REPETITIVE CONTROL OF SIMULATED MOVING BED PROCESS BASED ON CUBIC SPLINE COLLOCATION MODEL AND SUCCESSIVE LINEARIZATION

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Abstract: A new repetitive control (RC) technique for the simulated moving bed (SMB) process has been proposed. The RC technique was designed on the basis of a fundamental SMB model successively linearized around the operating trajectories in the previous period. It performs regulation of averaged product purities over each period at both extract and raffinate ports. To obtain a low-order but reliable fundamental SMB model for the RC design, we adopted a cubic spline collocation method combined with the far-side boundary condition. Through application to a numerical SMB process, it was found that the proposed RC technique performs quite satisfactorily against model error as well as set point and disturbance changes.

Keywords: simulated moving bed, repetitive control, reduced-order modeling, cubic spline collocation method

1. INTRODUCTION

The simulated moving bed (SMB) has received keen attention recently, especially for the separation of pharmaceutical and bio-chemical products. It has advantages of having less solvent consumption, smaller apparatus scale, lower investment cost, and higher yields over the batch chromatography (Lim, 2006). The SMB is a feasible realization of the conceptual counter-current continuous chromatography called true moving bed (TMB), where the adsorbent bed continuously moves in the reverse direction of the desorbent flow, by periodic switching of the inlet and outlet ports in the direction of the desorbent flow (Ruthven and Ching, 1989). By the port switching, complex adsorption phenomena, and inherent nonlinearity of the process, however, finding a desired operating condition of an SMB process is not a simple task but usually requires long trial and error attempts.

For the TMB model with equilibrium adsorption and no axial dispersion, Mazzotti *et al.*(1997) proposed the so called triangle theory that provides operating conditions for perfect separation of extract and raffinate products. However, significant discrepancy from pure separation is frequently observed when the condition is applied to the SMB. Feedback control is of great help in reducing the transient time for the SMB to reach a desired separation state. In the separation of small amount of high-valued products, highly performed feedback control might be crucial since the off-spec products during the transient period incur large economic loss.

Addressing such needs, Kloppenburg *et al.* (1999) considered a hypothetical TMB process and derived a nonlinear control method using the asymptotically exact input/output linearization. Klatt

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et al. (2000) proposed a two-layer control architecture where the optimal set points are calculated in the higher level optimizer for the lower level IMC controllers based on a MIMO ARX model. The previous researches didn't consider the repetitive nature of the SMB operation. In fact, the SMB operation is periodic and there is an opportunity to significantly improve the control performance through the period-wise information feedback. For such processes, Lee *et al.*(2001) proposed a new formulation of MPC called repetitive MPC (RMPC) that conducts period-wise feedback together with real-time feedback in the framework of MPC. Due to the period-wise integral action, it can eliminate the tracking offset overcoming model uncertainty and repetitive disturbances (Hara *et al.*, 1998; Ledwich and Bolton, 1993). The technique has been applied to the start-up problem, regulation, and dynamic optimization to the SMB process (Natarajan and Lee, 2000; Abel *et al.*, 2004; Erdem *et al.*, 2004). One of the shortcomings of the existing RMPC studies is that they relied on a linear time-invariant model for controller design and didn't take the nonlinear aspects of the SMB process into account. This may limit the operable region of the controller to some narrow region around the nominal input-output trajectories.

In this research, a novel repetitive control (RC) method for the SMB process has been proposed on the basis of the successive linearization of a fundamental SMB model. For this, we derived an ordinary differential equation (ODE) model of the SMB process using the cubic spline collocation method. At each switching period, the discrete-time nonlinear ODE model is repeatedly linearized along the operation trajectory of the previous period and used for renewing the repetitive controller. The control objective was chosen to steer product purities averaged over a switching period at the extract and raffinate ports to their respective targets by manipulating two flow rates while satisfying input constraints.

2. NUMERICAL SMB MODEL

2.1 *Mathematical model of SMB*

We consider a four zone SMB with eight identical columns as shown in Fig. 1 where the feed stream contains binary components, A and B. It is assumed that the fluid phase of each component satisfies a linear adsorption equilibrium with the adsorbed phase.

Assuming the linear adsorption isotherm, a single column model can be described as

$$\frac{\partial c_{ij}}{\partial \hat{t}} + \frac{(1-\varepsilon)}{\varepsilon}\frac{\partial w_{ij}}{\partial \hat{t}} + u_j \frac{\partial c_{ij}}{\partial \hat{z}} = D\frac{\partial^2 c_{ij}}{\partial \hat{z}^2} \quad (1)$$

$$\frac{\partial w_{ij}}{\partial \hat{t}} = k_i(c_{ij} - w_{ij}^*) \quad (2)$$

$$w_{ij}^* = H_i w_{ij} \quad (3)$$

where $i = A,\ B$; $j = 1,\ \cdots, 8$ denotes the column index; c_{ij}, w_{ij}, and w_{ij}^* represent the concentrations of the i^{th} species in the j^{th} column in the fluid, adsorbed phases, and equilibrated concentration with the adsorbed phase, respectively; ε, D, and k_i denote the overall void fraction of the bed, the apparent axial dispersion coefficient, and mass transfer coefficient, respectively; u_j represents the liquid interstitial velocity.

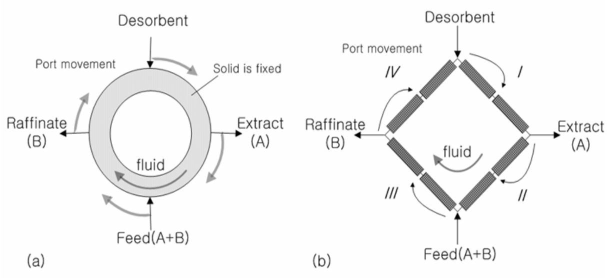

Fig. 1. Fixed circular bed with moving ports (a) and a four-zone SMB system(b).

Using the dimensionless space coordinate, $z \triangleq \hat{z}/L$ where L is the column length and dimensionless time $t \triangleq D\hat{t}/L^2$, (1) and (2) can be recast to

$$\frac{\partial c_{ij}}{\partial t} + \eta\frac{\partial w_{ij}}{\partial t} + N_{Pe,j}\frac{\partial c_{ij}}{\partial z} = \frac{\partial^2 c_{ij}}{\partial z^2} \quad (4)$$

$$\frac{\partial w_{ij}}{\partial t} = N_{Sh,i}(c_{ij} - H_i w_{ij}) \quad (5)$$

where $N_{Pe,j} \triangleq u_j L/D$ and $N_{Sh,i} \triangleq k_i L^2/D$ denote the Peclet and the Sherwood numbers, respectively, and $\eta \triangleq (1-\varepsilon)/\varepsilon$.

The initial and boundary conditions for this system are given as

$$\text{I.C. } c_{ij}(0,z) = w_{ij}(0,z) = 0 \quad (6)$$

$$\text{B.C. } c_{ij}(t,0) = c_{ij}^{in},\quad \left.\frac{\partial c_{ij}}{\partial z}\right|_{\infty} \approx \left.\frac{\partial c_{ij}}{\partial z}\right|_{z_L} = 0 \quad \text{for a sufficiently large } z_L \quad (7)$$

The second BC in (7) was proposed by Guiochon *et al.* (Guiochon *et al.*, 1994) and called the far-side boundary condition by Yun and Lee (2007). For finite difference/element/volume methods, (7) may increase complexity since the added region, $(1,\ z_L]$ should be discretized, too. However, collocation methods can easily adopt the BC without raising such complexity as will be shown later.

Referring to Fig. 1, the following material balances are satisfied at each node:

$$
\begin{aligned}
&Q_{IV} + Q_D = Q_I \ , \ c^{out}_{i,IV} Q_{IV} + c_{i,D} Q_D = c^{in}_{i,I} Q_I \\
&Q_I - Q_E = Q_{II} \ , \ c^{out}_{i,I} = c^{in}_{i,II} = c_{i,E} \qquad (8)\\
&Q_{II} + Q_F = Q_{III} \ , \ c^{out}_{i,II} Q_{II} + c_{i,F} Q_F = c^{in}_{i,III} Q_{III} \\
&Q_{III} - Q_R = Q_{IV} \ , \ c^{out}_{i,III} = c^{in}_{i,IV} = c_{i,R} \\
&c^{in}_{ij} = c^{out}_{i,j-1}
\end{aligned}
$$

The column and zone indices are rotated according to the port switching as shown in Fig. 1.

2.2 *ODE model by cubic spline collocation method*

The PDE model in eq. (4) is reduced a set of ODE's using the cubic spline collocation method (CSCM). The ordinary orthogonal collocation method (OCM) is prone to generate spurious ripples in the solution for the high Peclet number columns. The CSCM is same as OCM except that the cubic spline function is used as the interpolation function to improve the shortcoming of OCM.

Let the spatial domain $[0, z_L]$ be divided into $n+1$ intervals with the corresponding nodal points as $z_0(=0),\ z_1, \cdots, z_{n-1},\ z_n(=1)$, and $z_{n+1}(=z_L)$. Let $p_k(z)$ be the cubic spline function for the k^{th} interval. Then the interpolation function for a single column is

$$\bar{c}(z;\theta) \triangleq \sum_{k=1}^{n+1} \theta_k p_k(z) S_k(z) \qquad (9)$$

where $S_k(z) = 1$ over $[z_{k-1}, z_k]$ and 0 otherwise. After some straightforward manipulations, the interpolation function in (9) can be rearranged to have the output at the collocation points as its parameters (Choi *et al.*, 1991; Manickam *et al.*, 1998)

$$\bar{c}(\mathbf{c}(t), z) = \mathbf{m}(z)^T \bar{\mathbf{c}}(t) \qquad (10)$$

where $\mathbf{m}(z)$ is an $(n+2)\times 1$ vector and $\bar{\mathbf{c}} = [c(t,z_0)\ \cdots\ c(t,z_n)\ c(t,z_{n+1})]^T$. Using the above interpolation function, we have

$$\frac{\partial \bar{\mathbf{c}}}{\partial z} = \bar{\mathbf{A}}\bar{\mathbf{c}} \ \text{ and } \ \frac{\partial^2 \bar{\mathbf{c}}}{\partial z^2} = \bar{\mathbf{B}}\bar{\mathbf{c}} \qquad (11)$$

where

$$\bar{\mathbf{A}} \triangleq \text{col}\left[\mathbf{m}^{(1)}(z_i)^T\right] \ \text{ and } \ \bar{\mathbf{B}} \triangleq \text{col}\left[\mathbf{m}^{(2)}(z_i)^T\right], \quad \text{for } i = 0, \cdots, n+1$$

At the collocation points, (4) and (5) should be exactly satisfied by the interpolation function. Dropping the subscript $_{ij}$ to avoid notational complexity, this condition leads to

$$\frac{d\bar{\mathbf{c}}}{dt} + \eta \frac{d\bar{\mathbf{w}}}{dt} = \left(\bar{\mathbf{B}} - N_{Pe}\bar{\mathbf{A}}\right)\bar{\mathbf{c}} \qquad (12)$$

$$\frac{d\bar{\mathbf{w}}}{dt} = N_{Sh}(\bar{\mathbf{c}} - H\bar{\mathbf{w}}) \qquad (13)$$

where $\bar{\mathbf{w}}$ represents $[w(t,z_0)\ \cdots\ w(t,z_n)\ w(t,z_{n+1})]^T$. Indeed, (4) and (5) hold on the domain (open set) excluding the boundary points. Thus among the ODE's in (12) and (13), only the ones at the internal collocation points are valid. Omitting the ODE's at the boundaries from (12) and (13) and applying the inlet and far-side boundary conditions to the remaining equations yields

$$\frac{d\mathbf{c}}{dt} = \mathbf{E}(\mathbf{u})\ \mathbf{c} + \eta N_{Sh} H\ \mathbf{w} + \mathbf{g}(\mathbf{u})\ c^{in}(t) \qquad (14)$$

$$\frac{d\mathbf{w}}{dt} = N_{Sh}\ \mathbf{c} - N_{Sh} H\ \mathbf{w} \qquad (15)$$

where $\mathbf{c} \triangleq \left[\, c(t,z_1)\ \cdots\ c(t,z_n) \,\right]^T$ and $\mathbf{w}$ is similarly defined.

From (8), we can see that four flow rates are independently manipulable. In this study, Q_I and Q_{II} were chosen as manipulated variables whereas Q_D and Q_F were reserved for future steady state optimization and kept constant. In this way, the SMB is represented as a 2x2 MIMO system with Q_I and Q_{II} as input, and extract and raffinate concentrations as output variables.

After incorporating the models for eight columns and the switching logic, the SMB process can be expressed by a set of ODE's of the following form:

$$\frac{d\mathbf{x}}{dt} = F(\mathbf{u})\mathbf{x} + G(\mathbf{u}) \qquad (16)$$

where $\mathbf{x}$ denotes the state vector composed of the fluid phase and adsorbed phase concentrations of A and B at the collocation points for the eight columns and $\mathbf{u} \triangleq \left[\, Q_I \ \ Q_{II} \,\right]^T$.

3. DESIGN OF REPETITIVE CONTROL

The SMB model in (13) is nonlinear while the present RC method (Lee *et al.*, 2001) is based on a linear dynamic model. To accommodate the nonlinear aspects of the process as much as possible in the RC design, a linear model is derived around the operating trajectories after each cycle and used for the RC design for the upcoming cycle. Also the product purities at extract and raffinate streams averaged over a cycle were chosen as of controlled variables.

3.1 *Model for RC design*

Let the discrete-time equivalent model to (13) written for the k^{th} switching period with the purities as the output be

$$\mathbf{x}_k(t+1) = A(\mathbf{u}_k(t))\mathbf{x}_k(t) + B(\mathbf{u}_k(t)) \quad (17)$$
$$\bar{\mathbf{y}}_k(t) = C(\mathbf{x}_k(t))\mathbf{x}_k(t)$$

where $A(\mathbf{u}_k) \triangleq e^{F(\mathbf{u}_k)h}$, $B(\mathbf{u}_k) \triangleq F^{-1}(\mathbf{u}_k)[e^{F(\mathbf{u}_k)h} - I]G(\mathbf{u}_k)$, $\mathbf{y} \triangleq \left[\frac{c_A}{c_A+c_B}\Big|_{ext} \quad \frac{c_B}{c_A+c_B}\Big|_{raf}\right]^T$; h denotes the sampling interval. It is assumed that one cycle contains N sampling instants. To include the cycle-wise integral action, we write (17) for the $(k-1)^{\text{th}}$ cycle, too, and take the difference from (17). Assuming cautious control, *i.e.*, $\mathbf{u}_k(t) \approx \mathbf{u}_{k-1}(t)$ and $\mathbf{x}_k(t) \approx \mathbf{x}_{k-1}(t)$, we have

$$\mathbf{z}_k(t+1) \approx A(\mathbf{u}_{k-1}(t))\mathbf{z}_k(t) + \bar{B}(\mathbf{u}_{k-1}(t))\Delta\mathbf{u}_k(t)$$
$$\bar{\mathbf{y}}_k(t) \approx \bar{\mathbf{y}}_{k-1}(t) + \bar{C}(\mathbf{x}_{k-1}(t))\mathbf{z}_k(t) \quad (18)$$

where $\mathbf{z}_k(t) \triangleq \mathbf{x}_k(t) - \mathbf{x}_{k-1}(t)$, $\Delta\mathbf{u}_k(t) \triangleq \mathbf{u}_k(t) - \mathbf{u}_{k-1}(t)$, $\bar{B} \triangleq \partial(Ax+B)/\partial\mathbf{u}^T$, and $\bar{C} \triangleq \partial C/\partial\mathbf{x}^T$. The output equation is converted with respect to average purities over a switching period.

$$\mathbf{y}_k = \mathbf{y}_{k-1} + \frac{1}{N}\sum_{i=1}^{N}\bar{C}(\mathbf{x}_{k-1}(i))\mathbf{z}_k(i) \quad (19)$$

where $\mathbf{y}_k \triangleq \frac{1}{N}\sum_{i=1}^{N}\bar{\mathbf{y}}_k(i)$. Now, by lifting the equation over a switching period, a model that describes the state transition from the present cycle to the next can be derived in the following form:

$$\mathbf{z}_{k+1}(0) = \Phi_k\mathbf{z}_k(0) + \Gamma_k\Delta\mathbf{U}_k \quad (20)$$
$$\mathbf{y}_k = \mathbf{y}_{k-1} + \Pi_k\mathbf{z}_k(0) + \mathbf{G}_k\Delta\mathbf{U}_k$$

where

$$\Delta\mathbf{U}_k \triangleq [\Delta\mathbf{u}_k(0)^T \cdots \Delta\mathbf{u}_k(N-1)^T]^T$$

3.2 *Repetitive control (Lee et al., 2001)*

Recasting (19) to a standard state space model after defining $\mathbf{e}_k \triangleq \mathbf{y}_k - \mathbf{r}$ where $\mathbf{r}$ means the output set point results in

$$\begin{bmatrix}\mathbf{z}_{k+1}(0)\\ \mathbf{e}_k\end{bmatrix} = \begin{bmatrix}\Phi_k & 0\\ \Pi_k & I\end{bmatrix}\begin{bmatrix}\mathbf{z}_k(0)\\ \mathbf{e}_{k-1}\end{bmatrix} + \begin{bmatrix}\Gamma_k\\ \mathbf{G}_k\end{bmatrix}\Delta\mathbf{U}_k$$
$$\mathbf{e}_k = \begin{bmatrix}\Pi_k & I\end{bmatrix}\begin{bmatrix}\mathbf{z}_k(0)\\ \mathbf{e}_{k-1}\end{bmatrix} + \mathbf{G}_k\Delta\mathbf{U}_k \quad (21)$$

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

$$\min_{\Delta\mathbf{U}_k}\left[||\mathbf{e}_{k|k-1}||_Q^2 + ||\Delta\mathbf{U}_k||_R^2\right] \quad (22)$$

with input inequality constraints given by the restriction that the flow rate in each zone should be positive as shown in Fig. 2 and additional input constraints that restrict the maximum flow rates to prevent the column pressure from being excessive.

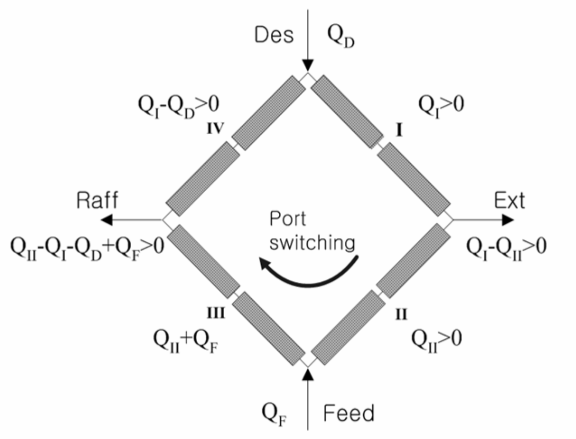

Fig. 2. Positive flow rate conditions imposed on QI and QII.

3.3 *Input blocking*

In the input calculation, it is demanding and moreover unnecessary to optimize all the elements in ΔU_k independently. Instead, it is sufficient and indeed beneficial to allow the input to change only at limited times within a switching period. Such a restriction is called input blocking and can be implemented using a blocking matrix. For demonstration, let us assume the single input case with $N = 4$. If the input is allowed to change only twice at the initial time and at a mid-time, the blocking matrix representation is

$$\Delta\mathbf{U}_k = \begin{bmatrix}1 & 0\\ 1 & 0\\ 0 & 1\\ 0 & 1\end{bmatrix}\Delta\mathbf{V}_k \quad (23)$$

Inserting the above into the associated equations modifies the minimization problem to determine ΔV_k instead of ΔU_k.

4. SIMULATION CONDITIONS

In Table 1, parameters and nominal operating conditions of the SMB process and some key parameters for the controller design are given. The port switching time was determined so that it corresponds to the average component transport speed under the nominal condition.

Table 1. Parameters for SMB and simulation conditions.

cross-sec. area = 3 cm^2, $L = 10$ cm, $\varepsilon = 0.5$,
$D = 3$ cm^2/min, $H_A = 3$, $H_B = 1.5$,
$c_A^{in} = c_B^{in} = 0.5$ g/cm^3,
$Q_F = 1.5,\ Q_D = 6$ cm^3/min
Initial $Q_I = 7.5,\ Q_{II} = 1.5$ cm^3/min
sw. period= 20 min, $z_L = 10$,
$N = 10$, $h = 2$ min

5. RESULTS AND DISCUSSION

5.1 *Improvement of purities*

Fig. 3 shows a set point tracking performance when the input blocking is not applied. During the first 40 cycles, the process was under an open-loop state resulting in average purities of c_A^{ext}=0.58 and c_B^{raf}=0.81. From the 41st cycle, closed-control began with set points of 0.66 and 0.92 for c_A^{ext} and c_B^{raf}, respectively. It can be observed that the closed-loop process shows quite satisfactory tracking performance.

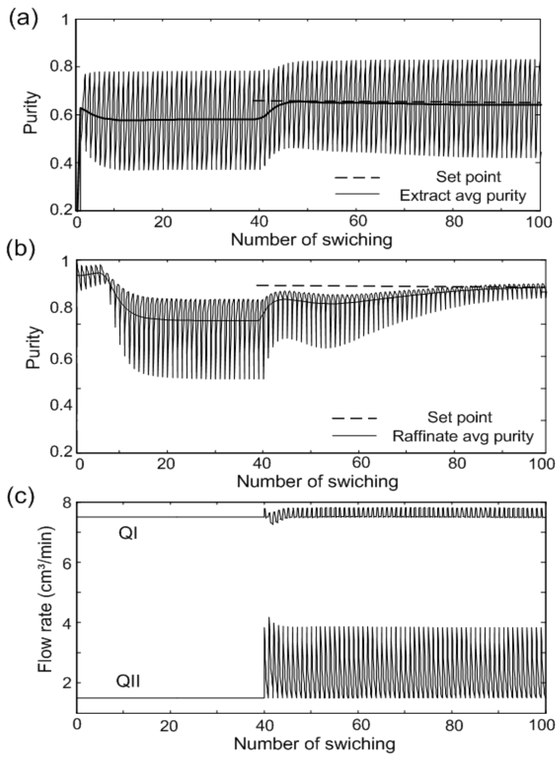

Fig. 3. Tracking performance with no input blocking.

5.2 *Input blocking*

Fig. 4 shows the results when the input is blocked to change only twice during a switching period. As can be seen, the output responses for the above two cases are virtually indistinguishable. From these results, we blocked the input movement to change only twice in the subsequent simulations.

5.3 *Disturbance rejection*

Fig. 5 shows the response when the mol faction of A in the feed changes from 0.5 to 0.3 at $k = 51$. We can see that the disturbance effect is gracefully rejected and the purities return to their respective set points after some transient.

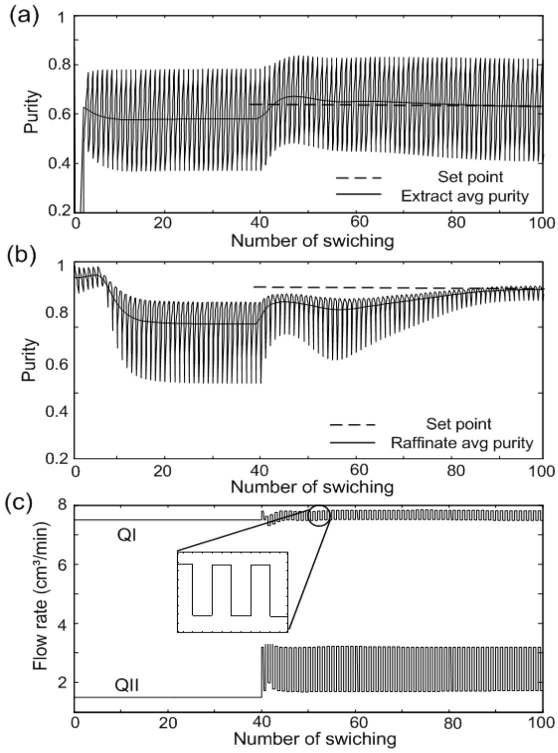

Fig. 4. Tracking performance with input blocking.

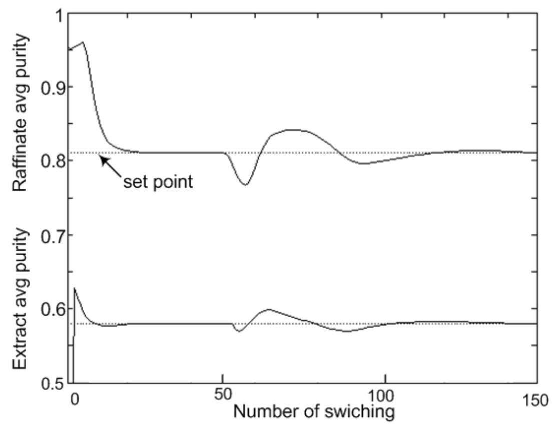

Fig. 5. Control performance against a change in feed concentration.

5.4 *Model error*

This time, we intentionally imposed parameter error from $k = 41$ on the control model by changing H_A and H_B to 2.4 and 1.2 from 3.0 and 1.5, respectively, while the process itself remains unchanged. Fig. 6 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 percent of uncertainties are given to the equilibrium constants.

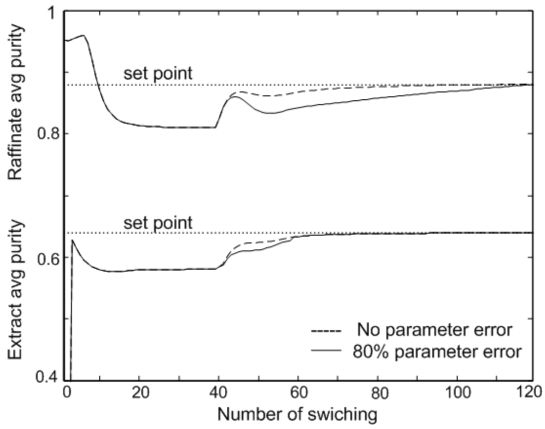

Fig. 6. Control performance against a model parameter change.

6. CONCLUSIONS

Through this study, a repetitive controller has been proposed for the SMB process. The controller was designed on the basis of the successive linearization of a fundamental SMB model around the operating trajectory of the previous cycle. 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 model error. With the robustly performing controller in hand, a 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 purities.

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