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Individual Column State and Parameter Estimation in the Simulated Moving Bed Process: an Optimization-based Method ⋆

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Abstract: The aim of this work is to propose a method for the simultaneous state and parameter estimation of the individual columns in the Simulated Moving Bed chromatographic process based on concentration measurements only in the switched product outlets. The method exploits the fact that the measurements switch from the inlets of the columns to their outlets sequentially. The estimation problem is cast as a dynamic optimization problem where the prediction error of the output profile is minimized. The initial concentrations in the individual columns and the parameters of the columns are treated as degrees of freedom of the optimization problem. As at each outlet the concentrations of one component are very small and therefore are subject to large relative measurement errors for given expected absolute errors of the concentration measurements, measurements for two different points in time, when the extract port and when the raffinate port is at the outlet of the column under consideration are taken into account simultaneously. The effectiveness of the method is demonstrated for the separation of an isopropanolol racemic mixture.

Keywords: State estimation; parameter estimation; distributed parameter systems; decentralized estimation; chromatography, SMB processes, multiple shooting.

1. INTRODUCTION

The Simulated Moving Bed (SMB) process is a preparative chromatographic separation method which has gained increasing importance in industrial sectors such as food, fine chemicals and pharmaceuticals, due to its efficiency in difficult separation tasks, such as the purification of substances with similar thermodynamic properties, or of temperature sensitive materials. The process is very efficient, but it is highly sensitive to disturbances, making the use of control schemes necessary for operating it reliably. The control of the process is difficult because the process shows large delays, and the availability of the measurement information is very limited in typical installations. The process performance is dependent on the process parameters, which in practice are distinct for each column in the plant, and which may change over time. For model-based control as well as for process monitoring, the estimation of the plant state and of process parameters is important. For this task, several approaches have been proposed in the literature. In Mangold et al. [1994] a simultaneous state and parameter estimation scheme to estimate the velocities of the components within the SMB plant by means of a distributed Luenberger- like observer was proposed. Similarly, in Kleinert and Lunze [2005] an estimation scheme which relied on a wavefront-based description of the concentration profiles within the chromatographic columns was developed, resulting in an observer of low order. In Alamir and Corriou [2003] a strategy in which the process was described by empirical functions, whose coefficients were obtained by means of a moving horizon estimator (MHE) was presented. In Kuepper et al. [2009] a MHE approach based on a full rigorous model of the SMB plant was proposed for the real-time simultaneous estimation of the states and the isotherm parameters in SMB processes.

A common feature of all aforementioned approaches is the assumption of uniform properties that are shared by all columns in the SMB plant. This however is not realistic, as it implies that all columns are packed identically with adsorbent, which is impossible in practice. In contrast, in Küpper and Engell [2006] a state and parameter estimation scheme was proposed which, by means of decentralized Extended Kalman Filters (EKF), estimated the adsorption isotherm parameters for each column separately. It was assumed that two measurements at the product outlets and one measurement at a fixed position in the SMB process are available. The EKF-based scheme exploits the fact that the measurements in the product stream move in the direction of the flow by using the state that was estimated for the preceding column in the prediction model for the current column. It was shown that the scheme is able to estimate column parameters which differ between the columns, however with a rather slow

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convergence to the true values.

In this contribution, an optimization-based scheme for the estimation of the individual column states and parameters is proposed. The measured concentration profiles that entered the column during the previous period and that leave it during the current period are used to estimate the initial state and some key parameters of a column. The paper is structured as follows: First, a brief description of the SMB chromatographic process is provided. Next, the process model is introduced, followed by the presentation and explanation of the proposed estimation scheme. The performance of the estimator is demonstrated by its application to the separation of the isopropanolol racemic mixture. The results are compared to the results obtained in Küpper and Engell [2006]. Finally, conclusions are presented.

2. DESCRIPTION OF THE SMB PROCESS

The Simulated Moving Bed is a continuous preparative chromatographic process for the separation of the components of fluid mixtures. The separation takes place due to the different adsorption affinities of the components to a solid adsorbent material packed in a chromatographic column. The idea behind the SMB process is to perform the continuous separation by approximating a counter-current flow between the fluid mixture and the solid, as a true counter-current operation is difficult to attain in practice. The SMB process consists of a series of individual chromatographic columns connected in a ring. The mixture and the solvent for recovering the most heavily adsorbed component are fed continuously at specific nodes between columns. Similarly, the resulting purified components are removed continuously from the plant. These feed and product ports are moved synchronously and periodically by one column in the direction of the liquid flow. Typically, a SMB plant is equipped with sensors for measuring the concentrations at the product ports (the extract, rich in the more strongly adsorbed component, and the raffinate, rich in the less strongly adsorbed component). This sensor configuration has been assumed in this work. A SMB plant is divided in four zones: in Zone I (between the solvent and extract ports) the more retained component is recovered and the solid is regenerated; in Zone II (between the extract and feed ports) the less retained component is desorbed; in Zone III (between the feed and raffinate ports) the more retained component is adsorbed and the other component is recovered; and in Zone IV (between the raffinate and solvent ports) the less retained component is adsorbed and the solvent is regenerated. The process is depicted in Figure 1.

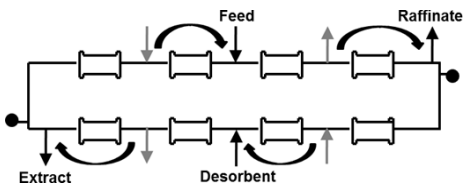

Fig. 1. Schematic representation of the SMB process.

3. PROCESS MODEL

The SMB process can be modeled by a composition of the individual chromatographic column models and the material balances at the interconnection nodes between the columns. In this work, the chromatographic columns are modelled by the so-called General Rate Model (GRM), which is comprehensively explained in numerous references, such as Schmidt-Traub [2012]. The GRM consists of two elements. The first one is a material balance for the bulk liquid phase in the column in the axial direction:

$$\begin{aligned}\frac{\partial C^{b,i}}{\partial t} &= D^i_{ax}\frac{\partial^2 C^{b,i}}{\partial z^2} - u\frac{\partial C^{b,i}}{\partial z} \\ &\quad - \left(\frac{1-\epsilon_b}{\epsilon_b}\right)\frac{3k^i_l}{r_p}\left(C^{b,i} - C^{p,i}|_{r=r_p}\right).\end{aligned} \tag{1}$$

The second part of the GRM is a material balance of the liquid in the adsorbent, in the particle radial direction:

$$(1-\epsilon_b)\frac{\partial q^i}{\partial t} + \epsilon_p\frac{\partial C^{p,i}}{\partial t} = \epsilon_p D^i_p \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C^{p,i}}{\partial r}\right). \tag{2}$$

It is assumed that the liquid in the particle pores is in equilibrium with the absorbed substance at the surface of the adsorbent. This equilibrium relation relationship is described by the so-called adsorption isotherm, which is dependent on the mixture, the solvent and the packing.

The boundary conditions for the bulk and pore phase material balances are shown in Eqs. 3 and 4:

$$\left.\frac{\partial C^{b,i}}{\partial z}\right|_{z=L} = 0; \quad \left.\frac{\partial C^{b,i}}{\partial z}\right|_{z=0} = \frac{u}{D^i_{ax}}\left(C^{b,i} - C^{b,i}_{in}\right) \tag{3}$$

$$\left.\frac{\partial C^{p,i}}{\partial r}\right|_{r=0} = 0; \quad \left.\frac{\partial C^{p,i}}{\partial r}\right|_{r=r_p} = \frac{k^i_l}{\epsilon_p D^i_p}\left(C^{b,i} - C^{p,i}|_{r=r_p}\right). \tag{4}$$

The model of the SMB process is completed by the material balances at the column interconnection nodes:

$$\begin{aligned}0 &= -Q_I + Q_{IV} + Q_{De} \\ 0 &= -Q_{II} + Q_I - Q_{Ex} \\ 0 &= -Q_{III} + Q_{II} + Q_{Fe} \\ 0 &= -Q_{IV} + Q_{III} - Q_{Ra} \\ 0 &= -C^{b,i}_{out,IV}Q_{IV} + C^{b,i}_{in,I}Q_I \\ 0 &= -C^{b,i}_{out,II}Q_{II} - C^i_F Q_F + C^{b,i}_{in,III}Q_{III},\end{aligned} \tag{5}$$

$$i = \{A, B\},$$

where Q_I, Q_{II}, Q_{III} and Q_{IV} are the flow rates of the zones I, II, III and IV.

4. DIFFICULTIES OF THE ESTIMATION PROBLEM

The main difficulty of the estimation problem lies in the scarcity of the available measurement information: the concentration profiles are measured only at the outlet ports in the raffinate and in the extract stream. In the ideal situation of an SMB process with exactly identical columns at the cyclic steady state, these profiles are the same in each switching period, so no new information is obtained after a switch of the ports. If the columns are not identical or if the plant is operated in a transient fashion, e.g. because of changes of the flow rate or in the switching times, the profiles differ, but not by very much. These small differences must be exploited to estimate the individual column parameters. Additionally, at the two

product ports the concentration of one of the substances is very low, as a high purity of one component in each port is the goal of the separation. This implies that the relative error of the concentration measurement for this substance will be high and that at very high purities, practically no information about the polluting component is obtained. In order to overcome these difficulties, a tailored optimization-based scheme is proposed in the next section.

5. A NEW METHOD FOR THE ESTIMATION OF COLUMN STATES AND INDIVIDUAL COLUMN PARAMETERS

The proposed estimation scheme considers a time horizon composed of two stages. The first stage corresponds to the interval in which the measurement position is located at the column inlet, and the second stage corresponds to the interval after the valve switching when the concentrations are measured at the outlet. The unknown internal concentration profiles at the beginning of the first stage are treated as degrees of freedom in the optimization problem, and the measured inlet concentrations are considered as inputs of the estimated column. It is well known that the estimation of initial conditions leads to ill-conditioning. To alleviate this problem, the estimated initial internal profiles are regularized by penalizing their deviations with respect to the values estimated one cycle before.

As only one of the ports (extract or raffinate) can be at the outlet of a column at one point in time, the sensors of each of the ports are expected to report relatively low concentrations of one of the components of the mixture due to the separation, i.e. there is little measurement information about these components. This is particularly true for high purity separations, and constitutes a problem for the estimation of the parameters that are strongly associated to that component. To overcome this difficulty, it is proposed that the measurement information obtained for each of the two sensors is combined in the optimization problem in order to estimate the states and the parameters of a given column. As the column is connected to the sensors at different points in time, the corresponding measurement data and the internal column concentration profiles at each of these time intervals are different. It is proposed to model the dynamics of the column at each of these time periods as decoupled columns (one for each port) sharing the same parameter set which must be fitted to describe the measured outlet profiles corresponding to that time interval.

The objective function which results from these considerations is:

$$\min_{\substack{\underline{\hat{p}}_i^{k+1},\ \underline{\hat{x}}_i(T^{k-1}),\\ \underline{\hat{x}}_i(T^{k-\Pi-1})}} \quad \frac{1}{2}\cdot\left|\left|\underline{\hat{p}}_i^{k-N_{col}+1}-\underline{\hat{p}}_i^{k+1}\right|\right|^2_{\sigma_p^{-1}} \tag{6}$$

$$+\frac{1}{2}\cdot\left|\left|\begin{array}{c}\underline{\hat{x}}_i(T^{k-N_{col}-1})-\underline{\hat{x}}_i(T^{k-1})\\ \underline{\hat{x}}_i(T^{k-\Pi-N_{col}-1})-\underline{\hat{x}}_i(T^{k-\Pi-1})\end{array}\right|\right|^2_{\sigma_x^{-1}}$$

$$+\frac{1}{2}\cdot\left|\left|\begin{array}{c}\underline{y}_i^{k+1,j}(t)-\underline{\hat{y}}_i^{k+1,j}(t)\\ \underline{y}_i^{k-\Pi+1,j}(t)-\underline{\hat{y}}_i^{k-\Pi+1,j}(t)\end{array}\right|\right|^2_{\sigma_m^{-1}}$$

$$\text{s.t.}\quad \underline{\hat{x}}_i(T^{\gamma+1})=\underline{\hat{x}}_i(T^{\gamma-1})+ \int_{T^{\gamma-1}}^{T^{\gamma}} f\left(\underline{\hat{x}}_i(t),\underline{u}_i^{\gamma-1}(t),\underline{\hat{p}}_i^{k+1}\right)dt+ \int_{T^{\gamma}}^{T^{\gamma+1}} f\left(\underline{\hat{x}}_i(t),\underline{u}_i^{\gamma}(t),\underline{\hat{p}}_i^{k+1}\right)dt, \tag{7}$$

$$\underline{\hat{x}}_i=[\underline{\hat{C}}_i^{b,j},\ \underline{\hat{C}}_i^{p,j}]^T,\quad j=\{A,B\} \tag{8}$$

$$u_i^{\gamma-1}(t)=\left[Q_i^{\gamma-1},\ \tau,\ \underline{y}_{i-1}^{\gamma-1}(t)\right]^T, \tag{9}$$

$$u_i^{\gamma}(t)=\left[Q_i^{\gamma},\ \tau,\ \underline{\hat{C}}_{out,i-1}^{\gamma}(t)\right]^T, \tag{10}$$

$$\underline{\hat{x}}_i^l\le\underline{\hat{x}}_i\le\underline{\hat{x}}_i^u, \tag{11}$$

$$\underline{\hat{p}}_i^l\le\underline{\hat{p}}_i\le\underline{\hat{p}}_i^u, \tag{12}$$

$$\gamma=\{k-\Pi,\ k\}, \tag{13}$$

$$\Pi=N_{col,I}+N_{col,IV}, \tag{14}$$

$$\underline{\hat{y}}=x_{N_{dis}} \tag{15}$$

where $\underline{\hat{p}}_i$ is the vector of estimated parameters of the column i, $\underline{\hat{x}}_i$ is the vector of state estimates, $\underline{u}_i$ is the vector of inputs applied to the column i, and $\underline{\hat{y}}_i^j$ and $\underline{y}_i^j$ are the simulated and the measured concentrations of component j at the outlet of the column i, respectively. The superindex Π represents the number of columns that separate the raffinate and extract ports, and it is equal to the sum of the lengths of the zones I and IV of the SMB plant. The input term $\hat{C}_{out,i-1}^{\gamma}$ deserves special attention. It represents the concentrations at the inlet of the column the parameters of which are estimated during the second stage. As these concentrations are unknown, they are calculated by simulation of the columns prior to the estimated ones during the second stage. This has been implemented by considering an arrangement of two decoupled pairs of columns. The columns at the front are the estimated ones, and their dynamics are considered during both time stages, while the columns at the rear are only simulated during the second stage in order to provide the input concentrations of the estimated columns. The arrangement of decoupled columns corresponding to the estimation of the parameters of a column i with measurement positions at its inlet during $T^{k-\Pi-1}<t<T^{k-\Pi}$ and $T^{k-1}<t<T^k$ and at its outlet during $T^{k-\Pi}<t<T^{k-\Pi+1}$ and $T^k<t<T^{k+1}$ is illustrated in Figure 2.

The first term in Eq. 6 provides the regularization of the estimated parameters in order to avoid abrupt changes in their values. The second term corresponds to the state regularization. The third term is the conventional squared residual error between the simulated and the measured concentrations at the column outlets. The states and parameters estimated by minimizing Eq. 6 correspond only to the column with a measurement position at its outlet at the two different intervals considered. The states of the rest of the SMB plant are calculated by dynamic simulation, replacing the simulated values of the concentrations at the outlet of the columns with the product ports by the measured values. The parameters of the simulation are updated once the optimization is finished.

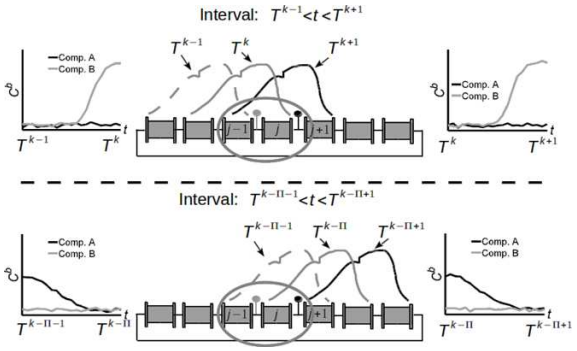

Fig. 2. Arrangement of decoupled columns used in the estimation of the parameters of a column j. The columns considered in the objective function are encircled.

6. RESULTS

The performance of the proposed estimation scheme has been tested for the case of the separation of an isopropanolol racemic mixture in a six-column plant with a 1/2/2/1 zone distribution. The adsorption behavior of the mixture is described by an extended Langmuir isotherm:

$$q_j = H_1^j C^{p,j} + \frac{H_2^A C^{p,j}}{1 + K^A C^{p,A} + K^B C^{p,B}}, \quad j = \{A, B\} \tag{16}$$

The adsorption isotherm parameters H_1^A and H_1^B, together with the individual column states were chosen as the variables to be estimated. Two scenarios were considered as test cases. The first scenario corresponds to the tracking of a step change of one of the adsorption parameters in one of the columns, starting from CSS conditions in a SMB plant with originally equal parameters in all columns. The second scenario corresponds to the estimation of the adsorption parameters in a SMB plant with different parameters in the columns, starting from the corresponding CSS conditions. In all cases, a sampling rate of 21 measurements per period is considered. The switching of the valves is assumed to be synchronous. The measurements are assumed to be contaminated with white noise with a standard deviation of 0.1138 g l^{-1}. In the two test cases, the estimator was activated after 10 periods of operation. The inputs corresponding to the operating point are $C_{A,feed} = C_{B,feed} = 7.25$ g l^{-1}, $Q_F = 0.31$ ml s^{-1}, $Q_D = 2.75$ ml s^{-1}, $Q_{Re} = 4.80$ ml s^{-1}, $Q_{Ex} = 1.94$ ml s^{-1}, $Q_{Ra} = 1.12$ ml s^{-1} and $\tau = 2.05$ min. The partial differential equations of the General Rate Model have been discretized with the Finite Element Method in the fluid phase, and with Orthogonal Collocation in the solid phase, as described in Gu [1995]. For each column, a total of 25 nodes were chosen for the fluid phase, and 1 collocation point for the pore phase, leading to a total of 400 state variables in the dynamic optimization problem. The estimator was parametrized with a measurement standard deviation $\sigma_m = 0.0447$ g l^{-1}, a state regularization $\sigma_x = 0.1$ g l^{-1} and with parameter regularizations $\sigma_p = \{0.0514, 0.0402\}$. This parametrization was found to provide the best compromise between the speed of convergence and the robustness against noise of the estimated parameters.

The two-stage dynamic optimization problem was solved with the multiple shooting method implemented in the software Package MUSCOD-II v.6. (Leineweber [2003]). Under this approach, the stages of which the time horizon is composed are divided into the so-called shooting intervals. The dynamic equations of the system are integrated over each interval with the differential equation solver DAESOL, using the states at the beginning of each interval as initial conditions. These are treated as degrees of freedom. The discretization of the states and of the inputs leads to casting the dynamic optimization problem into a large scale non-linear programming task. The continuity of the states between the shooting intervals (20 per stage in this work) is specified as a constraint of the optimization problem, which is enforced only at the solution in order to improve the convergence of the optimization. The resulting problem is solved by means of a tailored Sequential Quadratic Programming (SQP) algorithm, for which a Gauss-Newton approximation of the Hessian matrix, and a trust region globalization for the calculation of the SQP correction steps were chosen for the solution of the estimation problem. The concentrations measured at the inlet of the estimated column during the first stage of the time horizon were parametrized as piecewise continuous linear inputs. All the other inputs are constant.

6.1 Tracking of a step change of a parameter in a column

For this test case, two different scenarios were chosen. In the first scenario, a step change of 20% in the value of the Henry coefficient of column 3 with respect to its reference value (H_1^B=2.2) was introduced after 10 periods of operation, while the plant was operating at CSS conditions. At this moment the estimator was activated, and its performance was observed during a time period of 90 periods (i.e. 15 cycles) in order to verify its long term behavior. The time profiles of the estimated parameters are shown in Figure 3. It can be seen that the estimated value of H_1^B converges quickly to the real value. The parameter reaches its true value less than 30 periods after the start of the estimation. During the whole time horizon, the estimated values of H_1^A in all columns and of H_1^B in the rest of the plant fluctuate around their corresponding true values. The same occurs with H_1^B in column 3 once it has attained its real value, showing that the estimator delivers unbiased parameter estimates.

In the second scenario, a step change of 20% in the value of the parameter H_1^A of column 3 with respect to its reference value (H_1^A=2.68) was simulated, also after 10 periods of operation, while the plant was at CSS conditions. The time evolution of the estimated parameters is shown in Figure 4. It can be seen that, similarly as in the case of H_1^B, the parameter H_1^A reaches its true value in less than 30 periods of operation. In both cases, the parameter estimates remain unbiased, showing deviations around their true value of $\pm$2% or less. The convergence of both parameters can be accelerated by assigning lower weights to them, at the expense of a more fluctuating behavior.

6.2 Estimation of the parameters in a SMB plant with different column properties

For this case, it is assumed the true values of the parameters H_1^A and H_1^B of all columns in the plant deviate from

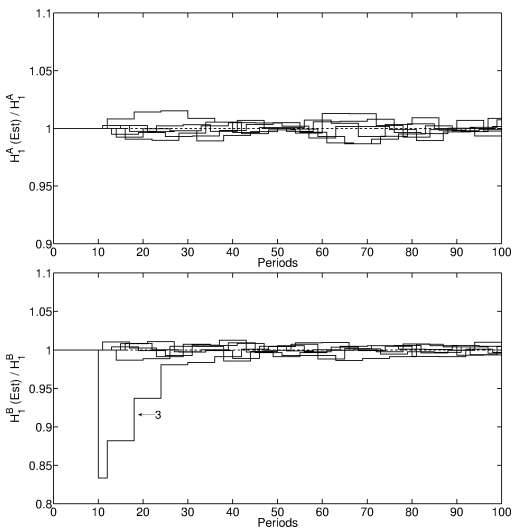

Fig. 3. Ratios between the estimated and the real values of H_1^A (above) and H_1^B (below) for all columns after a step change of 20% of H_1^B in column 3 after period 10.

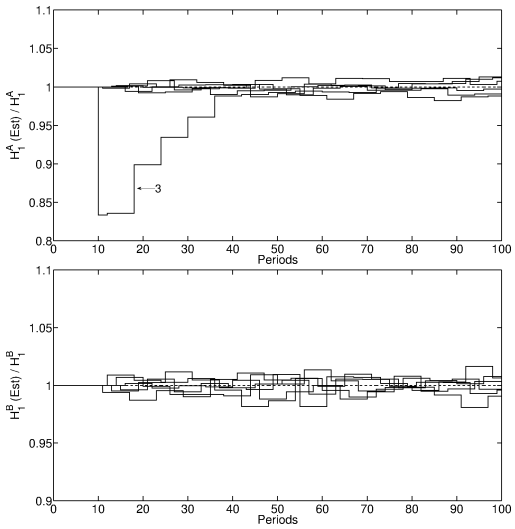

Fig. 4. Ratios between the estimated and the real values of H_1^A (above) and H_1^B (below) for all columns after a step change of 20% of H_1^A in column 3 after period 10.

their reference values (H_1^A=2.68, H_1^B=2.2) as described in Table 1, and that the plant is at the CSS conditions corresponding to this new parameter set when the estimator is activated.

The time profiles of the estimated parameters are shown in Figure 5 for a time horizon of 90 periods after the activation of the estimator. It can be observed that the scheme proposed in this work manages to bring the estimated values of H_1^A close to their true values approximately 40 periods after its activation. The estimated values of H_1^B require a similar amount of time to converge to the actual values of the plant. The results show once again that the estimator presented in this work is able to provide bias-free parameter estimates.

Column	1	2	3	4	5	6
ΔH_1^A	+8%	+8%	-18%	+10%	-7%	+4%
ΔH_1^B	+14%	+9%	-9%	+27%	+9%	-9%

Table 1. Deviations of the real parameters of the columns with respect to their reference values (H_1^A=2.68, H_1^B=2.2).

The performance of the proposed optimization-based method can be compared to the EKF-based approach presented in Küpper and Engell [2006]. Figure 6 shows the estimates of H_1^A and H_1^B reported in the reference for the same model-plant mismatch scenario, starting from the instant when the estimation scheme is activated. It can be seen that H_1^A converges relatively slowly, requiring up to 50 periods to attain the real values of the plant. In the case of H_1^B, the convergence to the actual values takes between 10 and 20 periods. This is comparable with the convergence rate obtained with the optimization-based approach. However, it must be taken into account that in Küpper and Engell [2006], besides the measurements at the extract and raffinate ports, a fixed measurement position is also considered. Additionally, a higher sampling rate (100 samples per period, Küpper [2011]) is assumed. Both factors can be expected to improve the performance of the estimator.

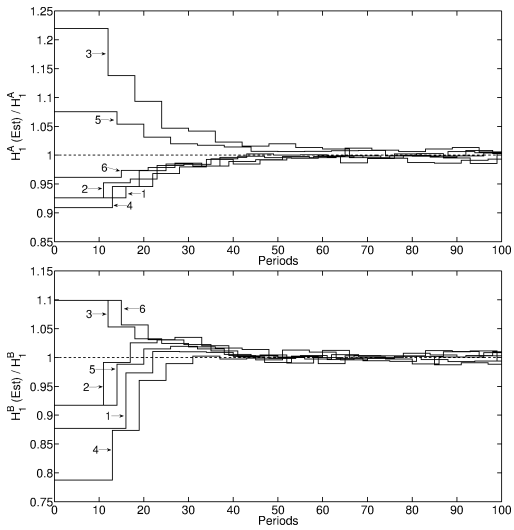

Fig. 5. Ratios between the estimated and the real values of H_1^A (above) and H_1^B (below) for all columns for the case of constant different column parameters.

Figure 7 shows the evolution of the accumulated state estimation error for the whole SMB plant at each sampling instant, defined in Eq. 17:

$$\hat{e} = \sqrt{\sum_{i=1}^{N_x} (\hat{x}(i) - x(i))^2}. \tag{17}$$

In Figure 7 it can be seen that the accumulated error, which originally fluctuates in a range between approximately 18 and 20 $g^2\ l^{-2}$, rapidly decreases once the estimator has been activated. The estimator manages to reduce the error to less than 5% of its initial value after approximately 50 periods of operation.

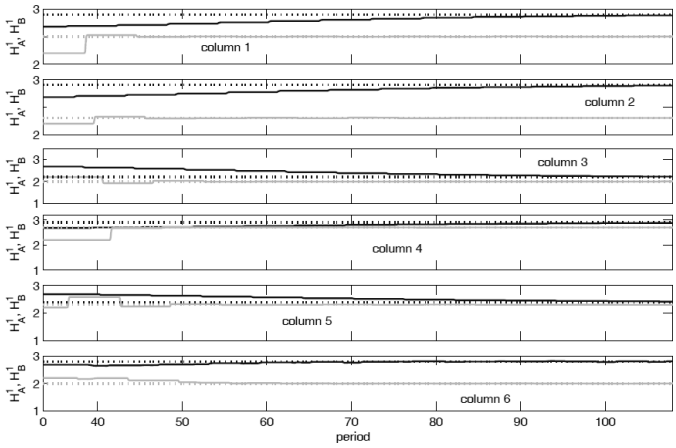

Fig. 6. Time evolution of the estimates of H_1^A (black lines) and H_1^B (gray lines) obtained with the approach proposed in Küpper and Engell [2006]

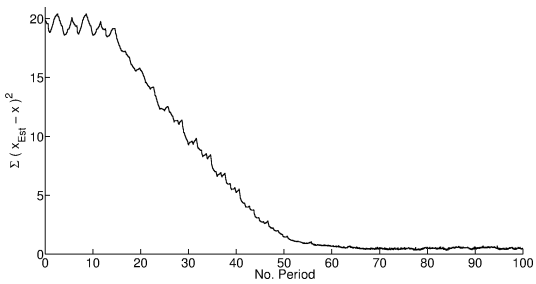

Fig. 7. Time evolution of the accumulated state estimation error for constant individual column parameters as indicated in Table 1.

7. CONCLUSIONS AND FUTURE WORK

In this work, a new optimization-based scheme for the estimation of the states and of the parameters of the individual columns in a SMB plant has been proposed. The scheme exploits explicitly that the measurement information at both the inlet and outlet of the columns is available due to the port switching, an intrinsic property of the SMB process. The proposed estimator was tested under the scenarios of tracking of step changes of individual column parameters and of state and column parameter estimation for a SMB plant with different adsorption parameters in all columns, showing in both tasks that the method is able to provide unbiased estimates at a reasonable speed of convergence.

The scheme presented here uses less measurement information than our previous work (Küpper and Engell [2006]) and is relatively easy to tune. In contrast to state and parameter estimation schemes for the whole SMB process, we propose a decentralized scheme in which only two columns are considered simultaneously which considerably reduces the computational effort and can handle the realistic situation of different parameters in all columns easily.

Future work includes the development of optimal experimental design strategies which enable the reliable estimation of parameters with minimal experimental effort.

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Appendix A. NOMENCLATURE AND PROCESS PARAMETERS

C^i	Concentration of i	g cm^{-3}
D	Column diameter	1.0 cm
D_{ax}^i	Axial dispersion coefficient (see Kuepper et al. [2009])	cm^2 s^{-1}
D_p^i	Particle diffusion coefficient	1x10^{-3} cm^2 s^{-1}
$H_1^{A,B}$	Henry coefficient of A, B (1)	2.68, 2.2
$H_2^{A,B}$	Henry coefficient of A, B (2)	0.9412, 0.4153
K^A	Isotherm coefficient of A	340 cm^3 g^{-1}
K^B	Isotherm coefficient of B	262 cm^3 g^{-1}
k_l^A	Mass transfer coefficient: A	5.6 s^{-3}
k_l^B	Mass transfer coefficient: B	3.3 s^{-3}
L	Column length	10 cm
N_x	States in the SMB plant	600
q^i	Concentration of i (solid)	g cm^{-3}
Q_i	Flow rate in the zone i	cm^3 s^{-1}
r	Radius	cm
r_p	Particle radius	0.002 cm
u	Interstitial velocity	cm s^{-1}
$\epsilon_b,\ \epsilon_p$	Porosity: column, particle	0.4, 0.5
ν	Viscosity	6.85x10^{-4} P
ρ	Density	1.0 g cm^{-3}
τ	Period length	123 s