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Nonlinear Model-based Repetitive Control of Simulated Moving Bed Process

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Abstract−The simulated moving bed (SMB) process, after more than 40 years of successful operation in the petrochemical industry, has emerged as one of the most important separation processes in the pharmaceutical, fine chemical, and biotechnology fields. However, optimal operation and automatic control of the SMB process is still challenging because of its complex dynamics caused by periodic port switching and inherent nonlinearity. In this research, a novel advanced control technique for the SMB process has been proposed. In the proposed technique, regulation of both extract and raffinate purities measured at the terminal time of each switching period is performed by a nonlinear repetitive controller which utilizes the past period data as feedback information. The repetitive controller was designed on the basis of a fundamental nonlinear model of the SMB process. Through application to a numerical SMB process, it was found that the proposed control technique performs quite satisfactorily against model error as well as set point and disturbance changes.

Key words: Simulated Moving Bed, Repetitive Control, Periodic System, Nonlinear System

INTRODUCTION

Chromatography is the most generic separation technique that can be applied to a truly wide variety of chemical and biological products. Although its major use is for analytical purposes, it has also been used for commercial separation of high valued food and pharmaceutical products. Especially, for separation of chiral mixtures that ubiquitously occur during the synthesis of pharmaceutical products, it is generally accepted that chromatography is the most viable, generic, and economical solution. Even with such wide-spread usage, conventional batch chromatography is too expensive for industrial use due to low productivity and excessive desorbent consumption.

The simulated moving bed (SMB) is an interesting alternative to conventional batch chromatography, where continuous feeding and product withdrawal are possible, and thus has received more and more attention recently, especially for chiral product separation. SMB technology is based on the concept of a counter-current continuous chromatography process called the true moving bed (TMB), where the adsorbent bed continuously moves in the reverse direction of the liquid flow. Since the bed moving is technically infeasible without damages and outflows of the solid adsorbent particles, the SMB periodically switches the position of the inlet and outlet ports in the direction of the liquid flow instead of moving the bed.

Indeed, SMB technology has more than forty years of history in the petrochemical industry. UOP first commercialized an SMB process for para-xylene production from the xylene mixture and has continuously extended its applications [Broughton et al., 1970; Johnson et al., 1993]. However, it is only recent as the bio- and pharmaceutical industries have become important that the SMB process has drawn a keen interest from academia [Juza et al., 2000; Pais et al., 1998]. By the research in academia over the past decade or more, considerable advances have been made in the process systems engineering aspect of the SMB technology, especially in the area of process design and optimization [Dunnebier et al., 1998; Ma et al., 1997; Storti et al., 1993; Zhong et al., 1996; Lim, 2004]. However, there still remain many problems to cope with in real applications. Regardless of the sophistication of the optimization scheme, the SMB practitioner eventually faces problems caused by the uncertainties from the process model and various disturbances. As has been exploited by previous researchers [Kloppenburg et al., 1999] and will also be demonstrated in this study, the theoretical optimum condition of an SMB process is quite sensitive to such uncertainties. In this respect, the operating condition provided by an off-line optimizer can only play as an initial trial point from which the true optimum is sought. The troubles with such uncertainties can be overcome only through feedback action, and the design of an appropriate feedback controller becomes critical in the SMB operation. The optimal operation and control of the SMB process, however, are still a challenging task because of the complex dynamics caused by periodic port switching and inherent nonlinearity of the process.

Until now, there have been limited publications on the control research of the SMB process. Kloppenburg et al. [1999] considered a hypothetical TMB process and derived a nonlinear control method using the asymptotically exact input/output linearization. Klatt et al. [2000] proposed a two-layer control architecture where the optimal operating trajectory is calculated in the higher level dynamic optimizer, whereas the lower level controllers try to regulate the process on the trajectory. They employed the IMC (internal model control) technique based on an MIMO ARX model. In the above two studies, the repetitive nature of the SMB operation was overlooked and conventional control techniques for continuous processes were attempted. Indeed, SMB operation is periodic and there is an opportunity to significantly improve the control performance through

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the period-wise information feedback in addition to the real-time feedback. Aiming at application to repetitive processes while entertaining the advantages of MPC (model predictive control), Lee et al. [2001] proposed a new formulation of MPC called repetitive MPC (RMPC) and applied the technique to the start-up problem of a numerical SMB process [Natarajan et al., 2000]. RMPC is a model-based control technique that can perform period-wise integral control together with real-time feedback in the framework of MPC. Due to the period-wise integral action, it can eliminate the tracking offset despite model uncertainty and repetitive disturbances. It should be mentioned that a similar extension of MPC has already been made for batch process control [Lee et al., 1999]. Following Natarajan et al.'s study [2000], a few more RMPC-based dynamic optimization and control studies for SMB operation have been presented [Abel et al., 2004; Erdem et al., 2004] demonstrating the advantages of RMPC. One of the drawbacks of the above RMPC studies is that they rely on a linear time-invariant model for controller design and do not take the nonlinear aspects of the SMB process into account. This limits the operable region of the controller to some neighborhood around the nominal input-output trajectories where the linear model is derived.

In this study, a new repetitive control method for the SMB process has been proposed on the basis of the nonlinear physical SMB model. The major benefits we anticipate from this approach are two: First, the controller can be better performed due to the reduced model error over a wider operating range. Second, an on-line optimizer which produces optimum set points from the upper level of the controller can be constructed by using the nonlinear physical model. For this, the fundamental SMB model was numerically approximated to a set of ordinary differential equations (ODE's) using the orthogonal collocation method and discretized in time using forward difference approximation. At each switching period, the discrete-time nonlinear ODE model is repeatedly linearized along the operating trajectory of the previous period and used for renewing the repetitive controller. The control objective was chosen to steer the purity of the extract and raffinate streams at the terminal time of a switching period to their respective target values by manipulating the flow rates inside the columns while satisfying input constraints. The proposed technique is shown to outperform the existing approaches and can be a practical gear for improved SMB operation.

PROCESS DESCRIPTION

The principle of SMB can be easily understood from hypothetical circular chromatography with continuous port moving, as shown in Fig. 1(a). It has two input ports for feed and desorbent streams,

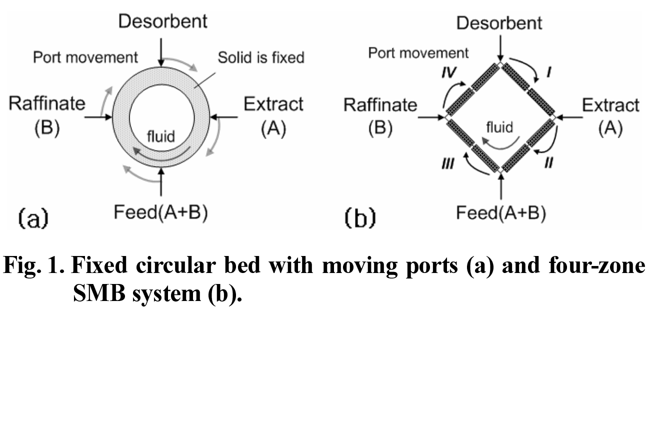

Fig. 1. Fixed circular bed with moving ports (a) and four-zone SMB system (b).

and two output ports for extract and raffinate streams. In fact, Fig. 1(a) is nothing more than a redrawing of the TMB by fixing the bed but moving the ports instead. In this system, the feed (A+B) is separated as in the usual chromatography. The components in the feed move along the desorbent flow and are split from each other by different affinities with the adsorbent. If the ports rotate in the same direction of the liquid flow with the average speed of the feed component moving, the stronger affinity component (A) can be removed from the extract port while the weaker affinity one (B) can be withdrawn from the raffinate port under continuously feeding and production. Fig. 1(b) shows a scheme of the SMB where the circular chromatography bed and the continuous port moving are replaced by several disjoint columns and discrete port switching, respectively. If the number of column is increased more, the SMB can be closer to the TMB. In this study, a four zone SMB with eight identical columns as shown in Fig. 1(b) is considered.

A dynamic model of the SMB can be obtained by connecting eight chromatography column models whose boundary conditions are periodically changing by port switching. A single column can be expressed differently with different levels of detail, especially on the mass transfer between the fluid and adsorbed phases and also within the adsorbent. In this study, the column is described by a dispersive model with linear adsorption equilibrium. It is assumed that the concentration of the adsorbed phase has no spatial distribution and is in equilibrium with that of the fluid phase. Under this condition, the model for a single column is written as

$$\frac{\partial c_i}{\partial t}+\frac{1-\varepsilon}{\varepsilon}\frac{\partial q_i}{\partial t}+v_j\frac{\partial c_i}{\partial z}=D_{ap,i}\frac{\partial^2 c_i}{\partial z^2},\ i=A,\ B \tag{1}$$

$$q_i=H_i c_i \tag{2}$$

$$\text{I.C.: } c_i(z, t=0)=0, \qquad q_i(z, t=0)=0 \tag{3}$$

$$\text{B.C.: } c_i^{in}=c_i\big|_{z=0^+},\ \frac{\partial c_i}{\partial z}\bigg|_{z=L}=0 \tag{4}$$

where c_i and q_i represent the concentration of the i^{th} species in the fluid and adsorbed phases, respectively; v, ε, D_{ap}, and H represent the liquid interstitial velocity, the bed void fraction, the apparent axial dispersion coefficient, and the equilibrium constant, respectively; t and z denote the time and axial distance, respectively. The boundary condition at z=L in Eq. (4) may be debatable, but we took this under the assumption that the column is long enough to satisfy the condition. In addition to the above, the material balance should be described at each node where the columns and ports are connected. Under the assumptions that the dead volume by the switching devices, connecting tubes, and other parts is negligible, the node balance is described as follows:

$$\begin{aligned}
&Q_D+Q_{IV}=Q_I,\ \ c_{i,IV}^{out}Q_{IV}+c_{i,D}Q_D=c_{i,I}^{in}Q_I\\
&Q_I-Q_E=Q_{II},\ \ c_{i,I}^{out}=c_{I,II}^{in}=c_{i,E}\\
&Q_{i,F}+Q_{II}=Q_{III},\ \ c_{i,II}^{out}Q_{II}+c_{i,F}Q_F=c_{i,III}^{in}Q_{III}\\
&Q_{III}-Q_R=Q_{IV},\ \ c_{i,III}^{out}=c_{i,IV}^{in}=c_{i,R}
\end{aligned} \tag{5}$$

In the above, Q represents volumetric flow rate, and zone indices I to IV are defined to be rotated according to the port switching as shown in Fig. 1(b). From Eq. (5), we can see that the eight flow rates are inter-related by four mass balance equations, and thus four

Table 1. Specifications of the concerned SMB process

SMB configuration	8 fixed columns {2 : 2 : 2 : 2}
Column length (L)	10 cm
Cross section area (S)	3 cm^2
Overall void fraction (~)	0.5
Axial dispersion coefficient (D_{ap})	1 cm^2/min
Feed concentration (C_F)	0.5 g/cm^3
Switching time (t*)	20 min
Linear isotherm parameter	H_A=3/H_B=1
Feed flow rate (Q_F)	1.5 cm^3/min
Desorbent flow rate (Q_D)	6 cm^3/min

flow rates are independently manipulable. In this study, Q_I and Q_{II} are chosen as manipulated variables, whereas Q_D and Q_F are reserved for future steady state optimization and kept constant. In this way, the SMB is represented as a 2×2 MIMO system with Q_I and Q_{II} as input, and extract and raffinate purities as output variables. In Table 1, dimensions and parameters of the SMB process considered in this study are given. The port switching time was determined so that it corresponds to the average component transport speed under the nominal condition.

The above model equations were approximated to a set of ordinary differential equations by using the orthogonal collocation method. For the process simulator, eight internal collocation points were used for each column. A larger number of collocation points had been tried but no appreciable improvement was observed. For a nonlinear nominal model for the controller design, five collocation points were used for each column. After incorporating the switching logic to the individual column models, we obtained a model equation of the following form for both the process simulator and the nominal model:

$$\frac{dx}{dt} = F(u)x + G(u)$$
$$y = C(x, u) \tag{6}$$

where $y = \left[\left. \frac{c_A}{c_A + c_B} \right|_{extr} \quad \left. \frac{c_B}{c_A + c_B} \right|_{raff} \right]^T$,

$u=[Q_I\ Q_{II}]^T$, and x for the nominal model is an 80×1 state vector that consists of the concentration of A and B at the five internal collocation points for the eight columns. Note that the columns were assumed to be identical. Therefore, port switching corresponds to one cyclic operation if x is defined such that its elements are relocated at each port switching so that their relative positions to u and y are invariant. In this case, F, G, and C are also invariant under the port switching.

The process simulator was solved by using the Runge-Kutta 4^{th}-order method (in MATLAB), and the nominal model was converted to a discrete-time version by applying the forward difference approximation to the time derivative.

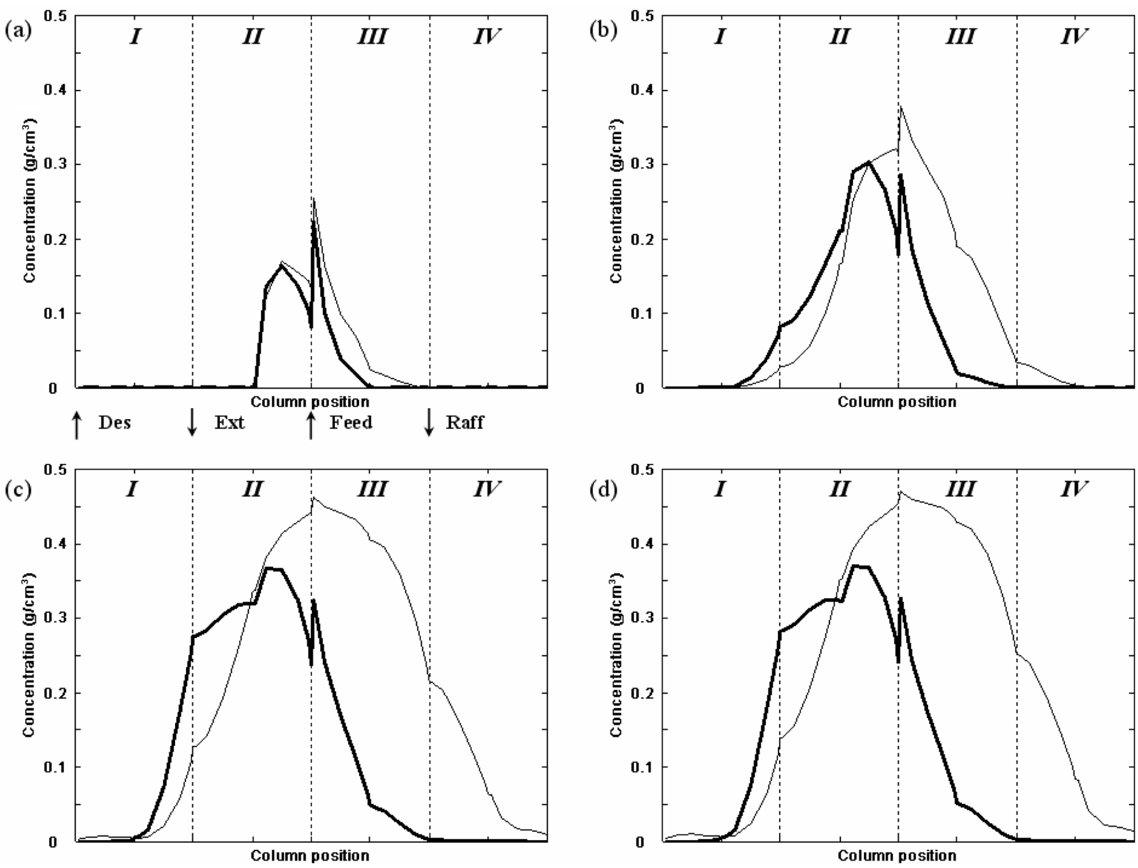

Fig. 2. Axial concentration profiles of component A and B at the last minute of the 2^{nd}, 5^{th}, 16^{th}, and 40^{th} switchings, respectively (thick-A, thin line-B).

PROCESS BEHAVIOR UNDER OFF-LINE OPERATION

1. Cyclic Steady State

Due to periodic switching, the SMB process is continuously under a dynamic state and hence never reaches a true steady state. Instead, it can reach a cyclic steady state where the same concentration profiles are repeated after each port switching. Fig. 2 demonstrates how the concentration profiles are developed from the starting cycle when the flow rates are fixed at constant values. We can see that the profiles of A and B converge to their respective limits in about two cycles (Fig. 2(c)). After then, the similar profiles are repeated. Such a periodic nature provides us with an opportunity of period-wise information feedback.

2. Operation at the Optimum Point by Triangle Theory

In the SMB process, determining the operating condition corresponding to a desired separation is a nontrivial task. For this, Mazzotti et al. [1997] have developed the so-called triangle theory on the basis of the TMB model with no axial dispersion. The theory offers us an operating window for pure separation and also an optimum operating condition that minimizes the desorbent consumption while satisfying the perfect separation. The Mazzotti condition is used as an initial operating point from which further improvement can be made through repeated simulation and/or experiments.

Fig. 3 shows the transient response of extract and raffinate purities when Mazzotti's optimum flow rates are applied to our SMB simulator. It is observed that the result shows significant discrepancy from pure separation, which comes from the periodic port switching and the axial dispersion effect that are not taken into consideration in the triangle theory.

CONTROLLER DESIGN

As observed above, it is not easy to steer an SMB process to a desired state by using off-line operation alone. To solve this problem, feedback control needs to be introduced. An appropriately designed controller can not only lead the process to the target state but also moderate the excessive and long transient response. In addition, the controller can mitigate the effects of various disturbances such as perturbation in the feed concentration, changes in the adsorption state, pulsation in the hydraulics during valve switching, etc.

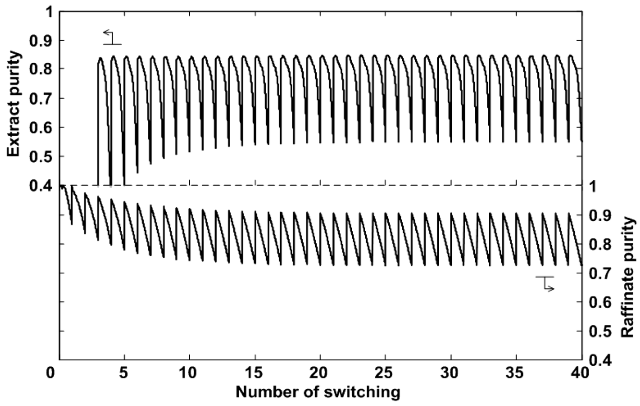

Fig. 3. Transient response of extract and raffinate purities by open-loop simulation with Mazzotti's condition.

In this study, we have devised a special control method by exploiting the repetitive nature of the SMB process. Such a control technique is called repetitive control (RC) in a generic term and has been studied by some researchers [Hara et al., 1988; Ledwich et al., 1993]. A key feature of RC is that an integral of the output error profile in the previous period is fed back in calculating the input profile for the upcoming period. Just as in ordinary integral control, the output profile error can be removed despite model error and period-wise repetitive disturbances as the number of periods increases. RC can be modified to include real-time feedback.

We assume that the measurements of product purity are available only once in a period at the last sampling instant before port switching with no analysis delay and the control objective is given to regulate the measured purities. Therefore, real-time control is not applicable and only RC was considered. In the existing RC control studies for the SMB process, the controller has been designed on the basis of a *linear time-invariant model*, which is obtained through either identification or linearization followed by spatial discretization (and sometimes together with model reduction) of a physical model. Unlike the existing studies, the RC technique presented in this study is based on a nonlinear physical model in order to reflect the inherent nonlinear aspects of the SMB process, especially from the bilinear term between v_i and $\partial c_i/\partial z$ in Eq. (1) and possibly nonlinear adsorption relationships to the controller. Benefits from the use of a physical model include the fact that the controller can properly behave over a large operating region and the on-line optimizer can be designed at the same time.

3. Algorithm Derivation

If Eq. (6) is converted to a discrete-time version and written for the k^{th} switching period, we have

$$\begin{aligned} x_k(t+1)&=A(u_k(t))x_k(t)+B(u_k(t)) \\ y_k(t)&=C(x_k(t),\ u_k(t)) \end{aligned} \tag{7}$$

To include the period-wise integral action, we write Eq. (7) for the $(k\text{-}1)^{th}$ switching period, too and take the difference from Eq. (7). Also we assume cautious control that implies $u_k \approx u_{k-1}$. Then we have

$$\begin{aligned} \Delta x_k(t+1)&=A(u_{k-1}(t))\Delta x_k(t)+\overline{B}(u_{k-1}(t))\Delta u_k(t) \\ y_k(t)&=y_{k-1}(t)+\overline{C}(x_{k-1}(t),\ u_{k-1}(t))\Delta x_k(t) \end{aligned} \tag{8}$$

where $\Delta x_k \triangleq x_k - x_{k-1}$, $\Delta u_k \triangleq u_k - u_{k-1}$, $\overline{B} \triangleq \partial B/\partial u^T$, and $\overline{C} \triangleq \partial C/\partial x^T$. Now, by lifting the equation over a switching period, a model that describes the state transition from the present period to the next can be derived. Since the output is assumed to be measured at the last sampling instant of a switching period, the resulting model equation can be represented as

$$\begin{aligned} \Delta x_{k+1}(0)&=\boldsymbol{\Phi}_{k-1}\Delta x_k(0)+\boldsymbol{\Gamma}_{k-1}\Delta \mathbf{U}_k \\ y_k(N-1)&=y_{k-1}(N-1)+\boldsymbol{\Pi}_{k-1}\Delta x_k(0)+\mathbf{G}_{k-1}\Delta \mathbf{U}_k \end{aligned} \tag{9}$$

where

$$\Delta \mathbf{U}_k \triangleq \begin{bmatrix} \Delta u_k(0) \\ \vdots \\ \Delta u_k(N-1) \end{bmatrix}$$

$$\boldsymbol{\Phi} \triangleq A(N-1)A(N-2)\cdots A(0)$$

$$\boldsymbol{\Gamma} \triangleq [A(N-1)\cdots A(1)\overline{B}(0) | A(N-1)\cdots A(2)\overline{B}(1) | \cdots | \overline{B}(N-1)]$$

$$\Pi \triangleq \overline{C}(N-1)A(N-2)\cdots A(0)$$
$$\mathbf{G} \triangleq [\overline{C}(N-1)A(N-2)\cdots A(1)\overline{B}(0)|\cdots|\overline{C}(N-1)B(N-2) \quad 0]$$

and N is the number of sampling instants in a switching period. In our process, both the extract and raffinate purities have minimum values at t=N−1, *i.e.*, $y_k(N-1)$ is the worst case purity in a switching period. In this respect, regulating $y_k(N-1)$ at a set point guarantees that the product purities are above certain specified values. In the above, we used the shorthand notations such as $A_{k-1}(t) \triangleq A(u_{k-1}(t))$ and so forth. Recasting Eq. (9) to a standard state space model after defining $e \triangleq y-r$ where r means the output set point results in

$$\begin{bmatrix} \Delta x_{k+1}(0) \\ e_k(N-1) \end{bmatrix} = \begin{bmatrix} \boldsymbol{\Phi}_{k-1} & \mathbf{0} \\ \boldsymbol{\Pi}_{k-1} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \Delta x_k(0) \\ e_{k-1}(N-1) \end{bmatrix} + \begin{bmatrix} \boldsymbol{\Gamma}_{k-1} \\ \mathbf{G}_{k-1} \end{bmatrix} \Delta \mathbf{U}_k$$

$$e_k(N-1) = [\,\boldsymbol{\Pi}_{k-1} \quad \mathbf{I}\,] \begin{bmatrix} \Delta x_k(0) \\ e_{k-1}(N-1) \end{bmatrix} + \mathbf{G}_{k-1}\Delta \mathbf{U}_k \tag{10}$$

or

$$\mathbf{z}_{k+1} = \overline{\boldsymbol{\Phi}}_{k-1}\mathbf{z}_k + \overline{\boldsymbol{\Gamma}}_{k-1}\Delta \mathbf{U}_k$$
$$e_k(N-1) = \overline{\boldsymbol{\Pi}}\mathbf{z}_k + \mathbf{G}_{k-1}\Delta \mathbf{U}_k \tag{11}$$

Now the input sequence $\Delta \mathbf{U}_k$ can be determined such that $e_{k|k-1}(N-1)$, an optimum prediction of $e_k(N-1)$ based on the information up to the $(k-1)^{th}$ switching period, is minimized. If we consider a quadratic criterion, the problem can be described as

$$\min_{\Delta \mathbf{U}_k} [\|e_{k|k-1}(N-1)\|_Q^2 + \|\Delta \mathbf{U}_k\|_R^2] \tag{12}$$

subject to constraints

In the above, the constraints include the input-output equality relationship between $\Delta \mathbf{U}_k$ and $e_{k|k-1}(N-1)$, and inequality constraints on the input movements. $e_{k|k-1}(N-1)$ can be estimated by using a Kalman filter applied to Eq. (11). For this Kalman filter to run, another Kalman filter (in fact, an extended Kalman filter) applied to Eq. (8) for estimation of $x_k(t|t)$ needs to be run in parallel since computation of $\overline{\boldsymbol{\Pi}}$ in Eq. (11) requires $\overline{C}$, which again requires x(t) for its computation (see Eq. (8)). The Kalman filter and extended Kalman filter equations can be found in various textbooks; for example, see Grewel et al. [2001].

The input inequality constraints are given by the restriction that the flow rate in each bed zone of the SMB should be positive as

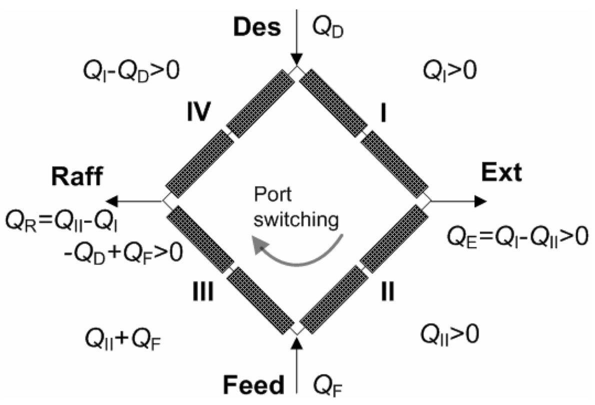

Fig. 4. Positive flow rate conditions imposed on Q_I and Q_{II}.

shown in Fig. 4. In addition, another set of input inequality constraints are derived from the safety reason that the maximum flow rate should be limited to prevent the column pressure from being excessive. From this consideration, inequality constraints are imposed on the liquid flow rates so that each of them is restricted by 50 ml/min. The input constraints on u need to be modified in terms of $\Delta \mathbf{U}_k$. For details on this procedure, please refer to Lee et al. [2000]. With the constraints formulated as linear inequalities of $\Delta \mathbf{U}_k$, the minimization of Eq. (12) becomes a standard QP (quadratic programming) problem.

4. Input Blocking

In the controller calculation, it is demanding and indeed unnecessary to optimize all the elements in $\Delta \mathbf{U}_k$ independently. Instead, it is sufficient and indeed beneficial to allow the sequence in $\Delta \mathbf{U}_k$ to have values only at pre-specified limited instants and optimize only those values. Then the input signal changes only at the specified time instants and remains constant in between. Such a restriction is called input blocking and can be implemented by using the blocking matrix. For demonstration, let us assume the single input case with N=4. Also, the input is allowed to change only twice at the initial time and at the mid-time in a switching period. Then we can represent the restriction as

$$\Delta \mathbf{U}_k = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{bmatrix} \Delta \mathbf{V}_k = J\Delta \mathbf{V}_k \tag{13}$$

Inserting the above relation into all the associated equations modifies the minimization problem to determine $\Delta \mathbf{V}_k$ instead of $\Delta \mathbf{U}_k$.

SIMULATION CONDITIONS

For discrete-time modeling and control, the sampling time was chosen to be 0.1 min, which means N=200 sampling instants in a switching period. Longer sampling times were found to cause too large model error.

The performance of the controller was investigated in terms of set point tracking, disturbance rejection, and robustness against model error. As a disturbance, we considered a step change in feed composition. The model error was simulated by applying step changes in the equilibrium constants for the linear isotherm.

The initial values of Q_I and Q_{II} were determined by using Mazzotti's triangle theory. For Q_F=1.5 cm^3/min and Q_D=6 cm^3/min, Q_I and Q_{II} were determined as 7.5 and 1.5 cm^3/min, respectively.

RESULTS AND DISCUSSION

1. Number of Input Movements

In Fig. 5, we compared the input and output transient responses during an initial start-up for three different cases. In the first case, the input movement is not blocked. In the second and third cases, the input is allowed to change twice and only once during a switching period, respectively. The set points for the extract and raffinate streams were given as 0.9 and 0.7, respectively. In this figure, the whole output profiles are displayed to demonstrate how the purities vary in real-time. It is assumed that only the output at the pit points

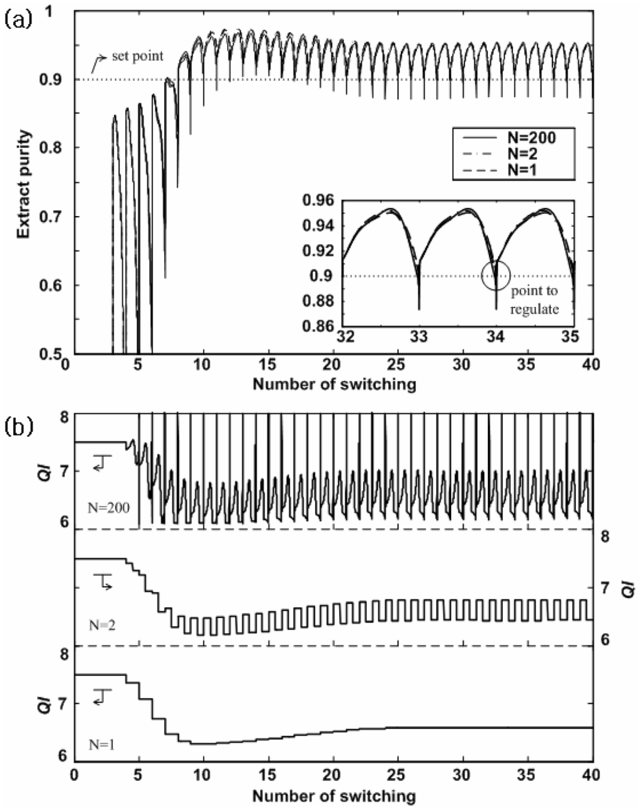

Fig. 5. Effects of the input blocking on the output response (N= number of allowed input change during one switching period).

is measured and regulated.

As can be seen, the output responses for the above three cases are virtually indistinguishable. From these results, we blocked the input movement to change only twice in the subsequent simulations.

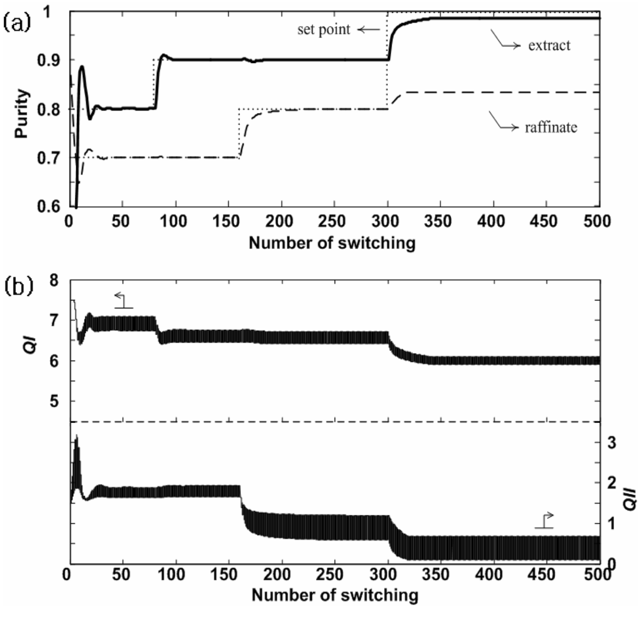

Fig. 6. Performance of the proposed controller for set point changes. Extract and raffinate purities at the controlled points (a) and controller outputs Q_I and Q_{II} (b).

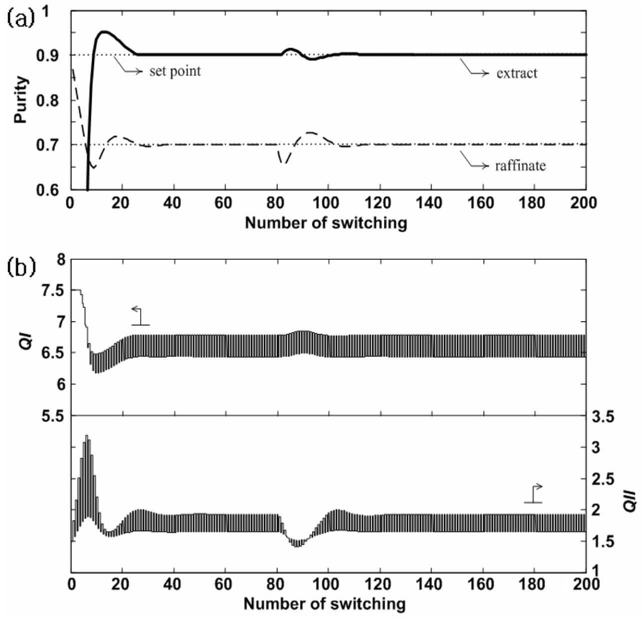

Fig. 7. Performance of the proposed controller against feed composition change. Extract and raffinate purities at the controlled points (a) and controller outputs Q_I and Q_{II} (b).

2. Set Point Tracking

Fig. 6 shows the input and output trajectories tracking the set point changes. In this figure, only the outputs at the controlled instants are displayed. It can be observed that the process shows quite satisfactory tracking performance for various set point scenarios. In the last change, both outputs were required to attain 100% purity, which is physically impossible for the present SMB. Nevertheless, the controller did its best and attained 0.99 and 0.85 for the extract and raffinate streams, respectively.

3. Disturbance Rejection

Fig. 7 shows the response when the mol faction of A in the feed changes from 0.5 to 0.25 at k=80. We can see that the disturbance effect is gracefully rejected and the purities return to their respective set points after a short transient.

4. Model Error

This time, we intentionally imposed parameter error on the control model by changing H_A and H_B to 4.5 and 1.5 from 3.0 and 1.0, respectively, while the process itself remained unchanged. Fig. 8 compares the output responses for the nominal case and parameter error case. We can see the response from the parameter error case is worse than the nominal case. However, the controller still works fine even when more than 100% of uncertainties are given to the equilibrium constants.

5. Low Selectivity Case

So far, the system was assumed to have a relatively high selectivity, $H_A/H_B=3$. To investigate whether the controller performs similarly in a low selectivity system, we modified H_A and H_B to 1.6 and 1.0 for both the process simulator and the nominal model. Q_F and Q_D were set at 0.45 and 6 [cm^3/min]. We conducted an open-loop simulation using Mazzotti's condition first and then closed simulation with the set points of extract and raffinate purities given at 0.7 and 0.6, respectively. In Fig. 9, the results are summarized. As can

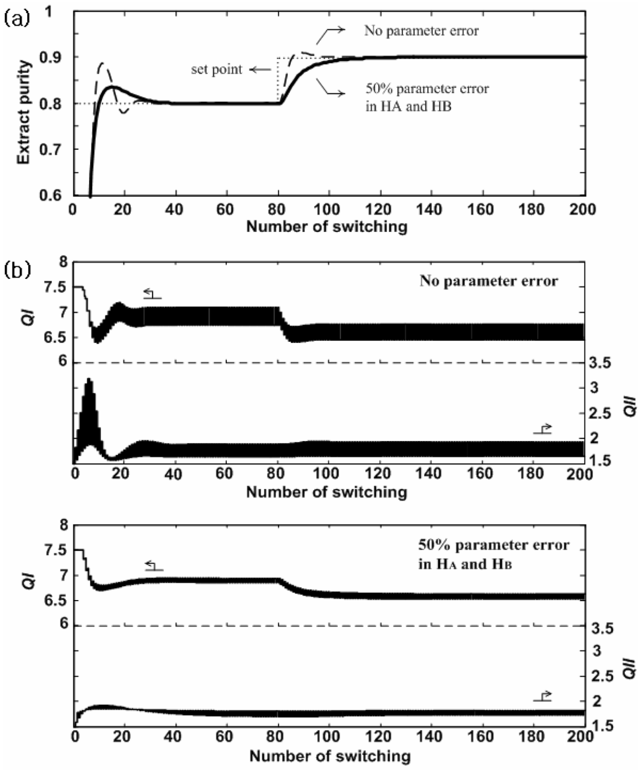

Fig. 8. Performance of the proposed controller when there is large error in H_A and H_B in the nominal mode. Extract purity at the controlled points (a) and controller output Q_I (b).

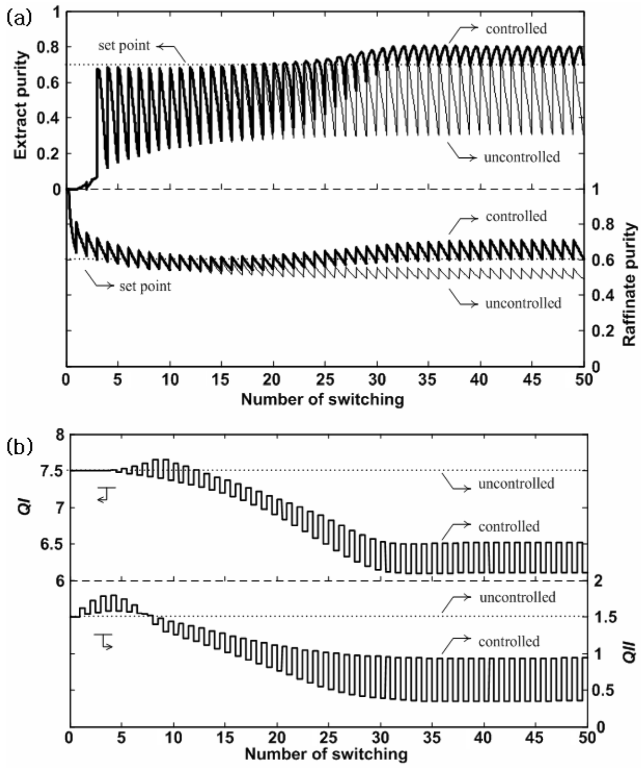

Fig. 9. Results for the low-selectivity separation case where H_A=1.5 and H_B=1 with Q_F=0.9 and Q_D=5 [cm^3/min]. Open-loop simulation was conducted under the Mazzotti's condition.

be observed, similar performance to the high selective case was obtained.

To recapitulate the performance of the proposed controller, results from some representative SMB control studies are compared with ours in Table 2. Since the details of the process situation and the control objectives are different from one to another, fair comparison is not possible. Nevertheless one can easily observe that the proposed controller can bear and handle much larger disturbances (in the feed concentration as well as isotherm constants) than the others. The tracking and regulation performance are found to be comparable or better. The main gear for the above performance is the nonlinear model-based approach, which enables the controller to appropriately perform in a larger operating region than the linear model-based controllers.

Table 2. Comparison of the present study with some representative SMB control studies

	Klatt et al. [2002]	Abel et al. [2004]	Schramm et al. [2003]	Our study
		Process and Controller Description		
SMB configuration	8 columns {2 : 2 : 2 : 2}	8 columns {2 : 2 : 2 : 2}	8 columns {2 : 2 : 2 : 2}	8 columns {2 : 2 : 2 : 2}
Isotherm	Linear	Linear	Langmuir	Linear
Modeling method	Linear ARX model	Reduced linearized model using FDM	No model	Nonlinear model using OCM
Control method	MIMO IMC (tracking of optimal conc. trajectory)	MIMO RMPC (dynamic optimization)	Multiple PI control (purity control)	MIMO RC (purity control)
		Results		
Settling cycle number (SP)		25 cycles	3 cycles	3 cycles
Settling cycle number (Dist.)	4 cycles (5% isotherm)	8 cycles (10% isotherm)	4 cycles (10% feed conc.)	5 cycles (+50% feed conc.) 5 cycles (+50% isotherm)

CONCLUSIONS

Through this study, a nonlinear model-based repetitive controller has been proposed for the SMB process. The objective of control has been placed in, under the assumption that the feed and desorbent flow rates are kept constant, regulating the extract and raffinate purities at a time instant in each switching period at the respective target values. The controller was designed on the basis of a nonlinear physical model of the SMB process or more precisely, a successive linearization of the nonlinear SMB model around the operating trajectory of the previous period. Thanks to the period-wise feedback and also by reflecting the nonlinear aspects to the controller, the proposed controller showed quite satisfactory performance against set point as well as disturbance changes, and also significant model error.

With the robustly performing controller in hand, further research is under way to design a nonlinear model identifier and an on-line optimizer that minimizes the desorbent consumption and maximizes the feed flow rate at the same time while the controller regulates the product purity.

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NOMENCLATURE

ARX : Auto-Regressive with eXogeneous variables
c_i : concentration in the fluid phase [g/cm^3]
c_F : feed concentration [g/cm^3]
conc. : concentration
cont. : control
D_{ap} : axial dispersion coefficient [cm^2/min]
Dist. : disturbance
e : vector of error variables
FDM : Finite Difference Method
H_i : equilibrium constant
IMC : Internal Model Control
k : switching period index
L : column length [cm]
N : number of time steps per switching period
OCM : Orthogonal Collocation Method
PI : Proportional and Integral
q_i : concentration in the adsorbed phase [g/cm^3]
Q_I : flow rate in the zone I [cm^3/min]
Q_{II} : flow rate in the zone II [cm^3/min]
Q_{III} : flow rate in the zone III [cm^3/min]
Q_{IV} : flow rate in the zone IV [cm^3/min]
Q_D : desorbent flow rate [cm^3/min]
Q_E : extract flow rate [cm^3/min]
Q_F : feed flow rate [cm^3/min]
Q_R : raffinate flow rate [cm^3/min]
RC : Repetitive Control
RMPC : Repetitive Model Predictive Control
S : cross-section area of the column [cm^2]
SP : Set Point change
t : time [min]
t^* : switching time [min]
traj. : trajectory
u : vector of manipulated variables
U : vector grouping the input values for one period
v : liquid interstitial velocity [cm/min]
V : vector grouping the input values for one period blocked
x : state vector
y : vector of output purities
z : axial distance of the column [cm]
z : state vector

Greek Letter

ε : void fraction

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