SMB 프로세스에 대한 식별 및 예측제어

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Identification and predictive control for a simulated moving bed (SMB) process

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Introduction

In recent years, several researchers have applied some advanced control strategies to simulated moving bed (SMB) units to treat the dynamic operation of SMB processes, ranging from the nonlinear control strategies such as the input-output linearizing control [4] to the repetitive model predictive control [5]. One of the shortcomings of these control strategies is that they use the first principles model. Although these controllers may be effective to treat various control problems, it may be difficult to implement them to actual SMB processes because of their heavy computational load and complex design procedure.

In this study we identify an SMB process using the conventional subspace identification method. The well-known input/output data-based prediction model is also used to obtain a prediction equation which is indispensable for the design of a predictive controller. The discrete variables such as the switching time are kept constant to construct the artificial continuous input-output mapping. With the proposed predictive controller we perform simulation studies for the control of the SMB process and demonstrate that the controller performs quite satisfactorily for both the disturbance rejection and the setpoint tracking.

SMB Process Description

The SMB chromatographic process is the technical realization of a countercurrent adsorption process, approximating the countercurrent flow by a cyclic port switching. In this study, the process is divided into four sections, each of which consists of 2 columns of chromatography playing a specific role in the separation. A feed mixture containing a proper inert solvent and the two components, *A* and *B*, is considered. The separation is carried out in the two central sections, in which component *A* (the more adsorbable component) is conveyed to the extract outlet and component B to the raffinate outlet, respectively.

The first principles model is considered to be the actual plant. The principle of operation can be best described with reference to the equivalent true countercurrently moving bed (TCC) configuration. Since the two configurations are equivalent, *i.e.,* they achieve the same separation performance provided the geometric and kinematic conversion rules are fulfilled, the simpler model of the equivalent TCC unit can be used to predict the steady state separation performances of SMB units especially for design purposes.

The first principles model of an SMB unit is constructed based on the previous works [2, 3]. With reference to a binary separation [2], the material balance equations are given by the following set of first-order partial differential equations:

$$\frac{\partial}{\partial\tau}\left[\varepsilon^* c_i^j + (1-\varepsilon^*)n_i^j\right] + (1-\varepsilon^p)\frac{\partial}{\partial\xi}\left[m_j c_i^j - n_i^j\right] = 0, \quad (i = A, B\ ,\ j = 1, 2, 3, 4) \tag{1}$$

where c_i^j and n_i^j represent the fluid phase and solid phase concentrations of species i in section j, respectively. Here τ and ξ are the dimensionless time and space coordinates and are defined as $\tau = t \cdot u_s / L$ and $\zeta = z / L$, while u_s, z, t and L denote the superficial solid phase velocity, axial coordinate, time and column length, respectively. $\varepsilon^* = \varepsilon + \varepsilon^p (1-\varepsilon)$ represent the overall void fraction of the bed, while ε^p and ε are the intraparticle porosity and the bed voidage, respectively. The solid phase concentration n^j_i is assumed to follow the linear driving force model

$$\frac{\partial n_i^j}{\partial t} = K_i a_p \left(n_i^{j*} - n_i^j \right) , \qquad n_i^{j*} = \frac{\gamma_i c_i^j}{1+\sum k_i c_i^j} + \frac{\delta_i c_i^j}{1+\sum h_i c_i^j} \tag{2}$$

in which K_i and a_p denote the overall mass transfer coefficient and the specific surface area, respectively. In this study the equilibrium concentration n_i^* is determined by the bi-Langmuir isotherm. k_i and h_i denote the adsorption equilibrium constants, while γ_i and δ_i are the bi-Langmuir parameters of component i.

The parameters m_j are the so-called flow rate ratios and are defined as the ratio of the net fluid flow rate over the solid phase flow rate in each section of the unit:

$$m_j = \frac{net\ fluid\ flow rate}{adsorbed\ phase\ flow rate} = \frac{Q_j^{SMB} t^* - V\varepsilon^*}{V(1-\varepsilon^*)} , \quad (j = 1,\ 2,\ 3,\ 4) \tag{3}$$

where Q_j, t^* and V denote the internal flow rate of fluid phase, the switching time and the volume of one column in the SMB unit, respectively. In the framework of equilibrium theory the design problem for an SMB unit is reduced to the development of criteria for the selection of the values of m_j. These values are considered as the input variables. For a complete modeling of an SMB process the node balance, the initial conditions and boundary conditions have to be set up for each column. For the details, one may refer to Migliorini *et al*. [2].

Predictive control of SMB Process

The input/output data-based predictive controller based on the identified model is designed and applied to a MIMO control problem for the SMB process. We use the input/output data-based prediction model in the MPC algorithm. The control parameters $\mathbf{L_w}$ and $\mathbf{L_u}$ are determined during the identification procedure and the past input/output data $\mathbf{w_p}$ are continuously updated so that the predicted output of the LTI part within the prediction horizon may also be updated. The QP method is usded to obtain the control input $\mathbf{u_f}$ by minimizing the objective function defined as

$$\min_{\mathbf{u_f}} J(\mathbf{u_f}) = (\mathbf{L_u u_f} + \mathbf{L_w w_p} - \mathbf{r_f})^T \mathbf{Q} (\mathbf{L_u u_f} + \mathbf{L_w w_p} - \mathbf{r_f}) + \mathbf{u_f}^T \mathbf{R u_f} \tag{4}$$

where $\mathbf{Q}$ and $\mathbf{R}$ are the weighting matrices for the output and input, respectively, and $\mathbf{r_f}$ denotes the set-point trajectory. It is well known that this type of objective function is very efficient to handle the input and output constraints. It is to be noted that we do not explicitly calculate the state estimate or the state space model. One may refer to our previous work [6] for the details of the controller design procedure.

The complete separation region in the triangle theory is considered as the input constraint and the output constraint comes from the requirement for the purity; *i. e.*,

$$\int_0^{\tau_{switch}} \frac{c_{A,Ex}(t)}{c_{A,Ex}(t) + c_{B,Ex}(t)} dt \ge Pur_{Ex,\min} \qquad \int_0^{\tau_{switch}} \frac{c_{B,Raf}(t)}{c_{A,Raf}(t) + c_{B,Raf}(t)} dt \ge Pur_{Raf,\min} \tag{5}$$

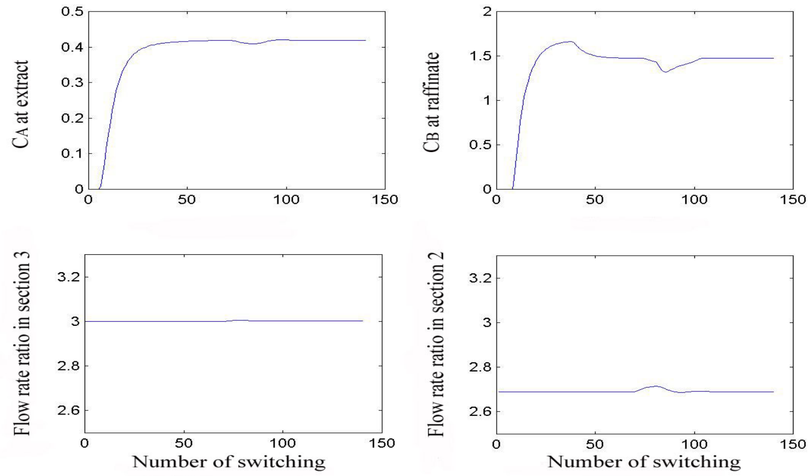

Figure 1. Disturbance rejection performance.

where $Pur_{Ex,min}$ and $Pur_{Raf,,min}$ represent the allowed minimum values of purity at extract and raffinate, respectively, and τ_{switch} indicates the switching time. The optimal conditions for complete separation are given by the following inequalities:

$$\begin{aligned}&[\gamma_A - \omega_G(1+K_A c_A^F)]m_2 + K_A c_A^F \omega_G m_3 < \omega_G(\gamma_A - \omega_G)\\&[\gamma_A - \gamma_B(1+K_A c_A^F)]m_2 + K_A c_A^F \gamma_B m_3 < \gamma_B(\gamma_A - \gamma_B), \quad m_2 < m_3\end{aligned} \tag{6}$$

where γ_A and ω_G denote the intersection points in the complete separation zone. For the detail one may refer to the work of Mazzotti and his coworkers [2].

Here we shall treat two typical control problems of practical interest; one is the disturbance rejection and the other is the setpoint tracking. For this purpose, the prediction and control horizons are set equal to 3 and 2 switching periods, respectively. As one can see in Figures 1 and 2, the SMB operation reaches the steady state after 60th switching and thus the disturbance or the setpoint change are to be introduced after 60th switching.

The SMB unit is usually operated at an optimal operating point but operating near an optimal point lacks robustness. Therefore, the matter of primary concern in the SMB process control would be the regulation and disturbance rejection. We shall assume that the feed concentrations of components *A* and *B* are reduced to one half of their original values, respectively, at 70th switching. These may be considered as unmeasured disturbances introduced to the process. The simulation results are presented in Figure 1, from which we notice that the sudden change in the feed concentration influences the state of raffinate more significantly than the state of extract. Accordingly, the flow rate ratio m_2 in section 2 increases to maintain the concentration of B in raffinate to its steady state value while the flow rate ratio m_3 in section 3 does not show any significant change. It is worth noting that the flow rate ratios, m_2 and m_3, do not violate the input constraints.

Next, we shall assume that, for some reason, there is a need to increase the product purities and thus the concentration of A in the raffinate is raised from 1.415 to 1.77 at 80 switching while that of B in the extract is increased from 0.418 to 0.439 simultaneously. The simulation results for the control performance are shown in Figure 2. It is noticed that the tracking for the raffinate concentration is successfully accomplished after a weak oscillatory behavior. However, the extract concentration shows a small offset and this may indicate that it is somewhat difficult to increase the purity of extract because it is already very high. It is expected that such a minor offset may be easily removed by tuning the controller with extra caution. After all, the flow rate ratios in sections 2 and 3 are slightly reduced

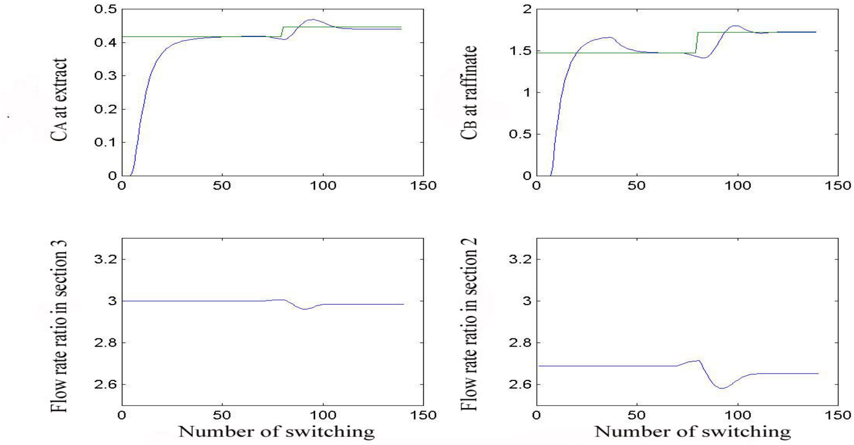

Figure 2. Tracking control performance.

to maintain the product purities as required.

Conclusions

In this study we identify an SMB process using the subspace identification method. The well-known input/output data-based prediction model suggested by Favoreel *et al.*[1] is used to obtain the prediction equation. The internal flow rate ratios are chosen as the input variables while the averaged concentrations of rich component in raffinate and extract, respectively, are selected as the output variables. The identified model based on the subspace identification method shows an excellent prediction performance. The input/output data-based predictive controller based on the identified model is designed and applied to MIMO control problems for the SMB process. The perfect separation region in the triangle theory and the bounds for the purity are considered as the input constraints and the output constraints, respectively. The simulation results show that the designed controller performed satisfactorily for the disturbance rejection and tracking control.

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References

[1] Favoreel, W.; De Moor, B.; Van Overschee, P.; Gevers, M*., Proceedings of the American Control Conference*, 3372-3381, (1999).
[2] Migliorini, G., Mazzotti, M. and Morbidelli, M., *Journal of Chromatography*, **A, 827**, 161-173, (1998).
[3] Dunnebier, G., Fricke, J., and Klatt, Karsten-Ulrich, *Ind. Eng. Chem. Res.,* **39**, 2290-2304, (2000).
[4] Kloppenburg, E. and Gills, E.D., *Journal of Process Control*, **9,** 41-50, (1999).
[5] Verhaegen, M. and Dewilde, P., *Int. J. Control*, **5**, 1187-1210, (1992).
[6] Song, I.-H., K.-Y. Yoo and H.-K. Rhee *Ind. Eng. Chem. Res.*, 40, 4292-4301, (2001).