Efficient Moving Horizon State and Parameter Estimation for the Varicol SMB Process

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Abstract: In this paper, a moving horizon state and parameter estimation (MHE) scheme for the Varicol process is presented. The Varicol process is an extension of the Simulated Moving Bed (SMB) process that realizes non-integer column distributions over the separation zones by an asynchronous switching of the inlet and outlet ports (the ports are shifted individually). These additional degrees of freedom can be used to yield an improvement in economical performance compared to SMB operation. The proposed estimation scheme is based on a rigorous SMB model that incorporates rigorous chromatographic columns and port switching. The absence of model simplifications allows the extension of the estimation scheme to the more complex Varicol process. The goal of the estimation scheme is to reconstruct the full state of the system, i.e. the concentration profiles along all columns, and to identify critical model parameters in the presence of noisy measurements. The estimation is based on measurements of the concentrations of the components at the two outlet ports (which are asynchronously switched from one column to the next) and at one fixed location between two columns. The state estimation scheme utilizes a deterministic model within the prediction horizon. State noise is only considered in the state and in the parameters up to the beginning of the horizon. By applying a multiple-shooting method and a real-time iteration scheme for solving the resulting optimization problem, the computation times are reduced and the scheme can be applied online. A numerical simulation for an enantiomer separation system with nonlinear adsorption isotherm is presented.

Keywords: Varicol, Simulated Moving Bed chromatography, moving horizon estimation, state estimation, model identification, real-time application, real-time iteration

1. INTRODUCTION

The Simulated Moving Bed (SMB) process is an efficient chromatographic separation technology that is increasingly applied in the food, fine chemicals, and pharmaceutical industries. Industrial applications have been reported especially for the separation of temperature sensitive components and for the separation of species with similar thermodynamic properties. A SMB process is realized by connecting several chromatographic columns in a closed loop as illustrated by Figure 1. The Varicol process switches the ports indvidually and thereby realizes non-integer column distributions over the zones ?), see Figure 2.

SMB processes and their variants are characterized by mixed discrete and continuous dynamics, spatially distributed state variables with steep slopes, and slow and strongly nonlinear responses of the concentrations profiles to changes of the operating parameters, therefore, they are difficult to control and to observe. In the literature, relatively few contributions that deal with state estimation of SMB processes can be found. The published work is based upon the approximation of the concentration profiles by a set of truncated exponential functions Alamir and Corriou (2003), or by using the equivalent True Moving Bed (TMB) model Mangold et al. (1994), Kloppenburg and Gilles (1999), or deals with the engineering of tailored estimation schemes Küpper and Engell (2006), Kleinert and Lunze (2005). Recently, a rigorous moving horizon estimation approach for SMB processes was proposed by Küpper et al. (2009). In this formulation of the MHE, a deterministic behaviour of the process on the estimation horizon and Gaussian independent identically distributed measurement noise are assumed. The initial state at the beginning of the horizon and its covariance are computed by an Extended Kalman Filter (EKF). The state noise covariance and the initial error covariance of this EKF are the only tuning parameters of this scheme. A fast online solution of the underlying constrained least-squares optimization problem is obtained by using the direct multiple shooting method Bock (1981, 1987). A full rigorous process



Fig. 1. Principle of the Simulated Moving Bed process

model is applied and therefore no assumption that the plant is close to the periodic steady state is needed. Along with the states, key adsorption parameters are estimated online. Simulations demonstrate that the states and critical model parameters can be reconstructed successfully. The scheme also works during transition periods including the start-up phase. The computation times are such that the estimator can be applied online. Since a rigorous full scale SMB model is used, the MHE approach can be extended to more complex variants of the SMB process. In this contribution, the moving horizon state and parameter estimation scheme is applied to the Varicol operation.

2. THE VARICOL SMB PROCESS

Chromatographic separation is based on the different adsorption affinities of the molecules in the liquid to an adsorbent which is packed in a chromatographic solid bed. The SMB process realizes a counter-current movement between the liquid and the adsorbent by switching the ports in the direction of the liquid flow periodically, as illustrated by Figure 1. In the Varicol process, the individual ports i(Eluent, Extract, Feed, Raffinate) are switched individually at the subperiod times δt_i , as illustrated by Figure 2. The individual port switching reduces the impurities by early switching of the Raffinate port and delayed switching of the Extract port. Since the Varicol process offers a larger number of degrees of freedom, it can be operated with better process economics than the SMB process, see Toumi et al. (2002), Toumi et al. (2003).

In the estimation scheme, the counter-current flow of the solid and of the liquid phases is modelled in the same way as it is achieved in the real plant by asynchronously switching the inlet and outlet ports in the direction of the liquid flow after subperiod n with subperiod length $(\delta t_n - \delta t_{n-1})\tau$ has passed. The state variables represent the concentrations in the physical columns and do not exhibit jumps. Only the input flow rates and the inflow concentrations change discontinuously. The dynamic simulation of the Varicol process is achieved by integrating the differential equation over the subperiods n



Fig. 2. Asynchronous switching in the Varicol process



Fig. 3. Concentration profiles of the Varicol process during one period with $\delta \tau_{Ra} = 0.3$, $\delta \tau_{Fe} = 0.6$, $\delta \tau_{Ex} = 0.9$, $\delta \tau_{De} = 1.0$, $\delta \tau_{Re} = 1.0$

$$\dot{\mathbf{x}} = f(\mathbf{x}, Q_n, \mathbf{p}) \tag{1}$$
$$t \in [(m-1)\tau + \delta t_{n-1}\tau, \ (m-1)\tau + \delta t_n\tau]$$
$$) = \mathbf{x}_{m,0} \tag{2}$$

 $\mathbf{x}(t_0) = \mathbf{x}_{m,0}$ followed by the switching of the flows $Q_{n,j,\delta t_j}$:

 $Q_{n+1,j,\delta t_j} = M_Q Q_{n,j,\delta t_j}$ j = De, Ex, Fe, Ra, Re,(3)with differential states $\mathbf{x}(t) \in \mathbb{R}^{n_x}$ and parameters $\mathbf{p} \in$ \mathbb{R}^{n_p} . The vector $Q_{n,j,\delta t_j}$ defines the inlet/outlet flow of port j (desorbent, extract, feed, raffinate) and the recycle stream at the individual switching time δt_i in period m (m denotes the full period count). The components of $Q_{n,j}$ represent the flows of the ports j to the columns. M_Q is a permutation matrix that shifts the flow ports after the asynchronous switching time δt_i of port j has passed (with individual period counter n). The recycle flow that defines the total flow rate in the zone in front of the desorbent port is switched with the last port. The zone flow rates result from the port flows and the recycle flow. The concentration profiles during one switching period are illustrated by Figure 3. The asynchronous switching of the feed port and of the extract port can be clearly seen in the profiles. In this paper, three positions where the concentrations of the two substances of the mixture are measured are assumed. The measurements are installed behind the extract port, behind the raffinate port, and behind one column in the process where physically the closing of the loop is realized (six measurements total). The extract and raffinate concentration measurements

move together with the ports. More measurements are not available in production plants.

2.1 Rigorous Dynamic Modelling

From mass balances of the components around the inlet and the outlet ports, the internal flow rates and the inlet concentrations can be calculated according to:

Desorbent node:
$$Q_{\rm IV} + Q_{\rm De} = Q_{\rm I}$$
 (4)

$$c_{i,\text{out,IV}}Q_{\text{IV}} = c_{i,\text{in,I}}Q_{\text{I}} \quad i = A, B \quad (5)$$

Extract node: $Q_{\text{I}} - Q_{\text{Ex}} = Q_{\text{II}} \quad (6)$
Feed node: $Q_{\text{II}} + Q_{\text{Fe}} = Q_{\text{III}} \quad i = A, B \quad (7)$

$$\text{tract node: } Q_{\text{I}} - Q_{\text{Ex}} = Q_{\text{II}}$$
 (0)

node:
$$Q_{\rm II} + Q_{\rm Fe} = Q_{\rm III}$$
 $i = A, B$ (1)

Raffinate node:
$$Q_{\text{Ra}} + Q_{\text{IV}} = Q_{\text{III}}$$
, (9)

where Q_{I-IV} are the flow rates in the corresponding zones, $Q_{\rm De}, Q_{\rm Ex}, Q_{\rm Fe}, \text{ and } Q_{\rm Ra}$ denote the external flow rates and $c_{i,\text{in}}$ and $c_{i,\text{out}}$ denote the concentrations of the component i in the streams leaving and entering the respective zone. The initial distribution of the columns over the four separation zones is 2/2/2/2 and the individual switching times are $\delta \tau_{Ra} = 0.3$, $\delta \tau_{Fe} = 0.6$, $\delta \tau_{Ex} = 0.9$, $\delta \tau_{De} = 1.0$, $\delta \tau_{Re} = 1.0$ from which the non-integer column distribution 2.1/2.3/2.3/1.3 results.

The chromatographic columns are modelled by the General Rate Model. It is assumed that there are no radial gradients in the column and that the particles of the solid phase are uniform, spherical, porous (with a constant particle porosity $\epsilon_{\rm p}$), and that the mass transfer between the particle and the surrounding layer of the bulk is in local equilibrium. The concentration of component i is denoted by c_i in the liquid phase and by q_i in the solid phase. D_{ax} is the axial dispersion coefficient, u the interstitial velocity, $\epsilon_{\rm b}$ the void fraction of the bulk phase, $k_{{\rm l},i}$ the film mass transfer resistance, and $D_{\rm p}$ the diffusion coefficient within the particle pores. The concentration within the pores is denoted by $c_{p,i}$. The following partial differential equations of a column can be derived from a mass balance around an infinitely small cross section area of the column assuming a constant radial distribution of the interstitial velocity uand the concentration c_i .

$$\frac{\partial c_i}{\partial t} + \frac{(1 - \epsilon_{\rm b})3k_{{\rm l},i}}{\epsilon_{\rm b}r_{\rm p}} \left(c_i - c_{{\rm p},i}|_{r=r_{\rm p}}\right) = D_{\rm ax}\frac{\partial^2 c_i}{\partial x^2} - u\frac{\partial c_i}{\partial x}$$
(10)

$$(1 - \epsilon_{\rm p})\frac{\partial q_i}{\partial t} + \epsilon_{\rm p}\frac{\partial c_{{\rm p},i}}{\partial t} - \epsilon_{\rm p}D_{\rm p}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_{{\rm p},i}}{\partial r}\right)\right] = 0,$$
(11)

with appropriate initial and boundary conditions. It is assumed that the concentration q_i is in thermodynamic equilibrium with the liquid concentrations in the particle and their relationship can be described by an extended Langmuir adsorption isotherm

$$q_i = H_i^1 c_{\mathrm{p},i} + \frac{H_i^2 c_{\mathrm{p},i}}{1 + k_{\mathrm{A}} c_{\mathrm{p},\mathrm{A}} + k_{\mathrm{B}} c_{\mathrm{p},\mathrm{B}}} \quad i = \mathrm{A}, \mathrm{B},$$
(12)

with H_i^j and k_i as isotherm constants. The resulting system of coupled differential equations can be efficiently solved by the numerical approach proposed in Gu (1995) where a Galerkin finite element discretization of the bulk phase is combined with orthogonal collocation for the solid phase. This numerical method was first applied to SMB processes in Dünnebier and Klatt (2000). The bulk phase is divided into $n_{\rm fe}$ finite elements and the solid phase is discretized by $n_{\rm c}$ internal collocation points. As a result, the set of initial values, boundary values, and partial differential equations (PDE) is transformed into a set of initial values and a system of ordinary differential equations (ODE)

$$\dot{\mathbf{x}} = f(\mathbf{x}, \mathbf{u}, \mathbf{p}),\tag{13}$$

where the flows Q are summarized in the input vector $\mathbf{u}(t) \in \mathbb{R}^{n_u}$. The system output is defined as

$$y = h(\mathbf{x}(\mathbf{u}, \mathbf{p})), \tag{14}$$

with $y \in \mathbb{R}^{n_y}$. For $n_{\text{fe}} = 5$, $n_{\text{c}} = 1$, number of components $n_{\rm sp} = 2$, and number of columns $n_{\rm col} = 8$ a system order of the SMB process of

 $n_x = n_{\rm col} * n_{\rm sp} * (n_{\rm c} + 1) * (2 * n_{\rm fe} + 1) = 352$ (15)results. The ODE-system is stiff due to large differences in the speeds of the interacting dynamics.

3. ESTIMATION IN THE VARICOL PROCESS

3.1 Moving Horizon Estimation

For the simultaneous estimation of the states and the parameters of SMB processes, we employ the Moving Horizon Estimation scheme introduced by Diehl et al. (2006); Kühl et al. (2008), which is modified in order to handle the shift of the inputs and of the measurements of the SMB process. The Moving Horizon Estimator estimates the states and the parameters based on the past measurements at specific time points that are located in the horizon $T_N = t_K - t_K$ t_L . t_K represents the current time and t_L is the time at the beginning of the horizon. A least-squares minimization is performed that minimizes the deviations of the real measurements η_k from the simulated measurements $h(\mathbf{x}(t_k; \mathbf{u}, \mathbf{p}))$ at times t_k . The expression $||.||_{V^{-\frac{1}{2}}}^2$ denotes $||\mathbf{x}||_{V^{-\frac{1}{2}}}^2 = \mathbf{x}^T V^{-1} \mathbf{x}$, where the matrix V is the positive semidefinite noise covariance matrix of the variables \mathbf{x} . $V^{-\frac{1}{2}}$ can be interpreted as weighting matrix of **x**. The measurement information prior to the moving horizon is considered in the estimation problem by an arrival cost term that is computed from the expected value of the state and the parameters and the estimation error covariance before the horizon. The optimization problem of the MHE results as:

$$\min_{\mathbf{x}(t_L),p} \left\{ \left\| \mathbf{x}(t_L) - \overline{\mathbf{x}}_L \right\|_{P_L^{-\frac{1}{2}}}^2 + \sum_{k=L}^K \left\| \eta_k - h(\mathbf{x}(t_k; \mathbf{u}, \mathbf{p})) \right\|_{V_k^{-\frac{1}{2}}}^2$$
(16)

s.t.
$$\dot{\mathbf{x}}(t) = f(\mathbf{x}(t), \mathbf{u}(t), \mathbf{p})$$
 (17)

$$_{min} \le \mathbf{x}(t) \le \mathbf{x}_{max} \tag{18}$$

 $\mathbf{p}_{min} \leq \mathbf{p} \leq \mathbf{p}_{max}$ (19)

$$\in [t_L, t_K] \,. \tag{20}$$

The second term represents the prediction errors within the horizon and the first term represents the arrival cost (the penalization of a change of the estimates of the initial values of the states and of the parameters), where $(\overline{\mathbf{x}}_L, \overline{\mathbf{p}}_L)$ are the expected values and $P_L \in \mathbb{R}^{(n_x+n_p) \times (n_x+n_p)}$ is the joint covariance matrix of $\mathbf{x}(t_L)$ and \mathbf{p}_L . Note that only the initial values of the states and the parameters are free parameters of the optimization problem because no state

noise is assumed within the horizon. The absence of state noise on the horizon is compensated by the simultaneous estimation of key model parameters which is an appropriate assumption since uncertainties are mostly due to model errors and not to disturbances. Furthermore, the inclusion of state noise at each point within the horizon would lead to a large number of degrees of freedom of the estimation and result in a considerably larger optimisation problem with additional $n_x \times (K - L)$ variables that, taking the system dimension into account, would be hard to solve online reliably. From the solution $\mathbf{x}(t_L)$ and \mathbf{p} of the optimization problem, the deterministic model is simulated forward to obtain the current estimated state \mathbf{x}_{K} . The MHE takes upper and lower bounds on the states and on the parameters into account. The expected value and the covariance of $\mathbf{x}(t_L)$ and \mathbf{p}_L in the arrival cost are determined by an Extended Kalman Filter. The smoothed Extended Kalman Filter Robertson et al. (1996) is employed where the recent state estimation $x_{L+1|K}$ and linearizations of the dynamics $G_{L+1|K}$ and the output matrix $C_{L+1|K}$ are utilized. In order to guarantee positive definite matrices in the presence of numerical errors, the smoothed Extended Kalman update is reformulated by two QR-decompositions yielding the equivalent smoothed Extended Kalman Filtering update in square-root formulation Diehl (2002); Kühl et al. (2008).

$$\begin{pmatrix} \overline{\mathbf{x}}_{L+1} \\ \overline{\mathbf{p}}_{L+1} \end{pmatrix} = \begin{pmatrix} \mathbf{x}(t_{L+1}; t_L, \mathbf{x}_{L|K}, \mathbf{u}_L, \mathbf{p}_{L|K}) \\ \mathbf{p}_{L|K} \end{pmatrix} + G_{L|K} R^{-1} Q^T \begin{pmatrix} P_{L|L-1}^{-\frac{1}{2}} \begin{pmatrix} \mathbf{x}_{L|L} - \mathbf{x}_{L|K} \\ \mathbf{p}_{L|L} - \mathbf{p}_{L|K} \end{pmatrix} \\ V_L^{-\frac{1}{2}} (\eta_L - h(\mathbf{x}_{L|K})) \end{pmatrix}$$
(21)

$$P_{L+1|L}^{-\frac{1}{2}} = \overline{Q}^T \begin{pmatrix} 0\\ W^{-\frac{1}{2}} \end{pmatrix}$$
(22)

with the linearizations of the dynamics

$$G_{L|K} = \begin{pmatrix} X_{x,L|K} & X_{p,L|K} \\ 0 & I_{n_p} \end{pmatrix}$$
(23)

$$X_{x,L|K} = \left. \frac{d\mathbf{x}(t_{L+1}; \mathbf{x}_{L|K}, \mathbf{p}_{L|K})}{d\mathbf{x}} \right|_{L|K}$$
(24)

$$X_{p,L|K} = \left. \frac{d\mathbf{x}(t_{L+1}; \mathbf{x}_{L|K}, \mathbf{p}_{L|K})}{d\mathbf{p}} \right|_{L|K}, \qquad (25)$$

the linearization of the output

$$H_{L|K} = \begin{pmatrix} H_{x,L|K} & H_{p,L|K} \end{pmatrix}$$
(26)
$$dh(\mathbf{x}(t_{x+1};\mathbf{x}_{x+1};\mathbf{p}_{x+1})) \mid$$

$$H_{x,L|K} = \left. \frac{dn(\mathbf{x}(\iota_{L+1}, \mathbf{x}_{L|K}, \mathbf{p}_{L|K}))}{d\mathbf{x}} \right|_{L|K}$$
(27)

$$H_{p,L|K} = \left. \frac{dh(\mathbf{x}(t_{L+1}; \mathbf{x}_{L|K}, \mathbf{p}_{L|K}))}{d\mathbf{p}} \right|_{L|K}, \qquad (28)$$

the QR-decompositions

$$\begin{pmatrix} P_{L|L-1}^{-\frac{1}{2}} \\ V_{L}^{-\frac{1}{2}} H_{L|K} \end{pmatrix} = (Q|\breve{Q}) \begin{pmatrix} R \\ 0 \end{pmatrix}$$
(29)

$$\begin{pmatrix} R\\ -W^{-\frac{1}{2}}G_{L|K} \end{pmatrix} = (\overline{Q}|\widetilde{Q}) \begin{pmatrix} \overline{R}\\ 0 \end{pmatrix},$$
(30)

and the state noise covariance matrix of the states and of the parameters

$$W = \begin{pmatrix} W_x & 0\\ 0 & W_p \end{pmatrix}.$$
 (31)

 $\mathbf{x}(t_{L+2}; t_{L+1}, \mathbf{x}_{L+1|K}, \mathbf{u}_{L+1}, \mathbf{p}_{L+1|K})$ denotes the prediction of the system based on the recent estimate at $_{L+1|K}$ while $\mathbf{x}_{L+2|L+1}$ is the smoothed prediction.

The MHE has to cope with jumps in the extract and raffinate measurements that are caused by the port switching. In order to obtain a smooth calculation of the gradients with respect to the simulated measurements which exhibit jumps due to the periodic movement of the ports, virtual measurements at constant positions at the outlet of each chromatographic column are included in the mapping h. In order to account for the actual existence of real measurements at the considered point of time k, the corresponding components on the diagonal of the measurement weight V_k^{-1} are set to $\frac{1}{\sigma_v^2}$ while nonexisting measurements cause zero entries on the diagonal of V_k^{-1} . A zero weight can be interpreted as infinite measurement noise. Thus, the correction terms of nonexisting measurements in the smoothed Extended Kalman Filtering update and in the moving horizon are zero. The switching of the measurement weights at the respective extract and raffinate switching times $\delta t_j \tau$ in period m is realized according to the movement of the extract and raffinate port:

$$\overline{V}_{m,j} = M_V \overline{V}_{m,j} \quad j = Ex, Ra \tag{32}$$

$$\overline{V}_m = \overline{V}_{m,Ex} + \overline{V}_{m,Ra} \tag{33}$$

$$V_m = \text{diag}(\overline{V}_{m+1}(1, \dots, (n_{\text{col}} - 1) * 2), \sigma_v^2, \sigma_v^2).$$
(34)

The permutation matrix M_V for shifting the extract and raffinate measurements around the plant for a new period m+1 is similar to the permutation matrix M_Q for shifting the port flows. The last two entries of V_k are the variances of the measurements at the internal measurement position (recycle) which are not shifted.

 $3.2~Multiple\mbox{-}Shooting~Real\mbox{-}Time~Iteration~Scheme~for~MHE$

The moving horizon optimization problem is solved by the multiple shooting method for parameter estimation Bock (1981, 1987). The basic idea of multiple shooting is to subdivide the time horizon into subintervals and to formulate autonomous initial value problems on each individual subinterval which are coupled by continuity conditions. The computational requirements are largely reduced by applying the *real-time iteration* scheme for the multiple shooting method introduced in Diehl et al. (2002, 2004); Diehl (2002) that updates the sensitivity matrices that are necessary to solve the optimization problem before the most recent measurement η_K is available. Another important feature is that the next optimization problem is initialized well at the current solution such that the number of iterations can be reduced to one.

4. RESULTS

For the demonstration of the performance of the moving horizon estimator, the separation of the enantiomer mixture EMD-53986 is considered which is described by a nonlinear adsorption isotherm of extended Langmuir type (12). Enantiomers are chemical molecules that are mirror images of each other, much as one's left and right hands. The separation of the enantiomers of EMD-53986 was studied experimentally in a joint project by *Merck* (Germany) and Universität Dortmund in 2001. From this work, an accurate simulation model is available. The parameters of the SMB model were taken from Jupke et al. (2002). More details on the process and the model parameters can be found in Jupke (2004). In order to demonstrate the performance of the MHE estimator, a simulation study is presented in which step changes of the Henry coefficients H_A^2, H_B^2 of the nonlinear adsorption isotherm are assumed. The performance of the moving horizon estimator is illustrated by the evolution of the parameters and of the overall state reconstruction error which is defined as

$$J = \sum_{j=1}^{352} (\mathbf{x}(j) - z(j))^2, \qquad (35)$$

where z is the true state. The measurements are corrupted by noise with a standard deviation of 0.025 g/l as observed in Jupke et al. (2002). No cross-correlations between the state noises and between the state noises and the parameters were assumed. Since the concentration profiles move around the simulated plant together with the ports, the same noise variances were assumed for each state. The tuning of the moving horizon estimator was performed by varying the covariances of the state variables and of the free parameters. The weighting matrix W incorporates a standard deviation of 0.00433 g/l for the state noise and a parameter standard deviation of 0.0316 for $H_{\rm A}^2$ and 0.0265 for $H_{\rm B}^2$: $W^{\frac{1}{2}} = \text{diag}(0.00433, \dots, 0.00433, 0.0361, 0.0265).$ The initial weight P_0 is set to $0.005 \times W$. The chosen state and parameter noises represent a compromise between the smooth estimation of the states and a quick adaptation of the parameters. The state and parameter bounds are chosen as -0.25 g/l $\leq x \leq 5$ g/l and $0 \leq H_i^2 \leq 50$ to prevent grossly wrong values. The lower bound on the states is chosen such that it remains inactive in the presence of large measurement noise. The sampling time of the estimator is 1/10 of the period length. The moving horizon length is five sampling intervals (half a period).

In the simulation scenario, $H_{\rm A}^2$ is increased by 10.6% from 19.90 to 22.00 at t = 14.58 min while $H_{\rm B}^2$ is increased by 10.3% from 5.85 to 6.45 at t = 68.04 min. It can be seen from figures 4 to 8, that the state is reconstructed correctly in the presence of the parameter variations and that the parameters are also estimated well. The Henry coefficient \hat{H}_B^2 is estimated faster than H_A^2 due to the stronger excitation of the raffinate dynamics by the parameter perturbation. The axial concentration profiles are reconstructed correctly by the MHE (not show here due to limited space). The MHE is more robust against measurement noise and wrong initializations of the states and parameters than an EKF, see Küpper et al. (2009). The MHE estimator can be applied online, as can be seen from Figure 8. The CPU times are below the sampling rate at all sampling points. The CPU times of the MHE are around 23 s on a standard PC^{1} , the maximum and minimum values being 28.0 s and 18.5 s. The CPU times for the estimator varies periodically. It was observed that the estimation problem requires a longer computation time when a shift of one of the inlet/outlet ports occurs within the moving horizon.



Fig. 4. Measurements (extract, raffinate, recycle)



Fig. 5. Enlarged measurements (extract, raffinate, recycle)



Fig. 6. Parameter estimates

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 $^{^1\,}$ Intel Xenon CPU 2.8 GHz, 4.0 GB RAM



Fig. 7. State reconstruction error



Fig. 8. CPU times of the estimator at each sampling point

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