotating the columns in the direction of the solid phase or by switching the valves connecting the pumps to the system in the direction of the liquid phase, by one column length. A precise balance between the velocities of the liquid and solid phases must be maintained in each zone, to ensure that the fronts of the internal concentration profiles remain in their designated zones.

These operating points can be obtained using triangle theory [2,3]. The degrees of freedom of the SMB process may be exploited to improve the productivity of the separation by variation of the column configuration (VariCol) [4–6], modulation of the flow rates (PowerFeed) [7,8], pulse modulation of the feed input (I-SMB) [9], feed concentration modulation (ModiCon) [10], or the optimization of all these parameters (SMB superstructure) [11].

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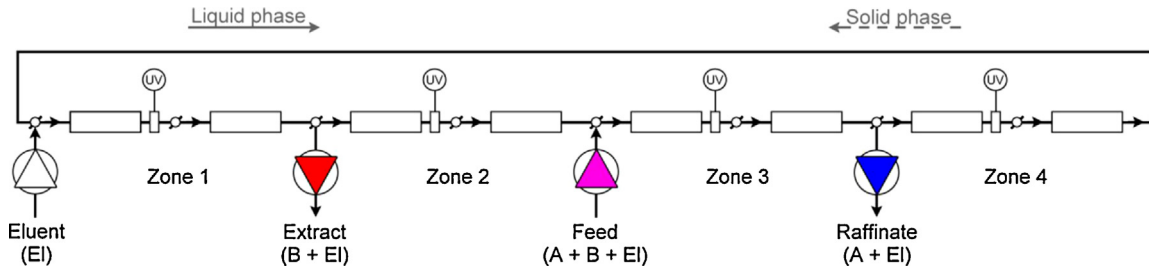


Fig. 1. SMB configuration.

Besides the selection of optimal operating conditions, the regulation of the process in order to reject potential disturbances has also attracted considerable attention. Many different techniques have been proposed, ranging from simple PI [12] or IMC [13] based controllers to more sophisticated techniques based on Model Predictive Control (MPC) (see for instance [14–18] and references therein). The main limitation of simple controllers is that the operating range in which stability can be ensured is usually small for plants with highly nonlinear behavior. On the other hand, advanced control techniques might require complex implementation and/or relatively high computational expenses.

The authors of the present paper have been involved in research at these two levels of control complexity. On the one hand, a simple PI controller for SMB processes has been proposed in [12], which makes use of the wave theory to control the purities at the two output streams and to maximize the productivity. The drawback of this approach is that it requires accurate information on the adsorption parameters and cannot compensate for their variations without an adaptation strategy. Such adaptation, using a receding-horizon strategy, can be found in [19], where Proper Orthogonal Decomposition (POD) is used to reduce considerably the computational costs.

The present work takes its root in [20], where a simple adaptive control scheme is proposed in the case of linear adsorption isotherms. The adaptive control concept is applied to the case of nonlinear adsorption isotherms which is non-trivial since the concept relies on simplifying assumptions which were derived from the analysis of the linear case. Extensive simulation studies, which account for plant model mismatch situations due to errors in the measured adsorption parameters, are conducted to investigate the control performance and robustness for separation of Fructo-OligoSaccharides (FOS) characterized by linear isotherms and separation of Cyclopentanone–Cycloheptanone (CC) characterized by nonlinear competitive Langmuir isotherms. Preliminary results were presented in a conference contribution [21]. In addition a stability analysis of the controller is presented for two different plant/sensor configurations under ideal conditions.

The proposed control scheme has several decisive advantages: (a) simplicity (a proportional controller with parameter adaptation is enough), (b) self-optimization (little a priori knowledge about the separation is required, the controller driving the process to the optimal operating point in a few periods), (c) flexibility (the available degrees of freedom allow to ensure productivity, purity, and production), and (d) straightforward implementation (in a standard industrial programmable logical controller).

The paper is organized as follows. The next section describes the mass-balance partial differential equation (PDE) model of the SMB plant. In Section 3, a discrete-time model of the concentration fronts movement is derived. This model is used in Section 4 to design a simple adaptive control scheme. Control performance and robustness is analyzed in depth in Section 5. Two different plant/sensor configurations are examined in Section 6. The stability

properties for the two different configurations are presented in Section 7. Conclusions and prospects are given in Section 8.

2. Process modelling and simulation

For the typical SMB unit of Fig. 1, with 2:2:2:2 column configuration, a system of 32 mass balance equations (1–2) is used. The mass transfer between the two phases is modeled using a Linear Driving Force model (Eq. (2)).

$$\frac{\partial C_{i,j}}{\partial t} + \frac{(1-\varepsilon)}{\varepsilon} \frac{\partial q_{i,j}}{\partial t} + v_l \frac{\partial C_{i,j}}{\partial z} = D_l \frac{\partial^2 C_{i,j}}{\partial z^2}, \quad D_l = \frac{Lv_l}{2N_{th}}; \quad (1)$$

$$i = A, B; j = 1, \dots, 8; l = 1, \dots, 4$$

$$\frac{\partial q_{i,j}}{\partial t} = K_i(q_{i,j}^{eq} - q_{i,j}) \quad (2)$$

In Eqs. (1) and (2), $C_{i,j}$ and $q_{i,j}$ represent the concentrations of the two components in the liquid and solid phase respectively, ε is the porosity, v_l is the speed of the liquid phase, D_l is the axial dispersion coefficient, L is the column length, N_{th} is the number of theoretical plates [19], K_i is the mass transfer coefficient, i identifies the component in the feed mixture, j the column and l the zone.

The number of theoretical plates can be determined experimentally from elution peaks resulting from low concentration single component injections.

The equilibrium between the two phases is described by linear isotherms (3) for the FOS separation and by nonlinear competitive Langmuir isotherms (4) for the CC separation.

$$q_{i,j}^{eq} = H_i C_{i,j} \quad (3)$$

$$q_{i,j}^{eq} = \frac{H_i C_{i,j}}{1 + b_A C_{A,j} + b_B C_{B,j}} \quad (4)$$

where H_i and b_i are the Henry coefficients and the adsorption equilibrium constants, respectively.

Dirichlet boundary conditions are considered at the input of each column. For the columns which are not at the feed or eluent ports, these conditions simply express concentration continuity:

$$C_{i,j}(0, t) = C_{i,(j-1)}(L, t), \quad i = A, B; \quad j = 2, 3, 4, 6, 7, 8 \quad (5)$$

whereas for the columns at the eluent or feed ports, the conditions are:

$$C_{i,1}(0, t) = C_{i,8}(L, t) \frac{v_4}{v_1} \quad (6)$$

$$C_{i,5}(0, t) = \frac{v_2 C_{i,4}(L, t) + v_{Fe} C_{i,Fe}}{v_3} \quad (7)$$

where L is the length of the column, $v_{1...4}$, v_{Fe} is the liquid phase velocity in each zone and at the feed port and $C_{i,Fe}$ is the concentration of component i in the feed mixture.

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