

Control of incomplete separation in simulated moving bed chromatographic processes

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Abstract: Simulated moving bed (SMB) is a continuous chromatographic process used for the separation of fluid mixtures. This paper presents a simple control strategy to handle incomplete separation, which requires tight control to achieve the desired purities. At first, a discrete-time nonlinear model is derived from wave theory, which will be the basis to estimate the position of the adsorption and desorption fronts. Four controllers are designed, two for the position of the concentration waves in zone 1 and 4, and two for the purities at the extract and raffinate outlets. The performance of the control strategy is evaluated with an experimental study of the separation of racemic Bicalutamide enantiomers in a 4 column-SMB.

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Keywords: chromatography, process control, adaptive control, parameter estimation

1. INTRODUCTION

Simulated Moving Bed (SMB) chromatographic separation processes allow the continuous separation of binary mixtures. They were first used in large scale production by universal oil products (UOP) in the early 60's (Broughton and Gerhold, 1961). Following their successful application to hydrocarbon and sugar separation, the technology was improved and increasingly applied to the separation of high-added value chemicals and pharmaceuticals.

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

The feed mixture 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. In a total separation configuration, the separation of the two components is performed in zone 2 and 3, whereas zones 1 and 4 are dedicated to adsorbent regeneration and solvent recycling, respectively.

The liquid-solid counter-current movement can be obtained by rotating the columns containing the adsorbent in the opposite direction to the liquid phase flow, as shown in figure 1. A specific equilibrium between the velocities of the liquid and solid phases must be achieved so as to ensure that the separation occurs in a desired way. The corresponding operating points for total separation can be obtained using the triangle theory (Storti et al., 1993; Mazzotti et al., 1997).

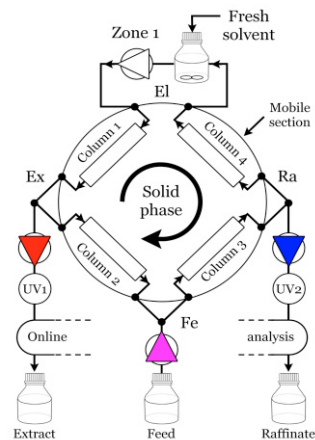


Figure 1. SMB configuration

Besides the selection of optimal operating conditions, the regulation of the process in order to reject potential disturbances has also attracted considerable attention, e.g. inferential PI controller (Schramm et al., 2003), the 'cycle to cycle' control concept based on model predictive control (Grossmann et al., 2008), (Erdem et al., 2005), (Song et al., 2006), (Engell and Toumi, 2005).

In (Fütterer, 2008; Suvarov et al., 2014), a simple adaptive control scheme has been proposed to achieve total separation. It is based on a discrete-time model of the front wave positions and on-line estimation of the optimal open-loop inputs to the plant to ensure total separation with maximum productivity. The resulting control scheme is extremely simple, combining feedforward actions (the estimated open-loop inputs) and feedback actions in the form of 4 proportional controllers regulating the position of the adsorption and desorption waves in their respective zones. Little prior knowledge about the adsorption properties

(isotherm parameters) is required, and the controller appears as a self-optimizing strategy as it allows the concentration fronts to be moved in optimal locations.

In the present study, the control concept is extended to handle the case of incomplete separation. In contrast with the total separation case, the concentration wave fronts do not stay confined in a zone, but can cross the extract and raffinate outlets (which is logical since the purity is reduced). The control strategy consists of 2 wave position controllers in zone 1 and 4, and 2 purity controllers at the raffinate and extract outlets. The operation of this controller is illustrated by experimental results obtained with the separation of racemic Bicalutamide. The experiments presented in this paper were carried out at low concentrations where a decentralized control approach seems sufficient. For higher feed concentrations, the interaction between the control loops becomes significant, so that some decoupling or a centralized control approach would be required.

The paper is organized as follows. The next section describes the mass-balance partial differential equation (PDE) model of the SMB plant. In the third section, a discrete-time model of the location of the foot point of the concentration fronts is derived. This model is used in section 4 to design a simple adaptive control scheme, which is tested in an experimental case study in section 5. Conclusions and prospects are given in section 6.

2. SMB MODELING AND SIMULATION

For the typical SMB unit of figure 1, with 1:1:1:1 column configuration, a system of 16 mass balance PDEs (1-2) can be derived. The mass transfer between the two phases is represented by a Linear Driving Force model (2).

$$\frac{\partial C_{i,j}}{\partial t} + F \frac{\partial q_{i,j}}{\partial t} + v_j \frac{\partial C_{i,j}}{\partial z} = D_j \frac{\partial^2 C_{i,j}}{\partial z^2}, \quad i = A, B; \quad j = 1, \dots, 4 \quad (1)$$

$$\frac{\partial q_{i,j}}{\partial t} = K_i (q_{i,j}^{eq} - q_{i,j}), \quad D_j = \frac{Lv_j}{2N}, \quad F = \frac{1-\varepsilon}{\varepsilon} \quad (2)$$

where $C_{i,j}$ and $q_{i,j}$ represent the concentrations of the two components in the liquid and solid phase, F is the phase ratio, ε is the column porosity, v_j is the speed of the liquid phase, D_j is the axial dispersion coefficient, K_i is the mass transfer coefficient, L is the length of a column, N is the number of theoretical plates, i identifies the component in the feed mixture and j the column.

The equilibrium between the two phases is described by a bi-Langmuir isotherm (3) for the racemic Bicalutamide separation (Kaemmerer et al., 2012).

$$q_i^{eq} = \frac{q_{s1,i} b_{1,i} C_i}{1 + b_{1,A} C_A + b_{1,B} C_B} + \frac{q_{s2,i} b_{2,i} C_i}{1 + b_{2,A} C_A + b_{2,B} C_B}, \quad i = A, B \quad (3)$$

The initial slope of the isotherms correspond to the Henry coefficients given by:

$$H_i = q_{s1,i} b_{1,i} + q_{s2,i} b_{2,i}, \quad i = A, B \quad (4)$$

Dirichlet boundary conditions are considered at the input of

each column. For columns 2 and 4, these conditions simply express concentration continuity.

$$C_{i,j+1}(0,t) = C_{i,j}(L,t), \quad i = A, B; \quad j = 2, 4 \quad (5)$$

while for columns 1 and 3, at the solvent or feed port, respectively, the conditions are:

$$C_{i,1}(0,t) = \frac{v_4 C_{i,4}(L,t)}{v_1}, \quad i = A, B \quad (6)$$

$$C_{i,3}(0,t) = \frac{v_2 C_{i,2}(L,t) + v_{Fe} C_{i,Fe}}{v_3}, \quad i = A, B \quad (7)$$

where $v_{1..4}$ are the liquid phase velocities in each zone, v_{Fe} and $C_{i,Fe}$ are the velocity and concentrations of the two components in the feed mixture injected.

At the output of each column, zero-dispersion and zero-adsorption conditions are expressed using a simple advection equation (Haag et al., 2001).

$$\frac{\partial C_{i,j}(L,t)}{\partial t} = -v_j \frac{\partial C_{i,j}(L,t)}{\partial z} \quad i = A, B; \quad j = 1, \dots, 4 \quad (8)$$

The counter-current movement needed for the separation is obtained by rotating the columns in the opposite direction of the liquid phase while the boundary conditions are fixed, by one column length every cycle.

The SMB model is simulated using a method of lines approach with finite elements and quadratic basis functions for spatial discretization, and a stiff differential ordinary differential equation solver, as available in Matlab and the MatMol library (Vande Wouwer et al., 2014). A typical simulation result obtained with 16 elements per column is shown in figure 3 for the separation of racemic Bicalutamide (total separation with optimal productivity).

3. WAVE FRONT MODELING

In order to regulate the purities at the extract and raffinate outlets, the position of the concentration waves must be controlled by adjusting the external flow rates and the cycle duration T_{SW} .

In this section, a model describing the movement of concentration waves is derived and used to set-up a one-cycle ahead predictor. UV detectors are assumed available at the extract and raffinate outlets, as shown in figure 1.

The foot point of a concentration wave is located at the intersection of the wave profile with a threshold chosen in accordance with the UV detector sensitivity and the presence of noise, as depicted in figure 2.

It is assumed that the velocity of the wave v_w is constant during one cycle and is directly proportional to the flow-rate in the corresponding zone.

The traveling time of the wave from its initial position to the UV detector can be determined from the measurements, and in turn the position of the wave (figure 3 and equations 9-10). This value is normalized with respect to the duration of the

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