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Engineering of Online Optimizing Control - A Case Study: Reactive SMB Chromatography

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Abstract: This contribution discusses the application of the idea of online optimizing control to a complex process from chemical engineering. The idea of online optimizing control is to minimize an economic objective over a finite moving horizon during plant operation based upon a rigorous nonlinear dynamic model. Plant limitations and product specifications are included in the optimization as constraints. The process discussed here is the so-called Hashimoto SMB process that combines reaction and continuous chromatographic separation in one plant. The degrees of freedom (flow rates and the switching time) are used to minimize the solvent consumption and to keep the product purity and product recovery above the specified values. The emphasis of this paper is on the modifications of the formulation of the optimization problem in order to cope with plant/model mismatch. *Copyright ©2008 IFAC.*

Keywords: Optimizing control, Chromatographic separations, SMB process, Plant-model mismatch.

1. INTRODUCTION

Direct online optimizing control is gaining increasing attention, see e.g. Engell (2007) and Rolandi and Romagnoli (2005). The idea of a direct online minimization of operating costs or plant profit with simultaneous satisfaction of constraints on operating ranges and product specifications is especially attractive for applications in the chemical and related industries. In this paper, the application of the direct optimizing control to a nonlinear, hybrid, multivariable process modelled by partial differential equations is presented. The process considered here is the Hashimoto Simulated Moving Bed (SMB) chromatographic process. In SMB processes, a counter-current movement of the liquid and of the solid phase is achieved by periodically switching the inlet and the outlet ports in a closed-loop of chromatographic columns. The integration of reaction and separation in one single plant is a promising approach to overcome chemical or thermodynamic equilibria and to increase process efficiency. The Hashimoto SMB (Hashimoto et al., 1983) process is established by placing reactors between the separation columns at specific positions around the feed port. SMB processes are complex, multivariable nonlinear processes and the complexity increases considerably with the integration of reactors in the system.

The most often proposed approach to feedback control of such processes is to control the positions of the concentration fronts in the columns in order to achieve desired product purities. For linear adsoption isotherms, a weakly coupled nearly linear multivariable system results after a transformation of the degrees of freedom (Hanisch, 2002). If plant/model mismatch is present, an additional purity control layer is necessary. Kleinert (2006) proposed to approximate the concentration profiles by wave fronts that are described by an exponential expression resulting from the solution of a True Moving Bed (TMB) model and under the assumption that the adsorption can be approximated linearly for the wave fronts (no multi-component adsorption). In contrast, Toumi and Engell (2004) and Erdem et al. (2006) employed variants of model-predictive control. In the latter approach, the online optimization is based upon a linearized reduced model which is corrected by a Kalman filter that uses the concentration measurements in the product streams. The switching period is fixed and not modified online. In Toumi and Engell (2004), online optimization was performed based on a rigorous nonlinear dynamic model and all degrees of freedom are included. This approach was applied successfully to a three-zone reactive SMB process for glucose isomerization on the pilot plant scale. An overview of recent achievements in the optimization and control of chromatographic separations can be found in Engell and Toumi (2005).

In Küpper and Engell (2006), it was first proposed to extend the optimizing control concept of Toumi and Engell (2004) to the Hashimoto SMB process. In Küpper and Engell (2007), results from real experiments were reported. Although the results are good, the dynamic behavior of the controlled process was not entirely satisfactory. This is mainly due to the presence of a considerable plant/model mismatch, caused by additional hold-ups in the real plant and a complex adsorption characteristic of the considered

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enantiomer separation system (Tröger's base) as reported in Mihlbachler et al. (2002). Therefore, in this paper we present a detailed analysis of the effects of plant-model mismatch and on modifications of the cost function that reduce the sensitivity to these errors by shifting the optimum to a different regime which is more robust. The remainder of this paper is structured as follows: In the next section, the Hashimoto SMB process and the rigorous process model are introduced. Section 3 describes the moving horizon online optimization control scheme and the measures that made the controller work for significant plant/model mismatch. Finally, the experience gained is summarized and directions for further developments are discussed.

2. PROCESS DESCRIPTION AND PROCESS MODEL

The Hashimoto SMB process is an integrated reaction and separation process. Reaction and chromatographic separation are performed in separate units such that optimal conditions for both reaction and separation can be chosen independently and the reactors are constantly placed at positions where the forward reaction of the equilibrium limited reaction system is advantageous. A countercurrent movement of the adsorbent is implemented by switching the ports in the direction of the liquid flow. The reactors, however, remain at their positions relative to the ports. The Hashimoto SMB process considered here is realized as a four-zone configuration, see Figure 1. Reactors and separators are placed in an alternating sequence in order to obtain the desired conversion by reaching the reaction equilibrium in the reactor and removing the valuable product in the following separation unit. Here, the desired component product is the more strongly adsorbed component which is obtained at the extract port. The second outlet flow at the raffinate port contains only little of the desired product and improves the desorption of the columns in zone IV by reducing the liquid flow leading to a lower solvent consumption compared to a three zone configuration. The raffinate stream can be converted back to the chemical equilibrium by a reactor and then be issued as feed again. In this paper, the integrated racemization (conversion of one enantiomer into another) and separation of Tröger's base (TB) is considered. Tröger's base consists of the enantiomers TB- and TB+. Enantiomers are chemical molecules that are mirror images of each other, much as one's left and right hands. The desired product TB- is which is used for the treatment of cardiovascular diseases. Both Tröger's base components form an equimolar reaction equilibrium. The separators are packed with the adsorbent Chiralcel. As the liquid phase, an equimolar mixture of the catalyst acetic acid and the solvent 2-Propanol is used. The catalyst has a high activity at a reactor temperature of $80°C$ but negligible activity at room temperature at which the separators are operated. The reactors are placed in a heated bath while the separating columns are operated at room temperature. Accurate dynamic models of multi-column continuous chromatographic processes consist of dynamic models of the single chromatographic columns and of the tubular reactors and of the node balances which describe the connections of the columns and the switching of the ports. The chromatographic columns are described accurately by the *general rate model* which accounts for

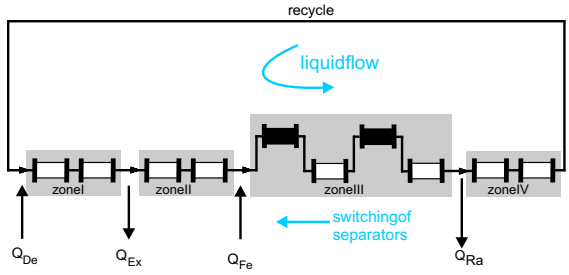

Fig. 1. Hashimoto SMB process four-zone configuration

all important effects of a radially homogeneous chromatographic column, i.e. mass transfer between the liquid and the solid phase, axial convection, and axial dispersion. It is assumed that the particles of the solid phase are uniform, spherical, porous (with a constant void fraction ϵ_p), and that the mass transfer between the particle and the surrounding layer of the bulk is in a 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, ϵ_b the void fraction of the bulk phase, $k_{l,i}$ the film mass transfer resistance, and D_p the diffusion coefficient within the particle pores. The concentration within the pores is denoted by $c_{p,i}$. The following set of partial differential equations for the separators and the tubular reactors can be obtained from a mass balance around an infinitely small cross-section of the column (TB- is referred to as A, while TB+ is denoted as B):

Separator

$$\begin{aligned} &\frac{\partial c_i}{\partial t} + \frac{(1-\epsilon_b)3k_{l,i}}{\epsilon_b r_p}\left(c_i - c_{p,i}|_{r=r_p}\right) \\ &= D_{ax}\frac{\partial^2 c_i}{\partial z^2} - u\frac{\partial c_i}{\partial z} \\ &(1-\epsilon_p)\frac{\partial q_i}{\partial t} + \epsilon_p\frac{\partial c_{p,i}}{\partial t} - \epsilon_p D_p \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_{p,i}}{\partial r}\right) = 0 \end{aligned} \tag{1}$$

Reactor

$$\frac{\partial c_i}{\partial t} + r^{\text{liq}}_{\text{kin},i} = D_{ax}\frac{\partial^2 c_i}{\partial z^2} - u\frac{\partial c_i}{\partial z} \tag{2}$$

with appropriate initial and boundary conditions. The adsorption equilibrium and the reaction kinetics have been determined experimentally in Borren et al. (2006). The adsorption equilibrium can be described by an asymmetric multi-component Langmuir isotherm

$$q_i = \frac{H_i c_i}{1 + \sum_j b_{i,j} c_j} \quad i = A, B, \tag{3}$$

where H_i denotes the Henry coefficient which dominates the adsorption. The racemization of Tröger's base is regarded as a homogeneous reaction described by first order kinetics:

$$r^{liq}_{kin,i} = \nu_i k_m (c_B - c_A). \tag{4}$$

The column inflows at each port position are obtained from simple mass and concentration balances. An efficient numerical solution approach is used following Gu (1995) where a finite element discretization of the bulk phase is combined with orthogonal collocation of the solid phase. Figure 9 shows the concentration profile within the Hashimoto SMB process at a periodic steady state for the

column+reactor distribution of 2/2/2+2/2 over the zones. The equimolar reaction equilibrium is reached within the reactors (columns 5, 7) and both components are separated in the chromatographic columns, such that TB- is obtained at a high purity at the extract port (column 2).

3. OPTIMIZING CONTROL

The optimizing control scheme is a non-linear finite horizon predictive controller. The goal of the online optimization is to minimize an economic objective while respecting important plant and product specifications such as product purity and recovery. The product specifications are treated as inequality constraints. Since a cost optimal operation is achieved at the brink of an infeasible solution some specifications will be active constraints at the optimum. Further relevant process constraints such as pump limitations or nonnegative concentrations can be included into the formulation. The objective function and the constraints are evaluated over the prediction horizon that consists of H_P time intervals. The operational degrees of freedom located within the control horizon H_C are considered as degrees of freedom for the optimization problem while the remaining inputs within the larger prediction horizon H_P are set equal to the values in the final control interval. The computed inputs in the first sampling interval are applied to the plant, and the optimization is then repeated for the next time interval $k+1$ with the control and prediction horizon shifted forward by one time interval.

3.1 Control formulation for the Hashimoto process

After discretization, the Hashimoto process is modelled by a nonlinear ode model with 1400 states. Online optimization is feasible for this process because the model can be solved efficiently and the process dynamics are slow. All degrees of freedom are fully utilized for the optimization: the flow rates and the period length. The period length also defines the sampling interval of the optimizing controller that is chosen as one cycle time (the period length times the number of separation columns). The flow rates and the period length are represented as the so called beta factors, Hashimoto et al. (1983). Hanisch (2002) modified the definitions of β_{III} and β_{IV} as given below, Toumi et al. (2002). The use of the beta factors has the advantage that they are scaled to the region around 1 and that their use leads to a decoupling of the influence of the inputs on the front positions and therefore on the purities.

$$\beta_I = \frac{1}{H_A}\left(\frac{Q_I}{Q_s} - \frac{1-\epsilon}{\epsilon}\right); \quad \frac{1}{\beta_{III}} = \frac{1}{H_A}\left(\frac{Q_{III}}{Q_s} - \frac{1-\epsilon}{\epsilon}\right)$$
$$\beta_{II} = \frac{1}{H_B}\left(\frac{Q_{II}}{Q_s} - \frac{1-\epsilon}{\epsilon}\right); \quad \frac{1}{\beta_{IV}} = \frac{1}{H_B}\left(\frac{Q_{IV}}{Q_s} - \frac{1-\epsilon}{\epsilon}\right)$$
$$Q_s = \frac{(1-\epsilon)V_{col}}{\tau} \ . \tag{5}$$

The objective function (6) of the online optimisation mainly penalizes the desorbent consumption Q_{De} over the horizon as the main objective of the optimizer. This is equivalent to minimizing the operating cost for a given throughput. The optimization problem is subject to the hybrid dynamics of the Hashimoto SMB process (7) and (8): the integration within period i and the switching of the states by the permutation matrix M at the beginning of the next state to account for the port switching. The purity and the product recovery averaged over the prediction horizon are demanded to be above the respective set points (9) and (11). Pump limitations are taken into account by the constraint (14). Thus, the following optimization problem results:

$$\min_{\beta_I,\beta_{II},\beta_{III},\beta_{IV}} \quad \sum_{i=1}^{H_P} Q_{De,i} + \Delta\beta R \Delta\beta \tag{6}$$

$$s.t. \quad x^i_{smb} = x^i_{smb,0} + \int_{t=0}^{\tau} f_{smb}(x_{smb}(t), u(t), p)dt \tag{7}$$
$$x^{i+1}_{smb,0} = M x^i_{smb,\tau} \tag{8}$$
$$\frac{\sum_{i=1}^{H_P} Pur^*_{Ex,i}}{H_P} \geq \left(Pur^*_{Ex,min} + \Delta Pur_{Ex}\right) \tag{9}$$
$$\Delta Pur_{Ex} = Pur^*_{Ex,model,k-1} - Pur^*_{Ex,plant,k-1} \tag{10}$$
$$\frac{\sum_{i=1}^{H_P} Rec_i}{H_P} \geq Rec_{min} + \Delta Rec \tag{11}$$
$$\Delta Rec = Rec_{model,k-1} - Rec_{plant,k-1} \tag{12}$$
$$\frac{\sum_{i=1}^{H_{P,short}} Pur_{Ex,i}}{H_{P,short}} \leq 99.995\% \tag{13}$$
$$Q_I \leq Q_{max} \tag{14}$$
$$Q_{El}, Q_{Ex}, Q_{Fe}, Q_{Re} \geq 0 \ . \tag{15}$$

Since an economical operation of SMB processes, as for many processes, is at the brink of an infeasible solution, (10) and 12 are satisfied as equalities.

3.2 Features to improve the control performance

In order to improve the performance of the controller, a few modifications of the formulation were made. A regularization term is added to the objective function to penalize changes of the degrees of freedom β and to obtain a smooth behavior of the controlled system such that aggressive changes of the control variables only take place when needed to obtain a feasible operation (e.g. in the presence of a setpoint change). In order to compensate for a plant/model mismatch, the recent differences of the predicted and the measured product purities (10) and recoveries (12) of the previous interval $k-1$ are added to the purity (9) and recovery (11) constraints for the present optimization. In order to realize purities near 100%, the purities have to be scaled since the error feedback otherwise can lead to an infeasible setpoint for the optimizer. Scaling (indicated by a *) of the purities is performed according to

$$Pur^* = log\left(\frac{Pur}{1-Pur}\right). \tag{16}$$

The feedback of the scaled purities (10) leads to optimizer set points (9) that asymptotically approach 100%. Furthermore, in order to avoid that the SQP problem loses sensitivity to the purity constraint (9) due to zero gradients at purities of 100%, an additional limit of the purity over a short prediction horizon $H_{P,short}$ of two intervals is

introduced (13). Due to the slow dynamic response of the concentration profiles of SMB processes to changes in the operating parameters, a modern PC is sufficient to solve the online optimization problems within a process cycle. The feasible path optimiser FFSQP Zhou et al. (1997) is utilized that searches for a feasible solution point first and then optimizes the objective function within the feasible region in order to ensure that the plant is always operated such that the product requirements specifications are met.

Simulation of the control scheme: A major problem in the application of such a model-based control scheme to the real plant is that the behavior of the plant differs considerably from the model, mainly due to differences in the adsorption isotherms. The first simulation scenario illustrates the control performance for a parametric plant/model mismatch. The adsorption isotherms of the (simulated) plant and of the model that is used in the controller are both of Langmuir type but the Henry coefficients of the model in the controller are perturbed by +10% and -5%, respectively. The recovery setpoint is set to 0.7 while the purity setpoint for the extract is initially at 75% and then successively increased to 90%, 95% and 99%. The controller is switched on at period 80. The axial profiles generated by the two models differ considerably, as shown by Figure 4. At the outlet of the reactors, the concentration is at the reactive equilibrium that reduces the effect of the plant/model match. The optimization of the solvent consumption leads to operating points where the impurity in the extract stream results from the impurity of the recycle stream (breakthrough) and not from the "simulated" solid flow as in conventional SMB operation. The controller manages to keep the product purity and the recovery at the specified minimal values for most of the simulation run and to reduce the solvent consumption. However, for the purity setpoint of 95% from period 448 to 728, the controller struggles to keep the purity of the plant above the setpoint. In the presence of slight changes of the manipulated variables by the controller (at period 608 the desorbent consumption is increased by 1% and the period length is decreased by 1%, see Figure 2), the breakthrough in the model at period 608 is reduced (the model purity is increased) over eight periods while the breakthrough in the plant remains the same, see figures 5, 6. The breakthrough of the model is then further reduced until period 728 (see the model purity in Figure 3). However, the purity of the extract in the plant hardly reacts to these changes at all. Thus, a change of the sign of the error feedback occurs at period 608, the feedback of the purity error for the optimizer is constantly increased and the controller does not manage to keep the plant purity above the required setpoint. Obviously, at this operating point, the model predictions become inaccurate. Physically, this is due to the fact that the liquid flow rate in zone 1 is very high, possibly leading to a strong reaction of the purities to small changes of the operating conditions. This effect is less pronounced for very high purities and for low purities.

3.3 Reformulation of the control problem

As the previous simulation demonstrates, the economic optimum is attained when a breakthrough of impurities in the liquid stream via the recycle line occurs that dominates the contamination of the extract via the solid flow. Since the Henry coefficient of the less retained component H_B is assumed to be smaller for the model than for the virtual plant, the model is affected more strongly by this phenomena than the virtual plant. Small changes in the operating parameters can lead to considerable changes of breakthroughs. In fact, this mode of operation is avoided in regular SMB operation. E.g. the triangle theory Mazzotti et al. (1997), a short-cut method for the design of the operating point of SMB processes, requires that the flow rates and period length are chosen such that no breakthrough of components over the recycle line occurs (all components are adsorbed in zone IV and desorbed in zone I). For the optimization problem (6)-(15), there is no constraint whether the impurity of the extract stream results form the usual SMB profiles or from a breakthrough. It turned out, however, that the economically more desirable operation with a breakthrough leads to a high sensitivity to model errors and a much less robust operation. Therefore, an additional penalty term was added to the objective function in order to penalize the flow of both components of the mixture over the recycle line:

$$\min_{\beta_I,\beta_{II},\beta_{III},\beta_{IV}} \quad \sum_{i=1}^{H_P} Q_{De,i} + \Delta\beta R \Delta\beta + \gamma \sum_{i=1}^{H_P} \int_{t=0}^{\tau_i} (c_{A,Re} + c_{B,Re}) Q_{Re} dt \tag{17}$$

Simulation of the reformulated control scheme: In the second scenario, the reformulated optimizing control scheme with the penalty term for the recycle breakthrough in the objective is applied for the same plant/model mismatch as in simulation I. The results of the simulation run are illustrated by the figures 7, 8, and 9. A conventional SMB operation is achieved (no breakthrough of contaminating components occurs, note the qualitative differences of the profiles in Figure 5 and Figure 10). The controller manages to keep the product purity and the recovery above the specified minimal values for the whole simulation horizon, regardless of the purity setpoint. Due to the penalty on the impurities in the stream that enters zone I, the purities of the model and of the virtual plant differ only slightly and do not exhibit a diverging behavior for any setpoint. Furthermore, the offset in the purity forecasts of the model and the virtual plant is reduced and an almost constant error feedback results. A calm behavior of the controller with constant error feedback is realized. However, the smooth control performance is paid for by a higher solvent consumption for high purities.

4. EVALUATION AND LESSONS LEARNED

The process at hand exhibits an extremely complex dynamic behavior. The development of a control scheme for this process based e.g. on the control of the front positions would have been rather tedious because of the strongly nonlinear and interacting behavior of the plant. The use of a nonlinear dynamic process model is indispensable to find a suitable operating regime for such plant, so there is no additional modelling effort involved in using the rigorous model also for control purposes. The concept of online optimization leads to a structurally simple control scheme in which the operating goals for the plant can be

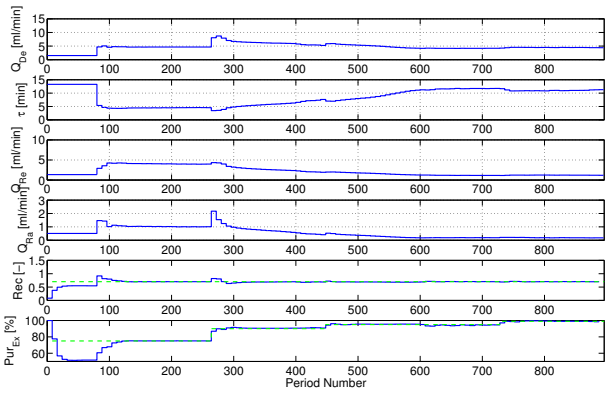

Fig. 2. Simulation I: manipulated and controlled variables

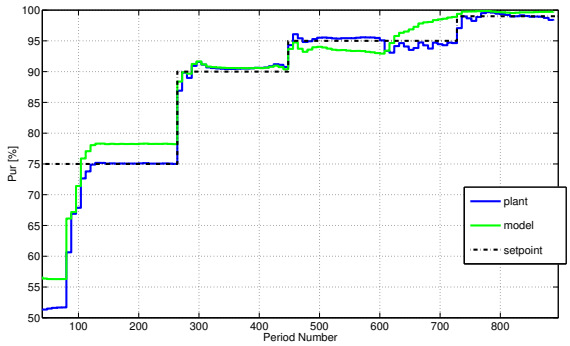

Fig. 3. Simulation I: model and plant purities and setpoint

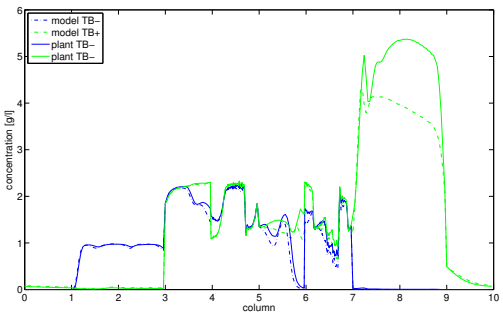

Fig. 4. Simulation I: axial concentration profiles of plant and model at the beginning of period 608

represented directly. In comparison to the classical solution of computing an optimal operating regime first and then implementing it via tracking of setpoints of all variables of interest, only critical constraints are tracked here. The use of a feasible path SQP algorithm ensures that a feasible solution is available whenever a new control input is needed. Experience showed that 5 iterations of the SQP algorithms were sufficient to obtain a good solution, this number of iterations can be performed during each full cycle of the process on a PC. By restarting the optimization from the previously obtained solution, a gradual convergence to the optimal point is achieved when the setpoint and the process behavior remain constant.

The issue of plant/model mismatch is a critical one. Constant error feedback is only adequate if the model predic-

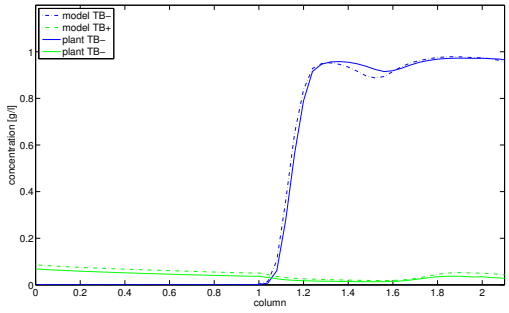

Fig. 5. Simulation I: enlarged axial concentration profiles of plant and model at the beginning of period 608

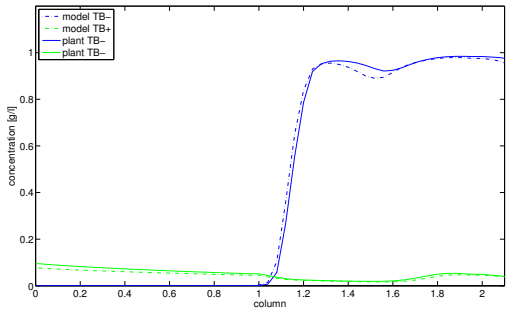

Fig. 6. Simulation I: enlarged axial concentration profiles of plant and model at the beginning of period 616

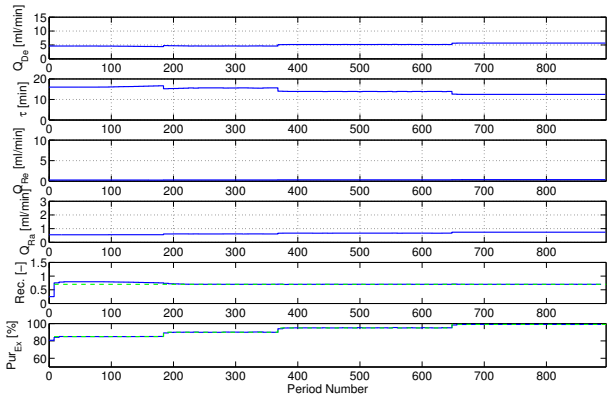

Fig. 7. Simulation II: manipulated and controlled variables

tions are at least locally qualitatively correct. In principle, the degrees of freedom of the process allow the optimizing controller to achieve the purity requirement at different operating points. Qualititavely different operating modes exist (conventional operation or breakthrough) and there is a conflict between economic optimality and robustness of operation. Forcing the process to conventional operation by adding a penalty term to the objective results in robust operation which is, however, paid for by an increased solvent consumption.

5. CONCLUSIONS

An optimizing controller for the Hashimoto SMB process was presented and the engineering of the cost function used

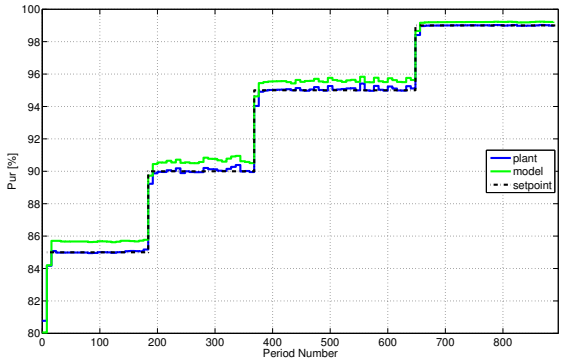

Fig. 8. Simulation II: model and plant purities and setpoint

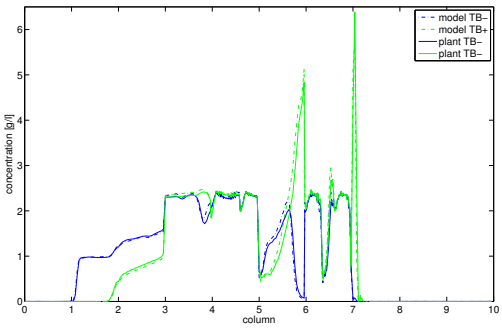

Fig. 9. Simulation II: axial concentration profiles of plant and model at the beginning of period 670

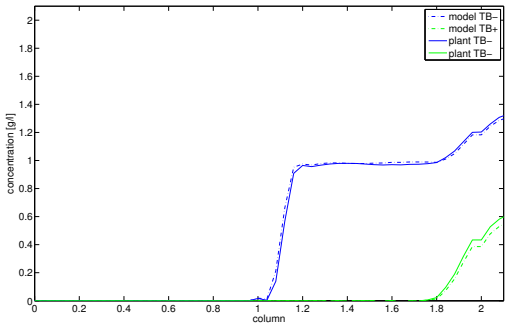

Fig. 10. Simulation II: enlarged axial concentration profiles of plant and model at the beginning of period 670

Table 1. Controller specifications

H_C	1 cycle = 8 periods
H_P	5 cycles = 40 periods
R	[0.5 0.5 0.5 0.5]
γ	0.2 (only for simulation III)

in the controller was discussed in detail. The advantage of the approach lies in the simultaneous pursuit of economical plant operation and satisfaction of product purity and recovery requirements and in the structural simplicity of the control scheme. The dynamic performance could be significantly improved by driving the plant to operating regions where the effect of plant/model mismatch is comparatively small and such that there is no change of the sign of the error feedback.

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