Determining SMB Superstructures by Mixed-Integer Optimal Control

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1 Introduction

We treat a simplified model of a Simulated Moving Bed (SMB) chromatographic separation process that contains time–dependent discrete decisions. SMB processes have been gaining increased attention lately, see [3], [4] for further references. The related optimization problems are challenging from a mathematical point of view, as they combine periodic nonlinear optimal control problems in partial differential equations (PDE) with time–dependent discrete decisions. For this problem class of mixed–integer optimal control problems (MIOCP) a novel numerical method, developed in [5], is applied.

2 Model

SMB chromatography finds various industrial applications such as sugar, food, petrochemical and pharmaceutical industries. A SMB unit consists of multiple columns filled with solid adsorbent. The columns are connected in a continuous cycle. There are two inlet streams, *desorbent* (De) and *feed* (Fe), and two outlet streams, *raffinate* (Ra) and *extract* (Ex). The continuous countercurrent operation is simulated by switching the four streams periodically in the direction of the liquid flow in the columns, thereby leading to better separation. Due to this discrete switching of columns, SMB processes reach a cyclic or periodic steady state, i.e., the concentration profiles at the end of a period are equal to those at the beginning shifted by one column ahead in direction of the fluid flow. A number of different operating schemes have been proposed to further improve the performance of SMB. These schemes can be described as special cases of the MIOCP (13).

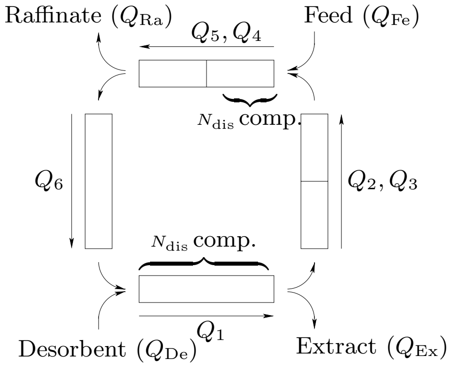

Fig. 1. In standard SMB, the positions of the ports for the four inlet and outlet flows are fixed and constant in time during one period.

The considered SMB unit consists of $N_{\mathrm{col}} = 6$ columns. The flow rate through column i is denoted by Q_{i}, $i \in I := \{1, \dots, N_{\mathrm{col}}\}$. The raffinate, desorbant, extract and feed flow rates are denoted by Q_{Ra}, Q_{De}, Q_{Ex} and Q_{Fe}, respectively. The (possibly) time–dependent value $w_{i\alpha}(t) \in \{0, 1\}$ denotes if the port of flow $\alpha \in \{\mathrm{Ra}, \mathrm{De}, \mathrm{Ex}, \mathrm{Fe}\}$ is positioned at column $i \in I$. As in many practical realizations of SMB processes only one pump per flow is available and the ports are switched by a 0–1 valve, we obtain the additional *special ordered set type one* restriction

$$\sum_{i \in I} w_{i\alpha}(t) = 1, \quad \forall \; t \in [0, T], \; \alpha \in \{\mathrm{Ra}, \mathrm{De}, \mathrm{Ex}, \mathrm{Fe}\}. \tag{1}$$

The flow rates Q_1, Q_{De}, Q_{Ex} and Q_{Fe} enter as control functions $u(\cdot)$ resp. time–invariant parameters p into the optimization problem, depending on the operating scheme to be optimized. The remaining flow rates are derived by mass balance as

$$Q_{\mathrm{Ra}} = Q_{\mathrm{De}} - Q_{\mathrm{Ex}} + Q_{\mathrm{Fe}} \tag{2}$$

$$Q_i = Q_{i-1} - \sum_{\alpha \in \{\mathrm{Ra}, \mathrm{Ex}\}} w_{\mathrm{i}\alpha} Q_\alpha + \sum_{\alpha \in \{\mathrm{De}, \mathrm{Fe}\}} w_{\mathrm{i}\alpha} Q_\alpha \tag{3}$$

for $i = 2, \dots N_{\mathrm{col}}$. The feed contains two components A and B dissolved in desorbent, with concentrations $c^{\mathrm{A}}_{\mathrm{Fe}} = c^{\mathrm{B}}_{\mathrm{Fe}} = 0.1$. The concentrations of A and B in desorbant are $c^{\mathrm{A}}_{\mathrm{De}} = c^{\mathrm{B}}_{\mathrm{De}} = 0$.

For our case study we use the simplified model presented in [2] for the dynamics in each column that considers axial convection and axial mixing introduced by dividing the respective column into N_{dis} perfectly mixed compartments. Although this simple discretization does not consider all effects present in the advection–diffusion equation for the time and space dependent concentrations, the qualitative behavior of the concentration profiles moving at different velocities through the respective columns is sufficiently well represented for our purposes. We assume that the compartment concentrations are constant. We denote the concentrations of A and B in the compartment with index i by c^{A}_i, c^{B}_i and leave away the time dependency. For the first compartment $j = (i-1)N_{\mathrm{dis}} + 1$ of column $i \in I$ we have by mass transfer for $K = \mathrm{A,B}$