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Combination of multi-model predictive control and the wave theory for the control of simulated moving bed plants

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ABSTRACT

In this work a new approach to the control of simulated moving bed (SMB) chromatographic separation processes is presented. This approach is based on the combination of the wave theory and Multi-Model Predictive Control (MMPC). The wave theory provides the theoretical framework in which the control law is formulated whereas receding-horizon MPC is used for determining the appropriate controller parameters. As SMB plants are distributed parameter systems (DPS) with nonlinearity arising from the expression of the adsorption isotherms, classical numerical methods for the solution of DPS are computationally demanding for MPC purposes. Reduced-order models are therefore derived using the proper orthogonal decomposition (POD) technique. To ensure stability, the POD model is updated on-line, resulting in MMPC.

1. Introduction

The simulated moving bed (SMB) process is a solid/fluid countercurrent chromatographic separation process. This technology is important in various industrial sectors, ranging from food to fine chemicals and pharmaceuticals. A schematic view of a typical SMB plant is presented in Fig. 1. The plant is subdivided into four zones delimited by the inlet and outlet streams. Each zone contains a given number of chromatographic columns which may vary between zones (1 or 2 columns per zone are typical). The difficulties arising from the practical implementation of a true countercurrent solid phase motion are solved in the SMB process by simulating such movement. To this end, the inlet and outlet ports are switched in the direction of the liquid flow as indicated in the figure by the dashed arrows. This results into an equivalent discrete-time countercurrent movement of the solid phase.

The binary mixture is fed between zones II and III. The solid phase is chosen such that components A and B are adsorbed at different rates, the less adsorbed component (A) being obtained at the raffinate drain, and the most adsorbed component (B) at the extract drain. The separation of the components occurs mainly in zones II and III while the aims of zones I and IV are the adsorbent regeneration and solvent recycling, respectively.

Several alternatives have been proposed for modeling mass transportation in the fluid phase and mass transfer between the liquid and solid phases in SMB plants. It is not the aim of this paper to review these several alternatives, the reader interested in these issues is referred to the literature (Guiochon et al., 1994; Grosfils et al., 2007b). Rather, a linear driving force (LDF) model is selected as a simulation model to test our nonlinear model predictive control (NMPC) approach. More details on the process can be found in Grosfils et al. (2007b) and Ruthven and Ching (1989) and references therein.

Regarding the control of SMB plants, many approaches have been presented in the literature. From simple PI (Schramm et al., 2003) or IMC (Klatt et al., 2002) based controllers to more sophisticated techniques based on MPC (see for instance Erdem et al., 2005; Song et al., 2006; Toumi and Engell, 2004 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 expense.

In this work, we propose to combine three different approaches or techniques for constructing a controller. First, the wave theory (see Helfferich and Carr, 1993; Helfferich, 1997) is used as a theoretical framework for the derivation of a PI controller following the ideas developed in Schramm et al. (2003). Second, the possible weaknesses of plain PI controllers are alleviated by an on-line adaptation of the controller parameters based on a receding horizon approach (Uduehi et al., 2001; Moradi, 2003; Xu et al., 2005). Since SMB plants are usually nonlinear distributed parameter systems, numerical methods

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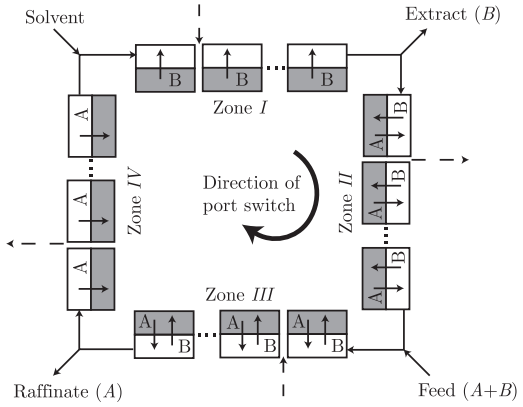

Fig. 1. Scheme of the separation of a binary mixture of components A and B in a simulated moving bed process.

have to be employed for simulation. Classical numerical methods like finite differences or finite elements (FEM) result into relatively high computational loads for on-line purposes. The proper orthogonal decomposition (POD) method (see Sirovich, 1987; Holmes et al., 1997) is thus considered as an efficient alternative.

However, even if the POD technique is a very efficient method, its main disadvantage is that, in general, it is only locally valid. In order to overcome this limitation, the POD model can be updated on-line so as to ensure the stability of MPC as initially proposed in Santos and Biegler (1999) and Santos et al. (2008) and extended in García (2008). Since this procedure uses different models, it is called multi-model predictive control (MMPC).

The paper is structured as follows: In the next section, the model equations for the SMB plant are presented and different issues regarding the simulation via the FEM and POD techniques are discussed. In Section 3, a brief introduction to the wave theory is presented and the connections with the controller are established. The MPC and MMPC frameworks will be described in Sections 4 and 5, respectively, and the advantages of the approach will be illustrated by means of simulation experiments. Finally, the main results of the work are summarized and possible future lines of research are discussed.

2. SMB modelling and simulation

Many different approaches have been proposed to describe the dynamic behavior of SMB plants. The differences between the proposed alternatives mostly lay in the modelling of mass transportation in the fluid phase and mass transfer between the solid and liquid phases. Some of the most popular approaches are: the *ideal model*, the *equilibrium dispersive model*, the *linear driving force model* (LDF), the *kinetic model* and the *general rate model*. As mentioned in the introduction, it is not the aim of this paper to discuss these several alternatives, the reader is referred to the literature for a deeper insight (Guiochon et al., 1994; Hassan et al., 1995; Azevedo et al., 1999). Rather, and for illustrative purposes, we concentrate on the LDF model. However, it is important to mention that other modelling approaches fit into the proposed methodology.

In this work, a binary mixture of components A and B has to be separated using a SMB plant with eight columns (2–2–2–2 configuration). Since the length of a column is much larger than its radius, the system can be considered perfectly mixed in the radial direction. Therefore, the original 3D model can be reduced to a 1D version in the axial direction. Additional simplifying assumptions are considered in modeling the SMB plant:

(i) only component A and B are absorbed by the solid phase;
(ii) the system is operated under isothermal conditions;
(iii) there is no void fraction and no turbulence;
(iv) the axial velocity within a zone is uniform.

Under these assumptions, the concentration of each component in the fluid phase $c_k^i(z,t)$ is, described in the LDF model, by[1]:

$$\frac{\partial c_k^i}{\partial t} = D_{k,j}\frac{\partial^2 c_k^i}{\partial z^2} - v_j\frac{\partial c_k^i}{\partial z} - k_\varepsilon\frac{\mathrm{d}q_k^i}{\mathrm{d}t}; \quad k_\varepsilon = \frac{1-\varepsilon}{\varepsilon}, \tag{1}$$

where the subindex k indicates the component ($k=$A,B), $j=$I, II, III, IV refers to each zone of the SMB plant mentioned in the introduction while the superindex $i=1,\ldots,N_c$ with $N_c=8$ indicates the column. $D_{k,j}$ represents the diffusivity, v_j the fluid velocity and ε the total porosity of the column. Note that since two columns per zone are considered, $j=$ I for $i=1,2$, $j=$ II for $i=3,4$, $j=$ III for $i=5,6$, $j=$ IV for $i=7,8$.

For the solid phase (q_k^i), a mass balance results into the following relation:

$$\frac{\mathrm{d}q_k^i}{\mathrm{d}t} = \kappa_k(q_k^{i,\mathrm{eq}} - q_k^i), \tag{2}$$

with κ_k and $q_k^{i,\mathrm{eq}}$ being, respectively, the mass transfer coefficient and the adsorbed equilibrium concentration, which can be related to the liquid concentration by means of a Langmuir isotherm (Mazzotti et al., 1997):

$$q_k^{i,\mathrm{eq}} = \frac{a_k c_k^i}{1+\sum_{k=1}^{2} b_k c_k^i}. \tag{3}$$

In this equation a_k and b_k are, respectively, the Henry coefficients and the adsorption equilibrium constants.

In order to complete the model description, boundary and initial conditions are required. Dirichlet boundary conditions are considered at the column inlet:

$$c_k^i(0,t) = c_{k,in}^i; \quad k=\mathrm{A,B}, \tag{4}$$

where $c_{k,in}^i$ is the column inlet concentration of component k in column i. Usually, for a given column p, the inlet concentration is taken as the outlet concentration in column $p-1$, this is

$$c_{k,in}^p = c_k^{p-1}(L,t).$$

with L being the column length. Note that for the columns located just after an inlet stream (eluent or feed) the inlet concentrations have to be modified. In the plant considered in this work, the feed is located between columns 4 (in zone II) and 5 (in zone III). A simple mass balance yields the following expression:

$$v_{\mathrm{III}}c_{k,in}^5 = v_{\mathrm{II}}c_k^4(L,t) + c_k^{\mathrm{Fe}}v_{\mathrm{Fe}},$$

Since the eluent stream is located between columns 8 (zone IV) and 1 (zone I) and the concentration in the eluent stream is zero for both components, we obtain

$$v_{\mathrm{I}}c_{k,in}^1 = v_{\mathrm{IV}}c_k^8(L,t).$$

In the last point of each column, dynamic boundary conditions are used to express zero-dispersion zero-adsorption conditions (Haag et al., 2001). This type of boundary condition is naturally derived from a minimum reduction of the PDE (Schiesser, 1996) and allows to alleviate spurious numerical oscillations in the presence of steep moving concentration fronts.

$$\frac{\partial c_k^i(L,t)}{\partial t} = -v_j\frac{\partial c_k^i(L,t)}{\partial z}. \tag{5}$$

The initial conditions are of the form:

$$c_k^i(z,0) = c_{k,0}^i. \tag{6}$$

[1] The arguments (z, t) in Eqs. (1)–(3) are omitted for brevity.