A FLEXIBLE NONLINEAR MODEL PREDICTIVE CONTROL SCHEME FOR QUALITY/PERFORMANCE HANDLING IN NONLINEAR SMB CHROMATOGRAPHY

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Abstract: A new state feedback scheme is proposed for the control of simulated moving beds with strongly nonlinear isotherms. The proposed scheme offers a unified framework enabling different performance criteria to be improved according to the active production constraints (achieving low cost, improving efficiency, respecting deadlines) that may unpredictably change during the production batch. The proposed scheme is illustrated through several examples showing the robustness of the closed-loop behavior against parameter uncertainties as well as its reactivity to changes in the active auxiliary criterion.

Keywords: Simulated Moving Bed, Nonlinear Predictive control.

1. INTRODUCTION

The Simulated Moving Bed **SMB** as a continuous chromatographic separation process, gains increasing importance in domains, such as food and fine chemical, where high purities of components, cannot be achieved by another separation tool with economical relative cost. The **SMB** process is realized by connecting in series several chromatographic columns to form four functional sections defined by their boundary ports see (Figure 1). These ports are outlet and inlet valves that are located between the columns and switch in the direction of the fluid flow in order to simulate the solid phase movement in opposite direction relative to the fluid phase. Ideally the solid phase is mobile, this is the case of the True Moving Bed **TMB**, however a moving solid phase is not realizable in practice due to technical limitations. The principle of separation in the binary **SMB** is

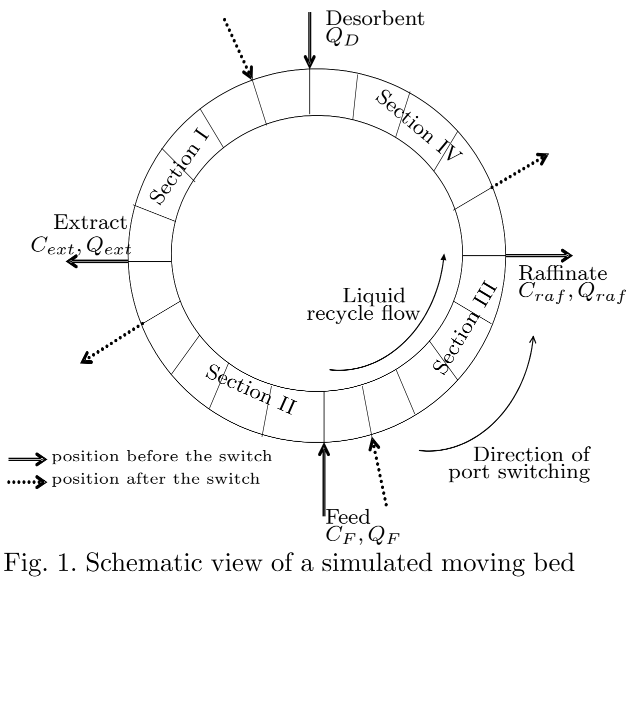

Fig. 1. Schematic view of a simulated moving bed

based on the difference of the adsorption affinities of the two components that are initially present in the feed inlet, that causes difference in the convection velocities through the sections. This results in the less adsorbed component being extracted at the raffinate outlet while the more adsorbed component is recovered at the extract outlet.

Due to its hybrid character including continuous and discrete dynamics, its operational conditions close to the optimum, its great sensitivity to operation parameters and disturbances, the control of the **SMB** process is complicated. Because of this complexity many proposed strategies use the equivalent **TMB** as an approximation, like in (Kloppenburg and Gilles, 1999) where an asymptotically input/output linearizing controller is based on this approximation which is used also in (Schramm *et al.*, 2003). Here, decoupled PI controllers are combined in order to induce slight movements of the wave fronts once a convenient and optimized cyclic regime is established. Note that when the amplitude of the set point changes considerably, the linearization based **TMB** model may be disqualified, and the high purities requirement not achieved, this renders the strategies based on the use of equivalent **TMB** inappropriate.

Due to the non convexity of the constrained optimal control problem of this process, the exact online solution of classical Nonlinear Predictive Control (NMPC) cannot be achieved; to overcome this difficulty, (Klatt *et al.*, 2002) propose a two-layers control architecture where the optimal operating trajectory is calculated off-line. A controller is then used in order to keep the process close to the optimized trajectory. But an off-line optimization strategy may be incompatible with an uncertain production scheduling. In this context and in order to overcome the difficulty of non realizable online solution and to be reactive to the probable change in the production planing, we solve the optimal control problem during the system lifetime in the sense that the iterations leading to its solution are distributed in time.

In this paper, we propose a multi-stage philosophy consisting in first achieving purities and yields requirements and then minimizing some cost function. This may be for instance the quantity of desorbant being used or the efficiency or production rate in order to meet the delivery time constraint. With this respect, (Abel *et al.*, 2003) propose a similar philosophy by using MPC scheme based on linearized equations while the present paper takes into account the **SMB** nonlinearity.

Quite similarly, a repetitive model predictive control scheme is proposed in (Seshatre and Lee, 2000) by assuming a constant switching period as it is usually taken in other existing feedback schemes; while in the present paper, the switching period is a decision variable which is a crucial feature when several auxiliary performance indexes may be used according to the production context.

The proposed feedback scheme incorporates an integrator effect to robustify the closed-loop against unavoidable parameter uncertainties, in particular, concerning the isotherm coefficients as well as the void fraction through the columns. Apart from (Kloppenburg and Gilles, 1999), few papers take the yields into account. In the present paper, the yields are explicitly used in the cost function. The paper is organized as follows : First the **SMB** modelling is recalled in section 2. The control problem is stated in section 3. Some definitions and notations are given in section 4. The proposed feedback algorithm is given in section 5 while illustrative scenarios are proposed in section 6 to assess the efficiency and underline some features of the proposed feedback scheme.

2. THE EQUATIONS OF THE SMB

Various mathematical models have been developed to describe the dynamic behavior of the chromatographic processes. (Ruthven and Ching, 1989) classify the models into three general categories : equilibrium theory, plate models and rate models. The particular model used in the forthcoming simulations is based on the use of a cascade of perfectly agitated reactors to model each single column, this belong to the plate models category. However, the feedback scheme proposed here is independent of the particular structure of the simulator. The latter is invoked by the feedback algorithm as a black box prediction tool that gives for some control profile the corresponding future evolution.

The performances of the **SMB** can be monitored by five independent variables. These are the delay $\tau_s > 0$ between switches and four flow rates that are chosen here to be as follows $U := \begin{pmatrix} Q_D & Q_{ext} & Q_F & Q_{IV} & \tau_s \end{pmatrix}^T \in \mathbb{U}$, where U denotes these decision variables and $\mathbb{U}$ denotes the compact set of possible values for which all the flow rates are positive and lower than their saturation levels.

Considering a binary **SMB** with n_c columns, the state vector $C \in \mathbb{R}_+^{2n_c}$ is obtained by concatenating $C_{a,i} \in \mathbb{R}_+^{n_c}$ and $C_{b,i} \in \mathbb{R}_+^{n_c}$ where $C_{a,i}$ [resp. $C_{b,i}$] is the concentration of species a [resp. b] in the i^{th} column. Since the system equations depend on the positions of the ports; let $\sigma \in \{1, \dots, n_c\}$ be the configuration index, say, the position of the feed inlet for instance. The evolution of σ is piece-wise constant with jumps occurring at the switching instants t_k, and assuming instantaneously reachable equilibrium between liquid and solid phases, the system equations under piecewise constant control $U(\cdot)$, that is, a control being constant between two successive switches, may be written as follows

$$\dot{C}(t) = F_{\sigma(t_k)}\Big(C(t), U(t_k), C_F(t)\Big) \quad t \in [t_k, t_{k+1}] \tag{1}$$
$$\sigma(t_k + U_5(t_k)) = [\sigma(t_k) + 1] \; mod \; (n_c) \tag{2}$$

here, $F_\sigma(\cdot)$ is the smooth convection-diffusion evolution law that holds under the configuration σ and $C_F(t)$ is the feed concentrations.

3. THE CONTROL PROBLEM

Denote by m_a^{ext} and m_a^{raf} [resp m_b^{ext} and m_b^{raf}] the mass of species a [resp b] collected at the extract [resp raffinate] ports over the operating interval $[t_0, t_0+T]$. The **SMB** operating over $[t_0, t_0+T]$ has to satisfy the following customer's order :

(1) The purity requirements :

$$\min\Big\{\frac{m_a^{ext}}{m_a^{ext}+m_b^{ext}} - p_{ext}^d, \frac{m_b^{raf}}{m_a^{raf}+m_b^{raf}} - p_{raf}^d\Big\} \geq 0 \tag{3}$$

where p_{ext}^d and p_{raf}^d are the minimal desired purities in the delivered product.

(2) The total produced quantities

$$m_a^{ext} \geq m_{ext}^d \quad ; \quad m_b^{raf} \geq m_{raf}^d \tag{4}$$

(3) The delivery deadline : $t_0 + T \leq t^d$

an optimal admissible strategy is therefore a one that meets the above requirements while minimizing some cost function. This may be the quantity of desorbent being used J_D, or alternatively, an efficiency criterion J_E, or the maximum production rate criterion J_P which is to be used when the production rate is to be maximized in order to meet the delivery time constraint. These cost functions are defined as following :

$J_D := \int_{t_0}^{t_0+T} Q_D(t)dt$; $J_E := \int_{t_0}^{t_0+T} \frac{Q_D(t)}{Q_F(t)}dt$;

$J_P := -\int_t^{t+T}\Big[Q_D + Q_F\Big]d\tau.$

4. SOME DEFINITIONS AND NOTATIONS

In order to properly define the feedback strategy, the following definitions are needed

Definition 1. (Steady mean solutions).
Given a constant profile $U(\cdot) \equiv U^0$, the corresponding steady mean solution is denoted by $\bar{C}(U^0)$, (Recall that , U_5^0 is the corresponding constant switching period), namely

$$\bar{C}(U^0) := \lim_{t\to\infty} \frac{1}{U_5^0}\int_t^{t+U_5^0} C(\tau)|_{U(\cdot)=U^0} d\tau \tag{5}$$

Definition 2. [Admissible constant profiles]
Given some positive real $\eta > 0$, $U_\eta \in \mathbb{U}$ is said to be η-admissible if the following holds

$$\Psi_{ext}(U_\eta) := \frac{\bar{C}_a^{ext}(U_\eta)}{\bar{C}_a^{ext}(U_\eta)+\bar{C}_b^{ext}(U_\eta)} - p_{ext}^d \geq \eta \tag{6}$$
$$\Psi_{raf}(U_\eta) := \frac{\bar{C}_b^{raf}(U_\eta)}{\bar{C}_a^{raf}(U_\eta)+\bar{C}_b^{raf}(U_\eta)} - p_{raf}^d \geq \eta \tag{7}$$

Hereafter, these constraints (6)-(7) are shortly written as ($J_{pur}(U_\eta, \eta) \leq 0$) where:

$$J_{pur}(U,\eta) := \eta - \min\Big\{\Psi_{ext}(U), \Psi_{raf}(U)\Big\} - \frac{\eta}{2C_F}\min\{\bar{C}_a^{ext}(U), \bar{C}_b^{raf}(U)\} \tag{8}$$

Here, the third term in (8) is a small weight term $(\leq \eta/2)$ is added to the cost function in order to take into account the concentrations of the components (the yields) at the extract and the raffinate ports.

The admissibility set can be defined equivalently as : $\mathcal{U}_\eta := \Big\{U \in \mathbb{U} \quad \text{s.t. } J_{pur}(U,\eta) \leq 0\Big\}$.

When the cost function $J_{pur}(U,\eta)$ becomes negative, it only guarantees that under the constant profile U, the purities meet the requirement after some finite time. The purity margin $\eta/2 > 0$ is used to compensate for potential "*lack of purity*" that would have been accumulated during the transient phase.

Definition 3. [Invariant admissible configuration]
The set of invariant admissible configurations $\mathcal{A}_\eta^{ad}$ is the set of all pairs $(C,U) \in \mathbb{R}^{2n_c} \times \mathcal{U}_\eta$ of initial states C and an admissible constant profile U such that for all $t \in [0,\infty]$:

$$\frac{1}{U_5}\int_t^{t+U_5} \frac{C_a^{ext}(\tau;C;U)}{C_a^{ext}(\tau;C;U)+C_b^{ext}(\tau;C;U)}d\tau - p_{ext}^d \geq \eta \tag{9}$$
$$\frac{1}{U_5}\int_t^{t+U_5} \frac{C_b^{raf}(\tau;C;U)}{C_a^{raf}(\tau;C;U)+C_b^{raf}(\tau;C;U)}d\tau - p_{raf}^d \geq \eta$$

where $C(\tau;C;U)$ is the solution at instant τ starting at $t=0$ with the initial state C.
$(C,U) \in \mathcal{A}_\eta^{ad}$ means that by applying the constant profile U, the resulting behavior satisfies the purity requirement over "*all the future*". With this respect, the following cost function is relevant :

$$J_{pur}^{inv}(C,U,\eta,T) := \min_{t\in[0,T]}\Bigg[\eta - \min\Big\{\Phi_{ext}(t), \Phi_{raf}(t)\Big\} - \frac{\eta}{2C_F}\min\{C_a^{ext}(t), C_b^{raf}(t)\}\Bigg] \tag{10}$$

where Φ_{ext} and Φ_{raf} are the l.h.s of the equations (9). Note that for sufficiently high T, the cost function J_{pur}^{inv} may be used to characterize the invariant admissible profiles set $\mathcal{A}_\eta^{ad}$ as follows $\Big\{(C,U) \in \mathcal{A}_\eta^{ad}\Big\} \Leftrightarrow \Big\{J_{pur}^{inv}(C,U,\eta,T) \leq 0\Big\}$ this results from the open-loop stability of the mean behavior over switching periods.

Definition 4. [Deadline-compatible constant profiles] Given a deadline t^d, for all $t \in [t_0, t_d[$ and all $\eta > 0$, a deadline-compatible constant profile is an admissible constant profile that meets the delivery deadline, namely :

$$\mathcal{U}_d(t,\eta) := \Big\{U \in \mathcal{U}_\eta \quad | \quad t + \Delta T_{ach}(C(t),U) \leq t^d\Big\} \quad (11)$$

where $\Delta T_{ach}(C(t),U)$ is the time necessary for the quality and the production requirement (3)-(4) to be achieved

5. THE PROPOSED FEEDBACK SCHEME

The control algorithm may be described as follows:

(1) **Initial data** : The production starts at $t = 0$ to satisfy an order defined by the quality parameters p_{ext}^d and p_{raf}^d, the total quantities to be produced m_{ext}^d and m_{raf}^d and the delivery deadline t^d. Let some initial security margin $\eta_0 > 0$ be given as well as some initial constant control profile $U(\cdot) = U^0$. Put the switching period index $k = 0$ and the initial switching instant $t_k = t_0 = 0$. Put $i = 1$.

(2) **During the switching period** $[t_k, t_k + U_5^k[$ The switching period being given by U_5^k, the constant flow rates $U(\cdot) \equiv U_{1,\dots,4}^k$ are applied over the switching period $[t_k, t_{k+1} := t_k + U_5^k[$. During this switching period, computations are done to find the control profile to be applied during the next switching period $[t_{k+1}, t_{k+1} + U_5^{k+1}]$. In order to do this, a prediction $\hat{C}(t_{k+1})$ is first computed by simulating the model starting from $C(t_k)$ under the constant control $U_{1,\dots,4}^k$. Two main situations are to be distinguished for which, different classes of updating policies are applied :

(a)- $(C(t_k), U^k) \notin \mathcal{A}_\eta^{ad}$: here, the system has not yet reached an invariant admissible configuration and U^k is improved in the sense of decreasing J_{pur} [see (8)]. Consequently, U^{k+1} is obtained by performing a given number of steps of some minimization subroutine starting from U^k as initial guess. This can be formally written as follows

Make N **iterations**

$(\alpha_i^{(k+1)}, U^{k+1}) \leftarrow \text{Improve}(J_{pur}, U^k, \alpha_i^{(k)}, i)$

$i \leftarrow (i+1)\ mod\ 5$

end

where i is the index of the component of U being updated while α_i is a corresponding trust region parameter, which is a kind of variation of the U^k admissible interval values, in order to find the global optimum while avoiding the local ones. Note that since J_{pur} cannot be indefinitely improved, the control profile becomes constant after a finite number of iterations and since the system is open-loop stable, an invariant admissible configuration is reached (provided that the purity requirements are achievable). The situation (b) hereafter is then "*fired*".

(b)- $(C(t_k), U^k) \in \mathcal{A}_\eta^{ad}$: now, an admissible configuration is reached that is invariant under U^k. However, better control profiles may improve the production cost, the efficiency or the possible delivery time. The choice of the cost function to be considered depends on the context. Regardless of the context, the principle is the following :

The decision variables are split into two categories, namely $U := \bigotimes_{i \in I_p \cup I_a} U_i \quad ; \quad I_p, I_a \subset \{1, \dots, 5\}$ where, I_p is the set of indexes of decision variables that are used to create purity margin by minimizing J_{pur}^{inv}. This margin enables the other decision variables indexed by I_a and called the auxiliary optimizing variables to decrease some auxiliary function J_a, for instance J_D, J_E or J_P defined above. More precisely, two situations may occur :

(i)- Either $U^k \in \mathcal{U}_d(t_k, \eta)$ in which case, the delivery deadline can be respected, therefore, auxiliary optimization may be focused on production cost. This is done hereafter by taking $J_a := Q_D$; with $\bigotimes_{i \in I_a} U_i = Q_D$; $I_a := \{1\}$. Alternatively, one may be interested in maximizing efficiency by taking $J_a := \frac{Q_D}{Q_F}$; with $\bigotimes_{i \in I_a} U_i = (Q_D, Q_F)^T, I_a := \{1,3\}$

(ii)- Or $U^k \notin \mathcal{U}_d(t_k, \eta)$ in which case cost consideration is temporarily dropped in favor of maximizing the production rate. In this case, one takes $J_a := -(Q_D + Q_F)$ with $\bigotimes_{i \in I_a} U_i = (Q_D, Q_F)^T;\ I_a := \{1,3\}$ The computations to be performed when $(C(t_k), U^k) \in \mathcal{A}_\eta^{ad}$ can now be given as follows

Make N **iterations**

$(\alpha_i^{(k+1)}, U^{k+1}) \leftarrow \text{Improve}(J^{(i)}, U^k, \alpha_i^{(k)}, i)$

under the constraint $(C(t_{k+1}), U^{k+1}) \in \mathcal{A}_\eta^{ad}$

and $U^{k+1} \in \mathcal{U}_d(t_{k+1}, \eta)$ if $U^k \in \mathcal{U}_d(t_k, \eta)$

$i \leftarrow (i+1)\ mod\ 5$

end

where $\quad J^{(i)} := \begin{cases} J_a & \text{if} \quad i \in I_a \\ J_{pur}^{inv} & \text{otherwise} \end{cases}$

A schematic view of the control philosophy is depicted on (Figure 2). Namely, at a first stage, all decision variables are used to decrease the cost function J_{pur}. As soon as J_{pur}^{inv} becomes negative, the decision variables with indices in I_p are used to create purity margin enabling those with indices in I_a to decrease the auxiliary cost.

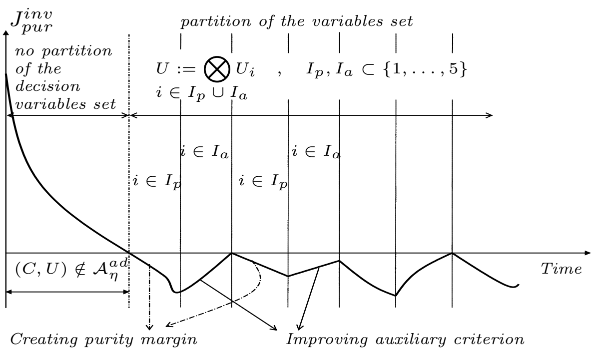

Fig. 2. Schematic view of the control algorithm

The integrator effect is introduced in order to robustify the closed-loop against the variables uncertainties. For, note that under free-uncertainty context and for sufficiently long prediction horizon, the property $J_{pur}^{inv} \leq 0$ is invariant, if J_{pur}^{inv} changes its sign from negative to positive, one must deduce that there are errors on the parameters used in the prediction. In such a case, the purity margin η must be increased in order to guarantee the purity requirements achievement. That is why whatever is the active configuration ($C(t_k, U^k) \in \mathcal{A}_\eta^{ad}$ or not) the following updating rule is used for η_k:

$$
\begin{aligned}
&\textbf{if } \left(J_{pur}^{inv}(k) > 0 \textbf{ and } J_{pur}^{inv}(k-1) \leq 0 \right) \textbf{ then} \\
&\qquad \eta_k \leftarrow \eta_k + \delta_\eta \\
&\textbf{Else} \\
&\qquad \eta_k \leftarrow \max\{\eta_{min}, \gamma \eta_{k-1}\} \quad ; \quad \gamma < 1 \\
&\textbf{Endif}
\end{aligned}
\tag{12}
$$

This decreasing rule aims to restore the initial margin when an increasing step has been fired by a transient disturbance.

6. ILLUSTRATIVE SIMULATIONS

The simulation was done by taking 5 columns in each section, each column is modelled by 4 reactors in series. A Langmuir nonlinear isotherm is used with constants $K_1 = 0.56$ and $K_2 = 0.2$. The diffusion coefficient is taken equal to the one used in (Klatt *et al.*, 2002) as well as the section area, length and void fraction of a columns, namely : $L = 53,6\ cm$; $\epsilon = 0.45$; $V = 2281\ cm^3$; where V is the total volume of the apparatus. Consequently, a system of 160 first order ODE is obtained that is solved by LSODA implemented in FORTRAN 90 code. As controller parameters, the saturation level $U_i^{max} = 0.15\ cm^3 s^{-1}$ on the flow rates is used. The number of iterations per switching period $N = 1$ is applied in order to carry on to its limit the distributed in time optimization principle. Note that the control scheme needs no initially optimized configuration to be available.

6.1 Simulations

Three different scenarios have been simulated, in the first one, a first step $y_d = (0.97, 0.97)$ is applied and after 150 switching periods, a step change is applied to require purities $y_d = (0.985, 0.985)$ (Figure 3). The corresponding flow rates evaluations are illustrated in (Figure 4), while the (Figure 5) shows the related switching period behavior. Note in particular that the initial values of the flow rates was not appropriate. This can be particularly seen on the J_{pur} evolution (Figure 6) where it can be observed that the initial value of J_{pur} is highly positive indicating that the mean steady state regime corresponding to the initial values of the flow rates and the switching time (the control U) does not satisfy the purity requirement $y_d = (0.97, 0.97)$. The auxiliary cost function J_a used in this experiment is $J_a = Q_D/Q_F$. (Figure 7) shows the role of the yield related weighting term in (8) in increasing the corresponding yield. The cyclic behavior as well as the corresponding mean values of the component (**a**) *"for example"*, are shown in (Figure 7).

In the second scenario, at $k = 150$, an unmeasured (-10%) step change in the void fraction ϵ (Figure 9) and unmeasured $(+15\%)$ step changes in the Langmuir coefficients K_1 and K_2 (Figure 8) are applied in order to test the robustness of the closed-loop system to parameter uncertainties. In the two related figures the feedback enables the purity requirement to be achieved while an open-loop control would fail.

The last scenario concerns the case where a delay in delivery time may occur and causes heavy penalties, here the production rate has to be accelerated. The results are shown on (Figure 10) that is to be compared with the first 150 switches of the first scenario see (Figure 3) where the same desired purities are required. (Figure 11), shows clearly how the related auxiliary cost function $J_a := Q_D + Q_F$ is maximised in order to meet the delivery deadline.

7. CONCLUSION

A nonlinear model predictive control is proposed for the control of a highly nonlinear SMB process. The key feature of the proposed scheme is that the optimization is distributed on the plant life-time. Furthermore, several performance indexes may be easily handled and on-line changed according to the production scheduling context. Simulations show good robustness of the closed-loop system against uncertainties on the system parameters

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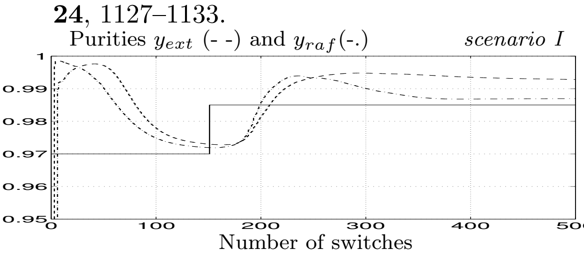

Fig. 3. Response of the controlled SMB to a step change of the desired purities y_d. y_d changes at $k = 150$ from $(0.97, 0.97)$ to $(0.985, 0.985)$

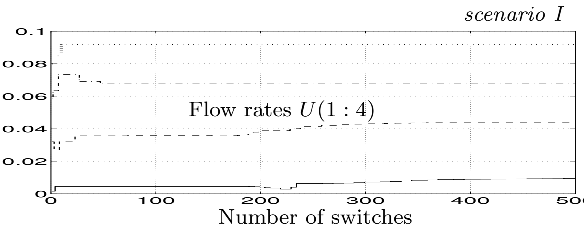

Fig. 4. The evolution of the control variables in response to the step change from $(0.97, 0.97)$ to $(0.985, 0.985)$

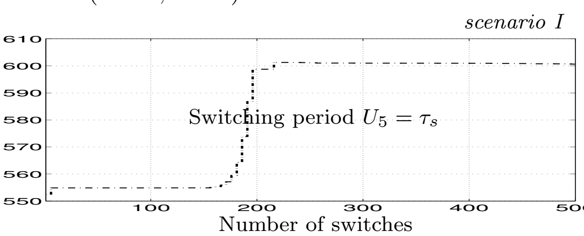

Fig. 5. The evolution of the switching time in response to the step change from $(0.97, 0.97)$ to $(0.985, 0.985)$

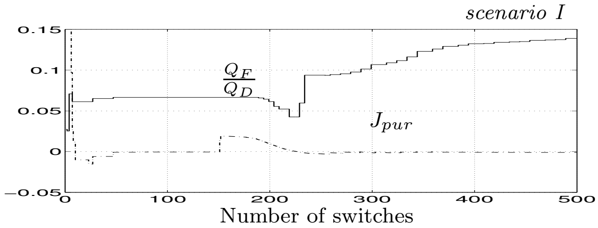

Fig. 6. The evolution of the cost functions in response to the step change from $(0.97, 0.97)$ to $(0.985, 0.985)$

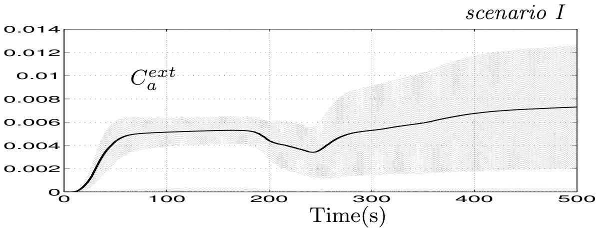

Fig. 7. The yields evolution

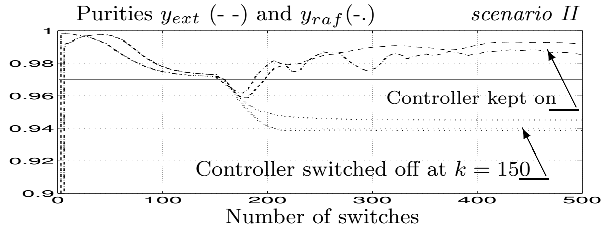

Fig. 8. Response of the controlled/uncontrolled SMB to a unmeasured +15% step change of the Langmuir coefficients

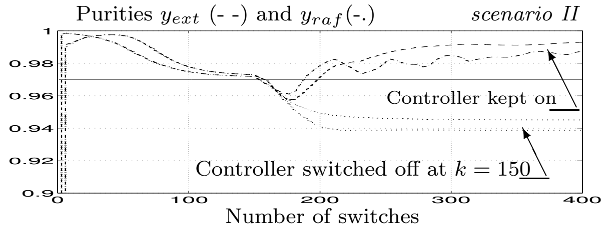

Fig. 9. Response of the controlled/uncontrolled SMB to a unmeasured -10% step change of the void fraction

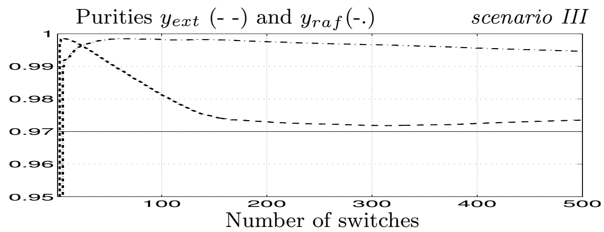

Fig. 10. Response of the controlled SMB to a step $y_d = 0.97$ under the maximum production rate constraint

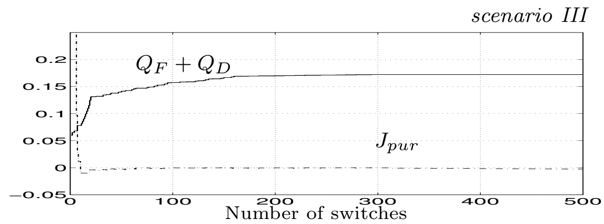

Fig. 11. The evolution of the cost functions under the maximum production rate constraint