Adaptive Control of Simulated Moving Bed Plants Using Comsol's Simulink Interface

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Abstract: The simulated moving bed (SMB) technology is an increasingly used separation process of binary mixtures. Several chromatographic columns are arranged to a ring where the feedings and drains are changed cyclically to maintain a continuous separation. This process is very sensitive to disturbances in the flow rates and changes in the process parameters. For this reason, an adaptive controller is proposed to adjust the flow rates automatically. The original process is described by several coupled partial differential equations, which are less suitable for control design. Therefore, a simpler model is used based on the movements of the foot points of the concentration fronts to construct an adaptive controller. This work implements the full model with aid of Comsol and validates the control loop in Matlab Simulink.

Keywords: SMB, simulated moving bed, chromatography, adaptive control

1. Introduction

Preparative chromatography is an important separation method. It uses the effect of different adsorption affinities of components in a multicomponent mixture. To maintain a continuous separation of a binary feed the simulated moving bed (SMB) technology was developed by Universal Oil Products (UOP) [1]. Several chromatographic columns are interconnected to a ring. The feedings and drains are changed cyclically to mimics a countercurrent operation between fluid and solid phase. For a proper operation, the volumetric flow rates as well as the switching time must be adjusted carefully. Further, this process is very sensitive to parameter variation and disturbances. It is therefore natural to require an automatic controller to adjust the flow rates and switching time.

In this contribution, the pde's of the full SMB model are implemented using the finite element package Comsol [2]. Based on a simplified model for the movements of the foot points of the concentration fronts, an adaptive controller is proposed [3]. The control loop is successfully tested within the Matlab Simulink [4] environment using Comsol's Simulink interface.

2. Plant description

As shown in Fig. 1 a SMB process consists of four zones that are coupled by the volumetric flow rates of the liquid phase. In this contribution, each zone consists of two chromatographic columns. The binary mixture is fed in between zone II and III. The product drain for component B is called extract and lies between zone I and II. On the other side, the product drain for component A is called raffinate and lies between zone III and IV. Additional a pure solvent feed is necessary between zone I and IV. The flow rates are adjusted by four pumps. The flow directions of the liquid phase are indicated. After a time interval defined by the switching time, the ports are shifted synchronous in the flow direction.
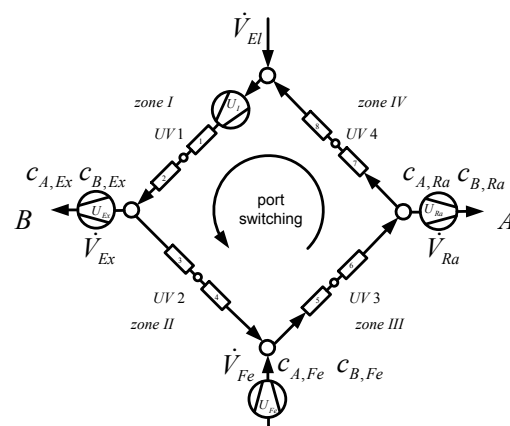

Figure 1. Configuration of SMB process.

The propagation velocity of the more retained component B must be slower than the virtual solid phase velocity that is the ratio of column length and switching time. Therefore, the component B will move to the direction of the extract. The propagation velocity of component

A needs to be higher than the virtual solid phase velocity to move to the direction of the raffinate.
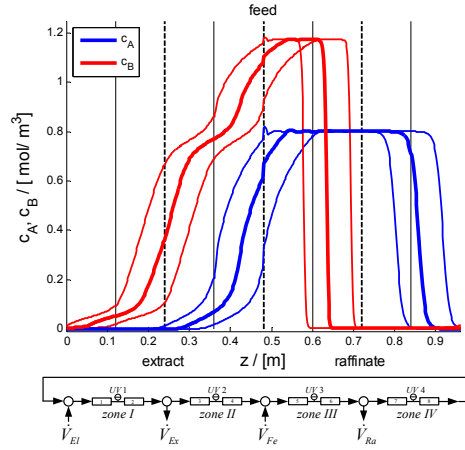

Figure 2. Concentration profiles in controlled cyclic-steady-state.

As indicated in Fig. 2, the four zones may be arranged in a plane to plot the associated concentration profile in cyclic-steady-state above the columns. The spatial coordinate is chosen such that its start with zone I. Within a time interval, the concentration profiles move from the left to the right. The broader lines correspond to the concentration profile in the middle of a time interval, whereas the thin lines are the profiles to the beginning and end of a time interval.

2.1 Governing equations for one column

The mass transports of the two components of a chromatographic column are described with aid of the volume concentration by the following two partial differential equations [5], [6].

$$\frac{\partial c_i}{\partial t} + F \frac{\partial q_i(c_i)}{\partial t} = -v_l \frac{\partial c_i}{\partial z} + D \frac{\partial^2 c_i}{\partial z^2}, \quad i = A, B, \tag{1}$$

$$F = \frac{1-\varepsilon}{\varepsilon}, \quad v_l = \frac{\dot{V}}{\varepsilon A} \tag{2}$$

The boundary conditions are:

$$c_{i,in}(t) = c_i(t,0) - \frac{D \, \varepsilon \, A}{\dot{V}} \frac{\partial c_i(t,z)}{\partial z} \bigg|_{z=0}, \tag{3}$$

$$\frac{\partial c_i(t,z)}{\partial z} \bigg|_{z=L} = 0, \quad i = A, B. \tag{4}$$

The initial conditions are:

$$c_i(0,z) = c_{i,0}(z), \quad i = A, B. \tag{5}$$

To complete the model, a static relationship between the adsorbed and liquid phase has to be chosen. In this contribution, the non-competitive Langmuir isotherms are selected.

$$q_i(c_i) = \frac{H_i \, c_i}{1 + K_i \, c_i}, \quad i = A, B \tag{6}$$

2.2 Comsol implementation

To implement the system one needs to compare the model equations with Comsol's pde equation in general form.

$$\mathbf{d_a} \cdot \frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{\Gamma} = \mathbf{F} \tag{7}$$

Comsol's vector variables are identified to be:

$$\mathbf{u} = (c_A \quad c_B)^T, \tag{8}$$

$$\mathbf{d_a} = \begin{pmatrix} 1 + F \dfrac{dq_A}{dc_A} & 0 \\ 0 & 1 + F \dfrac{dq_B}{dc_B} \end{pmatrix}, \tag{9}$$

$$\mathbf{\Gamma} = \left(\frac{\dot{V}}{\varepsilon \cdot A} c_A - D \frac{\partial c_A}{\partial z} \quad \frac{\dot{V}}{\varepsilon \cdot A} c_B - D \frac{\partial c_B}{\partial z} \right)^T, \tag{10}$$

$$\mathbf{F} = \begin{pmatrix} 0 & 0 \end{pmatrix}^T. \tag{11}$$

The boundary condition in general forms are:

$$-\mathbf{n} \cdot \mathbf{\Gamma} = \mathbf{G} + \left(\frac{\partial \mathbf{R}}{\partial \mathbf{u}} \right)^T \cdot \mathbf{\mu}, \tag{12}$$

$$\mathbf{R} = \mathbf{0}. \tag{13}$$

One possible solution is:

$$\mathbf{G}_{|z=0} = \left(\frac{\dot{V}}{\varepsilon \cdot A} \cdot c_{A,in} \quad \frac{\dot{V}}{\varepsilon \cdot A} \cdot c_{B,in} \right)^T, \tag{14}$$

$$\mathbf{G}_{|z=L} = \left(-\frac{\dot{V}}{\varepsilon \cdot A} \cdot c_A \quad -\frac{\dot{V}}{\varepsilon \cdot A} \cdot c_B \right)^T, \tag{15}$$

$$\mathbf{R}_{\substack{|z=0 \\ |z=L}} = \begin{pmatrix} 0 & 0 \end{pmatrix}^T. \tag{16}$$

2.3 Coupling of Columns

Under the assumption that there is a stationary flow, the following coupling equations will hold.

External flow rates:

$$0 = \dot{V}_{El} + \dot{V}_{Fe} - \dot{V}_{Ex} - \dot{V}_{Ra}. \tag{17}$$

Eluent feed:

$$\dot{V}_I = \dot{V}_{IV} + \dot{V}_{El}, \quad c_{i,in,I} \, \dot{V}_I = c_{i,out,IV} \, \dot{V}_{IV},$$
$$i = A, B. \tag{18}$$

Extract drain:

$$\dot{V}_{II} = \dot{V}_I - \dot{V}_{Ex}, \quad c_{i,in,II} = c_{i,out,I} = c_{i,Ex},$$
$$i = A, B. \tag{19}$$

Feed:

$$\dot{V}_{III} = \dot{V}_{II} + \dot{V}_{Fe},$$

$$c_{i,in,III} \, \dot{V}_{III} = c_{i,out,II} \, \dot{V}_{II} + c_{i,Fe} \, \dot{V}_{Fe}, \tag{20}$$
$$i = A, B.$$

Raffinate drain:

$$\dot{V}_{IV} = \dot{V}_{III} - \dot{V}_{Ra}, \quad c_{i,Ra} = c_{i,in,IV} = c_{i,out,III},$$
$$i = A, B. \tag{21}$$

The coupling of the chromatographic columns can be done in Comsol by extrusion or identity coupling variables.

3 Determine an operating point

To start up the SMB plant a specification of the volumetric flow rates and the switching time is necessary. For non-competitive Langmuir isotherms, the following equations can be used to determine operating points of a dispersion-free SMB plant for high feeding concentrations.

Given the feed concentrations $c_{A,Fe}$, $c_{B,Fe}$, the feed flow rate $\dot{V}_{Fe}$ and the normalized residence times $0 \ll \tau_{B,I} \leq 1$ and $0 \ll \tau_{A,IV} \leq 1$ one can compute the necessary flow rates $\dot{V}_I$, $\dot{V}_{Ex}$, $\dot{V}_{Ra}$ and switching time T_S for $H_A < H_B$ in the following way.

$$c_{B,0} = \frac{1}{K_B} \frac{H_B - H_A}{\sqrt{H_A H_B} + H_A} \tag{22}$$

$$c_{B,Fe} > c_{B,0} \tag{23}$$

$$c_{B,P} = \frac{H_B - H_A}{K_B} \frac{\left(\sqrt{H_B} + \sqrt{H_A}\right)^2 K_B c_{B,Fe} - (H_B - H_A)}{H_A \left(\sqrt{H_B} + \sqrt{H_A}\right)^2 K_B c_{B,Fe} + (H_B - H_A)^2} \tag{24}$$

$$c_{A,P} = \frac{H_B - H_A}{2} \frac{\left(\sqrt{ \begin{array}{c} (H_B - H_A)^2 (1 + K_A c_{A,Fe})^2 \\ +4 H_A \left(\sqrt{H_B} + \sqrt{H_A}\right)^2 K_A K_B c_{A,Fe} c_{B,Fe} \end{array} } -(H_B - H_A)(1 - K_A c_{A,Fe}) \right)}{K_A \left[H_A \left(\sqrt{H_B} + \sqrt{H_A}\right)^2 K_B c_{B,Fe} + (H_B - H_A)^2 \right]} \tag{25}$$

$$\dot{V}_I = \frac{\left(\sqrt{H_B} + \sqrt{H_A}\right)^2 \left[F\left(H_B - H_A\left(1 - \tau_{B,I}\right)\right) + \tau_{B,I}\right]}{F\,\tau_{B,I}\left(H_B - H_A\right)^2} K_B\,c_{B,Fe}\,\dot{V}_{Fe} \tag{26}$$

$$\dot{V}_{Ex} = \frac{\left(\sqrt{H_B} + \sqrt{H_A}\right)^2}{\tau_{B,I}\left(H_B - H_A\right)} K_B\,c_{B,Fe}\,\dot{V}_{Fe} \tag{27}$$

$$\dot{V}_{Ra} = \frac{c_{A,Fe}}{\tau_{A,IV}\,c_{A,P}}\,\dot{V}_{Fe} \tag{28}$$

$$T_S = \frac{F}{1+F}\,\frac{AL}{\dot{V}_{Fe}}\,\frac{\left(H_B - H_A\right)^2}{\left(\sqrt{H_B} + \sqrt{H_A}\right)^2 K_B\,c_{B,Fe}} \tag{29}$$

Similar equations exist for low feeding concentrations as given in the parameter file "SMB8AdaptiveControlComsol_param.m". This file contains also formulas for Henry isotherms, competitive Langmuir isotherms and Anti-Langmuir isotherms. More details can be found in the associated publications, e.g. [7].

4. Simple modeling

To control SMB plants it is helpful to construct a simple model, which is based on the propagation of the foot points of the concentration fronts [3].
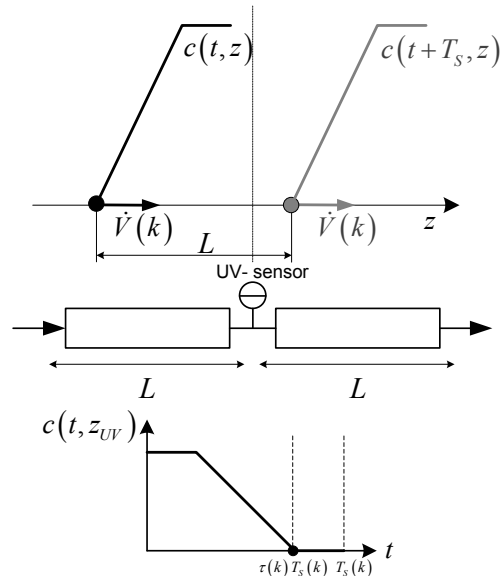

Figure 3. On foot point movement and definition of normalized residence times.

For further simplification, all flow rates are kept constant during the switching interval. This opens an advantageous discrete model representation.

In Fig. 3 two chromatographic columns are indicated where a sensor which measures a concentration related signal is mounted between them. In cyclic-steady-state, this sensor records the concentration trajectory within one switching interval as shown below the columns. The goal is to keep the foot point, indicated by a big black dot, at the desired location. It is useful to express this time stamp by a normalized residence times τ [3,7] that makes the control design independent of the actual value of the switching time.

4.1 Computing normalized residence times

To control this time stamp it is necessary to measure τ reliable. This can be done with aid of the correlation technique. To this, two intermediate signals given by Eq. (30) and (31) are constructed for every switching interval. The small offset c_0 defines the concentration value which propagation will be investigated. For faultless work, this value should lie above the expected sensor noise level. The sign of α takes care on the different qualitative course of the concentrations between extract and raffinate side.

$$x(t) = sign\big(c(t) - c_0\big) \tag{30}$$

$$x_{ref}(t) = \alpha\,sign\big(t - \tau_{ref}\,T_S\big) \tag{31}$$

$$\alpha = \begin{cases} -1 & \text{extract side} \\ +1 & \text{raffinate side} \end{cases} \tag{32}$$

The cross correlation of both signals will get a maximum at the shift $\Delta\tau_{max}$, as shown in Fig.4. This shift is a measure of the control error.

$$R_{x_{ref}x}(\Delta\tau) = \lim_{T\to\infty} \frac{1}{2T}\int_{-T}^{T} x_{ref}(t)\,x\big(t + \Delta\tau\,T_S\big)dt$$
$$\Delta\tau \in [-1,1] \tag{33}$$

The sum of the shift $\Delta\tau_{max}$ and reference τ_{ref} results in the actual value τ. The maximum may be determined by a simple one-dimensional search.
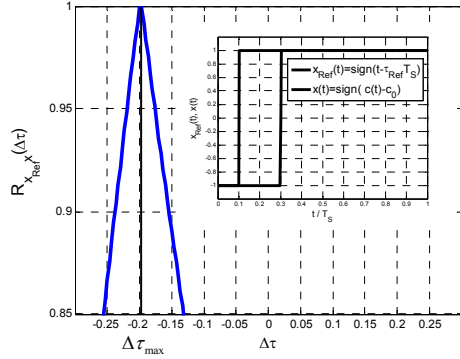

Figure 4. On cross correlation of two phase shifted sign signals.

4.2 Simple model equations

The equations of the simple model are derived in [3] and may be expressed in the traditional notation style of the control community.

$$u_i(k) = \dot{V}_i(k), \quad i = 1, 2, 3, 4 \tag{34}$$

$$u_5(k) = T_S(k) \tag{35}$$

$$\widehat{u}_i(k) = u_i(k)u_5(k) \tag{36}$$

$$y_i(k) = \tau_i(k-1) \tag{37}$$

$$y_i(k+1) = \frac{\theta_i - \widehat{u}_i(k-1)(1 - y_i(k))}{\widehat{u}_i(k)} \tag{38}$$

In steady-state, the input is equal to the parameter. This opens a simple way to compute the parameters by Eq. (39) from existing design rules for complete separations directly from the parameters of the full model, e.g. by Eq. (22)-(29) and Eq. (34)-(36).

$$\theta_i = \widehat{u}_i^*, \quad i = 1, 2, 3, 4 \tag{39}$$

Often the operators of such plants already know the flow rates and switching time for complete separation through experiments.

5. Control design

5.1 Proportional feedback control law

To maintain the concentration fronts at the desired positions the following simple proportional feedback law is suggested [3].

$$\widehat{u}_i(k) = \hat{\theta}_i - 0.25\left(y_{i,ref} - y_i(k)\right)\hat{\theta}_i \tag{40}$$

$$i = 1, 2, 3, 4, \quad y_{i,ref} \in [0,1] \tag{41}$$

5.2 Computing optimal switching time

For a fixed feed throughput, it is necessary to use the switching time as control input. The optimal switching time is computed with aid of the normalized control inputs.

$$T_S(k) = \frac{\widehat{u}_3(k) - \widehat{u}_2(k)}{\dot{V}_{Fe}} \tag{42}$$

The volumetric flow rates of the four zones are computed by following formula.

$$u_i(k) = \frac{\widehat{u}_i(k)}{T_S(k)}, \quad i = 1, 2, 3, 4 \tag{43}$$

Notice, that the scaling property of the switching time may also be used to satisfy upper constraints on the volumetric flow rates. Such constraints arise from a maximum allowable pressure drop across the columns. More details can be found in the file "AdaptiveSMB8 Controller_sfun.m" that implements the proposed controller.

5.3 Estimator design

To be able to track parameter changes through aging and changes in the operating conditions, it is necessary to estimate them from measurements. The following simple estimator, which uses (38) to compute $\hat{y}_i$, is proposed [3].

$$\hat{\theta}_i(k) = \hat{\theta}_i(k-1) + (1-a_\theta)\hat{u}_i(k-1)\left(y_i(k) - \hat{y}_i(k)\right)$$
$$|a_\theta| < 1, \quad i = 1,2,3,4, \quad e.g. \ a_\theta = 0.5 \quad (44)$$

6. Simulation results

To validate the control concept a simulation using the detailed model is carried out. The model parameters are given in table 2. The initial flow rates, the switching time, and therefore the initial parameters of the simplified model were computed using Eq.(22)-(29). The set points are chosen to $\tau_{I,ref} = \tau_{II,,ref} = 0.85$ and $\tau_{III,ref} = \tau_{IV,ref} = 0.15$. In Fig.5, the time trajectories of the measured normalized residence times are represented. It can be seen that after a transient time the controller is able to set the locations of the concentration fronts as desired. Additional to the start-up phase of the plant a probably unrealistic high counter step in the feed concentrations to the double and half of the nominal feed concentration was simulated after 44 minutes. As shown in Fig.5 the adaptive controller is able to reject this disturbance.
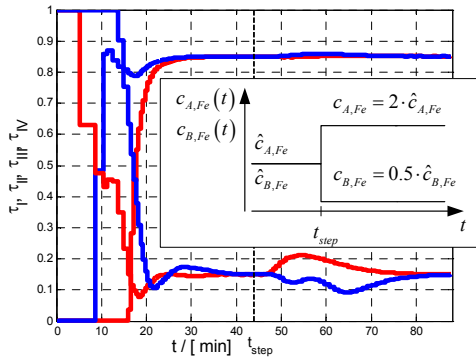

Figure 5. Adjustments of normalized residence times during start-up phase and a counter-step in feed concentrations.

In Fig.6, the time trajectory of the switching time is represented. Initially the switching time is high so that the concentration fronts can appear quickly at the sensor locations. After the step disturbance in the feed concentrations, a different steady-state value takes place.

The parameters are adjusted as soon as the concentration fronts appear at the associated sensor locations, as seen in Fig.7. Again, the step disturbance leads to different steady-state values.
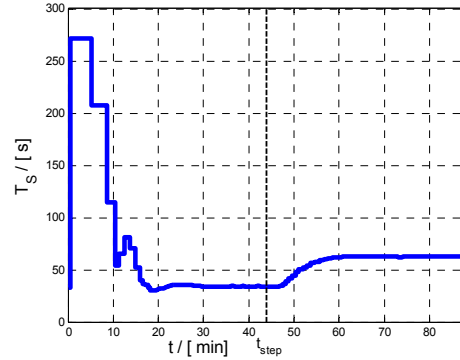

Figure 6. Adjustments of switching time during start-up phase and a counter-step in feed concentrations.
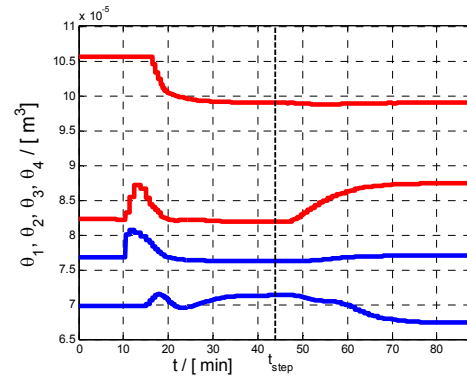

Figure 7. Adjustments of parameters during start-up phase and a counter-step in feed concentrations.

7. Conclusions

The proposed control concept is a simple and effective way to control SMB plants. The only knowledge to initiate the control loop are the volumetric flow rates and switching time for complete separation, which are always known by the operators. Further, the proposed controller works independently of the in fact occurring adsorption behavior. In this contribution, the adsorption behavior was modeled by non-competitive Langmuir isotherms. However, a simulation study with Henry and competitive Langmuir isotherms turns out to give similarly good results using the same controller. Therefore, the proposed control concept is ideally suitable for the industrial use.

This concept can also be extended easily to control the drain purities [8], if the drain concentrations can be measured.

8. References

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8. Appendix

Table 1: Notation

H	Henry constant
K	Langmuir constant
c	fluid concentration (volumetric)
q	adsorbed concentration (volumetric)
$\dot{V}$	volumetric flow rate
T_S	switching time

Table 2: Model parameter

column length	L	$0.12 \cdot m$
column diameter	d	$0.02 \cdot m$
void fraction	ε	0.7407
diffusion	D	$5 \cdot 10^{-6} \cdot \frac{m^2}{s}$
Henry constant A	H_A	5.00
Henry constant B	H_B	7.50
Langmuir constant A	K_A	$0.15 \cdot \frac{m^3}{mol}$
Langmuir constant B	K_B	$0.30 \cdot \frac{m^3}{mol}$
feed concentration A	$c_{A,Fe}$	$1.50 \cdot \frac{mol}{m^3}$
feed concentration B	$c_{B,Fe}$	$1.50 \cdot \frac{mol}{m^3}$
feed flow rate	$\dot{V}_{Fe}$	$10.00 \cdot \frac{ml}{min}$
number of columns	NC	8 (2 / 2 / 2 / 2)

List 1: Files in zip archive SMB8Control.zip

- SMB8Control.mph

  Comsol model for competitive Langmuir isotherms.

- SMB8ControlNonCompetitive.mph

  Comsol model for non-competitive Langmuir isotherms.

- SMB8AdaptiveControlComsol.mdl

  Simulink model for specifying the control loop.

- AdaptiveSMB8Controller_sfun.m

  Matlab S-function to implement the adaptive controller.

- SMB8Decoder_sfun.m

  Matlab S-function to decode the outlet concentrations of the chromatographic columns from Comsol to rotating observer.

- SMB8AdaptiveControlComsol_param.m

  Matlab M-file to define parameter of the model and compute an initial operating point.

- SolveLangmuirSMB.m

  Matlab M-file to compute operating points for competitive Langmuir isotherms under reduced purity requirements.

- TestSolveLangmuirSMB.m

  Matlab M-file to construct the concentration trajectories at the drains in cyclic-steady-state for competitive Langmuir isotherms.

- PlotResults.m

  Matlab M-file to plot the simulation results after simulation.