# A NONLINEAR OBSERVER FOR CONCENTRATION PROFILES IN SIMULATED MOVING BED

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Abstract: In this paper, a state observer is proposed for the reconstruction of the concentration profiles in a simulated moving bed. The approach is based on a simple Luenberger-like correction term. Validating simulations are proposed to assess the efficiency of the proposed profile reconstruction and its robustness against uncertainties on modelling parameters. Comparisons are also done with open-loop simulation based-observer in order to strengthen the relevance of the correction term. 

Keywords: State observer; Nonlinear; Process control; Robust Estimation; Large Scale Systems.

## 1. INTRODUCTION

The Simulated-Moving-Bed (SMB) is an efficient counter-current separation process that is extensively used in the process industry. The SMB has been studied in the literature concerning different aspects including design, modelling and simulation (Charton and Nicoud, 1995; Dnnebier and Klatt, 2000; Ludemann-Hombourger and Nicoud, n.d.), optimization for selection of optimal operating conditions and respect of operating constraints (Mazzotti *et al.*, 1997; Couenne *et al.*, 2002) and control using multivariable linear constrained control (Couenne *et al.*, 2002), model-based control (Natarajan and Lee, 2000; Klatt *et al.*, 2002), nonlinear geometric control (Kloppenburg and Gilles, 1999).

Papers concerning the design of observers for the SMB are less common though it is an important issue. In, (Mangold *et al.*, 1994) a state observer is proposed based on the linearized model. In this approach however, the observer's gain is computed by heuristic approach based on physical considerations and simulation studies.

A very different observer is developed by (Kleinert and Lunze, 2003). Here, only the stationary regime which results in a periodic behaviour of the SMB is considered. The model includes convection and diffusion and the binary system is described by a linear isotherm. A simple three-dimensional parameterization of a wave form is proposed and used to build a corresponding low dimensional state observer in which the states are the wave parameters.

In (Alamir and Corriou, 2003), a nonlinear receding horizon estimation scheme with adjustable precision is proposed. The scheme approximates the concentration profiles over a suitable truncated functional basis. The resulting vector of unknowns is first reduced using available measurements. The remaining part is then computed by nonlinear optimization. The scheme is conceptually very general. However, in order to achieve high precision estimation, high dimensional optimization problems have to be invoked that may be difficult to solve in real time.

In this paper, an estimation scheme is proposed that is dedicated to processes in which the main phenomena are linear and where nonlinearities are present but as second order terms (this is typically the case of many SMB processes with nonlinear isotherms).

The paper is organized as follows: the estimation scheme is first presented in section 2 in a general context. The SMB equations are recalled in section 3 and the way they can be put in the general form of section 2 is detailed. Finally, illustrative simulation results are proposed in section 4 in order to assess the efficiency of the proposed scheme in estimating the concentration profiles in the the columns despite significant errors in the system's parameters knowledge.

## 2. THEORETICAL BACKGROUND

### *2.1 definition of the class of systems*

Consider a nonlinear system given by :

$$\dot{x}(t) = A(u(t_{k-1}))x(t) + B(u(t_{k-1}))w(t) + \\ +\phi(x(t), u(t_{k-1}), w(t)) \quad ; \quad t \in ]t_{k-1}, t_k] \quad (1)$$

$$x(t_k^+) = Mx(t_k) \quad (2)$$

$$y(t) = H(u(t_{k-1}))x(t) \quad (3)$$

where $x \in \mathbb{R}^n$ is the state of the system; $y$ is the measured output; $u$ is a piece-wise constant control input while $w$ is a measured exogenous signal. $(t_k)_{k\geq 0}$ is a strictly increasing sequence of switching instants w.r.t which the piece-wise constant control $u$ is defined. $x(t_k^+)$ stands for the state "*just after*" instant $t_k$ in order for (2) to define a jump on the state arising at instant $t_k$. The control input $u$ and the measured exogenous signal $w$ are assumed to belong to two compact sets respectively denoted by $\mathcal{U}$ and $\mathcal{W}$. Namely :

$$\forall t \in \mathbb{R}_+ \quad ; \quad (u(t), w(t)) \in \mathcal{U} \times \mathcal{W} \quad (4)$$

furthermore, the following assumptions are needed :

**Assumption 1.** The nonlinear term in (1) is globally Lipschitz as a function of $x$ uniformly in $u$ and $w$. More precisely, there is a constant $K_\phi > 0$ such that $\forall (u, w) \in \mathcal{U} \times \mathcal{W}$

$$\|\phi(x_1, u, w) - \phi(x_2, u, w)\| \leq K_\phi \cdot \|x_1 - x_2\| \quad (5)$$

**Assumption 2.** There exists a positive real $\tau_{min}$ such that $\forall k, \quad t_{k+1} - t_k \geq \tau_{min}$

**Assumption 3.** For all $u \in \mathcal{U}$, the pair $(A(u), H(u))$ is observable. Moreover, there exists a positive real $\mu > 0$ such that for all $u \in \mathcal{U}$, there exists a positive definite matrix $Q(u)$ and a matrix gain $L(u)$ such that the following conditions hold

(1) for all $u \in \mathcal{U}$ :

$$-\lambda_{min}(Q(u)) + 2K_\phi\|P(u)\| \leq -\mu \quad (6)$$

where $P(u)$ is the solution of the Lyapunov equation :

$$\Big[A(u) - L(u)H(u)\Big]^T P(u) \\ +P(u)\Big[A(u) - L(u)H(u)\Big] = -Q(u) \quad (7)$$

(2) for all $u \in \mathcal{U}$ there exists a positive $\gamma > 0$ such that :

$$\mathcal{C}(\mathcal{U}) \cdot \lambda^2_{max}(M) \cdot e^{-\mu\tau_{min}/\lambda_{max}(P(u))} \leq \gamma < 1 \quad (8)$$

where $\mathcal{C}(\mathcal{U})$ is the positive real defined by

$$\mathcal{C}(\mathcal{U}) := \sup_{(u_1,u_2)\in\mathcal{U}\times\mathcal{U}} \left[\frac{\lambda_{max}(P(u_1))}{\lambda_{min}(P(u_2))}\right] \quad (9)$$

(3) There is a positive definite matrix $P_0 > 0$ such that

$$\forall u \in \mathcal{U}, \quad P(u) \geq P_0 > 0 \quad (10)$$

### *2.2 Observer's definition*

In order to estimate the state of the dynamical system (1)-(3), the following observer is used

$$\dot{\hat{x}}(t) = A(u(t_{k-1}))\hat{x}(t) + B(u(t_{k-1}))w(t) + \\ +\phi(\hat{x}(t), u(t_{k-1}), w(t)) + \\ +L(u(t_{k-1}))\Big[y(t) - H(u(t_{k-1}))\hat{x}(t)\Big] \quad (11)$$

$$\hat{x}(t_k^+) = M\hat{x}(t_k) \quad (12)$$

The following proposition can then be proved (see the appendix) :

**Proposition 1.** Under assumptions 1-3, the dynamic system (11)-(12) is an asymptotic dynamic observer for the switched nonlinear system (1)-(3).

## 3. APPLICATION TO THE SMB

### *3.1 Model*

The SMB has been modeled by the following partial differential equations (Dnnebier *et al.*, 1998) representing respectively the mass balance for component $i$ and the mass transfer from the liquid phase to the solid phase

$$\frac{\partial c_i}{\partial t} + \frac{1-\epsilon}{\epsilon}\frac{\partial q_i}{\partial t} - D_{ax}\frac{\partial^2 c_i}{\partial x^2} + v\frac{\partial c_i}{\partial x} = 0 \\ \frac{\partial q_i}{\partial t} = k_{eff,i}\frac{3}{R_p}(c - c_i^{eq}) \tag{13}$$

where $c_i$ and $q_i$ are respectively the concentrations in the liquid and solid phase, $\epsilon$ is the porosity, $D_{ax}$ is the apparent dispersion coefficient, $v$ the fluid velocity in given section, $R_p$ the adsorbent particle radius, $k_{eff,i}$ the mass transfer coefficient, $c_i^{eq}$ the equilibrium concentration. The binary system is described by a competitive Langmuir nonlinear isotherm

$$q_i = \frac{N_i K_i c_i}{1 + \sum_{j=1}^{n_c} K_j c_j} \tag{14}$$

with $N_i$ the saturation loading capacity of component $i$ and $K_i$ the Langmuir equilibrium constant. The values of the parameters used in the simulation are given in Table 1.

Table 1. Values of the parameters for SMB simulation.

| System parameters | | | |
|---|---|---|---|
| $D$ | 5 cm | $L$ | 50 cm |
| $\epsilon$ | 0.4 | $D_{ax}$ | $3\times10^{-2}$ cm$^2$/s |
| $K_A$ | 1500 cm$^3$/g | $K_B$ | 2000 cm$^3$/g |
| $N_A$ | 5 | $N_B$ | 5 |
| $k_{eff,A}$ | $3\times10^{-4}$ cm/s | $k_{eff,A}$ | $2.5\times10^{-4}$ cm/s |
| **Operating parameters** | | | |
| Feed concentration $c_{f,i}$ | | $5\times10^{-4}$ g/cm$^3$ | |
| Feed flow rate $Q_f$ | | 5.62 cm$^3$/s | |
| Desorbent flow rate $Q_D$ | | 100.644 cm$^3$/s | |
| Extract flow rate $Q_E$ | | 75.14 cm$^3$/s | |
| Recycle flow rate $Q_{IV}$ | | 103.56 cm$^3$/s | |
| Switching period $t_{switch}$ | | 30 s | |

### 3.2 Obtaining the canonical form (1)-(3)

After noticing that the mass transfer equation can be neglected with very little error and using classical finite difference discretization, the system equations become

$$E(c)\dot{c} = F(u)c + G(u)c_f \tag{15}$$

where $c_f$ is the feed concentration which is a measured exogenous signal. $m$ being the number of discretization elements, the chemical system being binary, the vector $c$ has dimension $2m$ and is formed by the successive vectors $[c_{A,i}, c_{B,i}]$ where $i$ is the index of a spatial element. $F(u)$ and $G(u)$ depend on the flow rates and thus on the manipulated inputs $u$. The matrix $E(c)$ can be easily inverted resulting in

$$\dot{c} = E^{-1}(c)F(u)c + E^{-1}(c)G(u)c_f \tag{16}$$

Then, $E^{-1}(c)$ is decomposed into two contributions, one equal to $E^{-1}(c=0)$ and denoted by $E_0^{-1}$, the other one depending on $c$ and is equal to $[E^{-1}(c) - E^{-1}(c=0)]$ and denoted by $E_c^{-1}$, so that the system becomes

$$\dot{c} = E_0^{-1}F(u)c + E_c^{-1}F(u)c + E^{-1}(c)G(u)c_f \tag{17}$$

with a linear term, a nonlinear term and one disturbance terms.

The matrix $M$ representing the shift operation is easily obtained from the representation of the vector $c$ just before and after the shift

$$c^+ = Mc^- \tag{18}$$

The measured outputs are the concentrations $c_A$ and $c_B$ at the different streams of the SMB, i.e. the extract, the inlet of section III, the raffinate and lastly the recycle or outlet of section IV. Furthermore, the measurements are assumed to be instantaneous. From this definition of the outputs, the matrix $H$ is deduced.

To summarize, the system can be put in the general form (1)-(3) with the following definitions (with $x = c$ and $w = c_f$)

$$A(u) = E_0^{-1}F(u) \quad ; \quad \phi(x,u) = E_c^{-1}F(u)c \\ B(u) = E_0^{-1}G(u) + E_c^{-1}G(u)$$

### 3.3 Some implementation issues

The computation of the observer gain $L(u)$ that is used in the observer equations (11) has been done using the dual linear quadratic regulator design [1] with some suitably chosen weighting matrices $Q_{Reg} \in \mathbb{R}^{160\times160}$ and $R \in \mathbb{R}^{8\times8}_{Reg}$. This enables to find $L(u)$ such that the Lyapunov equation (7) is satisfied with $Q$ given by

$$Q(u) = Q_{Reg} + L(u)R_{reg}L(u)^T$$

This is possible if the pair $(A(u), H)$ is observable which has been tested for some hyper-cube centered on some nominal value of the flow rates corresponding to good separation regime.

## 4. SIMULATION RESULTS

In all simulations, the states of the process are initially equal to zero. At time zero, the model

[1] This has been done using the Matlab's subroutine LQR in which the matrices $A^T(u), H^T, Q_{Reg}$ and $R_{Reg}$ have been used.

of the process starts but the observer starts only after three switching periods and starts with non-zero initial estimated states.

Different scenarii have been successively tested to check the influence of various model errors and of measurement noises following the normal law, as well as the influence of the correction term in the observer. The chosen times were the end of the 1st switch corresponding to a time close to initialization, the end of the 8th switch to an intermediate time, the end of the 30th switch to a time when normally the stationary regime is established.

The spatial profiles of real and estimated components show that in absence of of any noise or modeling errors are shown on figure 1. The model errors have various influences on the estimated spatial profile. In Figure 2, it appears that the errors on the equilibrium coefficients influence the estimated states more than the errors on the flow rates or on the feed concentration. However, in spite of relatively large errors on all these parameters, the states are correctly estimated. The influence of the correction term of the observer is clearly demonstrated in Figure 3. In the absence of this correction term, after 30 switches, the deviation between the real and the estimated profiles is considerable and the presence of this correction term is necessary.

The convergence has been shown for a point of a wave front located at mid-distance between two measurements in the third section. In the absence of model errors, the observer with correction term converges in approximately three switching periods towards the real state (Figure 4.(a)) while the free-correction term simulation based observer converges much more slowly since about 10 switching periods are necessary for the estimated profiles to converge to the real ones (Figure 4.(b)).

Finally figure 5 enables to appreciate the noise level by showing the behavior of the feed point measurements and the corresponding estimation under several modelling errors.

## Appendix A. APPENDIX

### A.1 *Proof of proposition*

Using $e$ to denote the estimation error, namely

$$e(t) = x(t) - \hat{x}(t) \tag{A.1}$$

direct computation leads to the following error dynamics

$$\dot{e}(t) = \Big[A(u(t_{k-1})) - L(u(t_{k-1}))H(u(t_{k-1}))\Big]e(t) + \\ +\phi(x(t), u(t_{k-1}), w(t)) - \phi(\hat{x}(t), u(t_{k-1}), w(t)) \quad \text{(A.2)}$$

$$e(t_k^+) = Me(t_k) \tag{A.3}$$

Using the notation $V(e,u) = e^T P(u)e$, one can write for all $t \in [t_{k-1}^+, t_k[$ using (7)

$$\dot{V}(e(t), u(t_{k-1})) \leq \Big[-\lambda_{min}(Q(u(t_{k-1}))) \\ +2K_\phi \cdot \|P(u(t_{k-1}))\|\Big]\|e(t)\|^2 \quad \text{(A.4)}$$

hence, by virtue of (6), it comes that for all $t \in [t_{k-1}^+, t_k]$

$$\dot{V}(e(t), u(t_{k-1})) \leq -\frac{\mu}{\lambda_{max}(P(u(t_{k-1})))}V(e(t), u(t_{k-1}))$$

therefore

$$V(e(t_k, u(t_{k-1}))) \leq e^{-\mu\tau_{min}/\lambda_{max}(P(u(t_{k-1})))} \cdot \\ \cdot V(e(t_{k-1}^+, u(t_{k-1}))) \quad \text{(A.5)}$$

Let us now compute $V(e(t_k^+), u(t_k))$ . By definition, one has

$$V(e(t_k^+), u(t_k)) := e^T(t_k)M^T P(u(t_k))Me(t_k) \\ \leq \lambda_{max}^2(M)\lambda_{max}(P(u(t_k)))\|e(t_k)\|^2 \\ \leq \lambda_{max}^2(M)\lambda_{max}(P(u(t_k)))\frac{V(e(t_k), u(t_{k-1}))}{\lambda_{min}(P(u(t_{k-1})))}$$

and using (A.5), one obtains

$$V(e(t_k^+), u(t_k)) \leq \lambda_{max}^2(M)\mathcal{C}(\mathcal{U}) \cdot \\ e^{-\mu\tau_{min}/\lambda_{max}(P(u(t_{k-1})))} \cdot V(e(t_{k-1}^+, u(t_{k-1})))$$

which, by virtue of (8) gives

$$V(e(t_k^+), u(t_k)) \leq \gamma \cdot V(e(t_{k-1}^+, u(t_{k-1})))$$

therefore, according to assumption (10)

$$\lim_{k\to\infty} e^T(t_k^+)P_0 e(t_k^+) \leq \lim_{k\to\infty} V(e(t_k^+), u(t_k)) = 0$$

and since $P_0$ is positive definite, it comes that

$$\lim_{k\to\infty} e(t_k^+) = 0$$

This together with the consistency if the observer equation and the continuity of the jump map clearly prove the result. $\diamondsuit$

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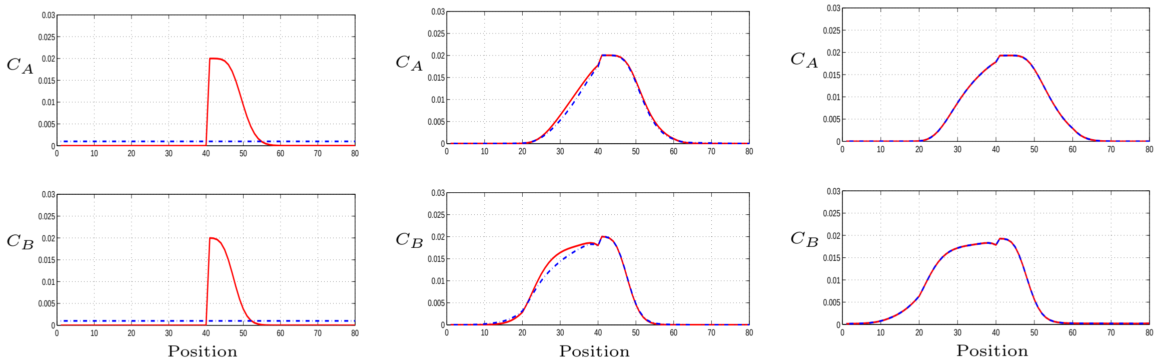


Fig. 1. Spatial profiles of component A (top) and B (bottom) in the SMB at the end of the 1st, 8th and the 30th switching periods. Continuous line (real states), dashed line (estimated states). (Conditions: no measurement noise, no model errors, **correction term in the observer**).

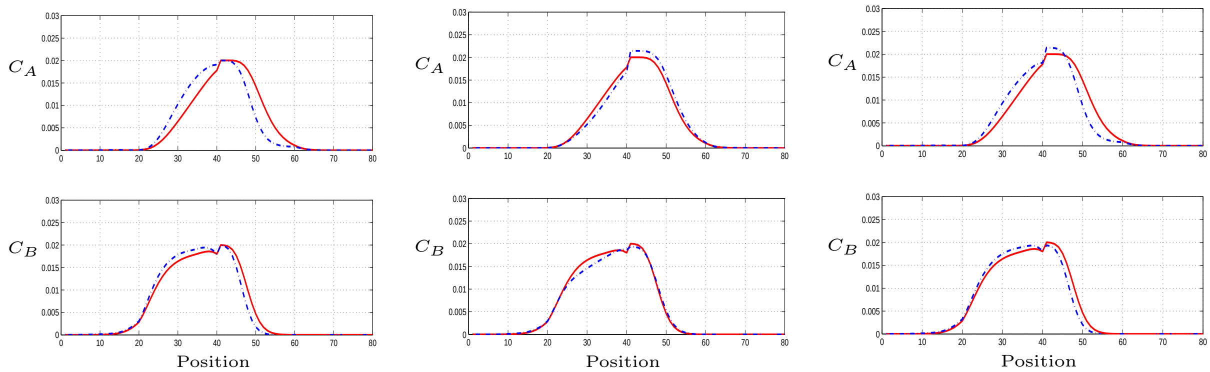


Fig. 2. Influence of various modelling errors on the spatial profiles of component A (top) and B (bottom) in the SMB at the end of the 8th switching period. Continuous line (real states), dashed line (estimated states). In all cases, measurement normal noise ($\sigma = 0.25$) and **correction term in the observer**. (Left conditions: model errors on the equilibrium constants $K_i$ and $N_i$ (5%), correction term in the observer). (Middle conditions: model errors on the flow rates (±5%) and the feed concentration (±5%), correction term in the observer). (Right conditions: model errors on the equilibrium constants $K_i$ and $N_i$ (5%), the flow rates (±5%) and the feed concentration (±5%)) .

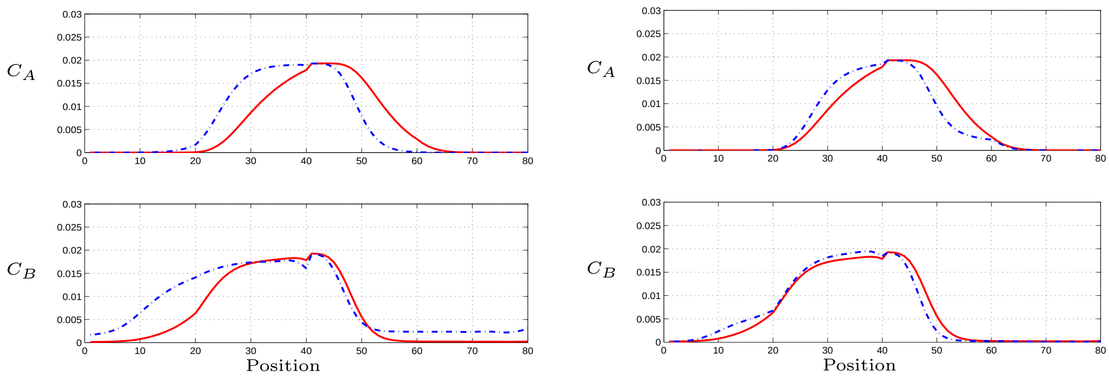


Fig. 3. Influence of the correction term of the observer on the spatial profiles of component A (top) and B (bottom) in the SMB at the end of the 30th switching period. Continuous line (real states), dashed line (estimated states). In both cases, measurement normal noise ($\sigma = 0.25$), model errors on the equilibrium constants $K_i$ and $N_i$ (5%). (Left conditions: **no correction term in the observer**). (Right conditions: **correction term in the observer**).

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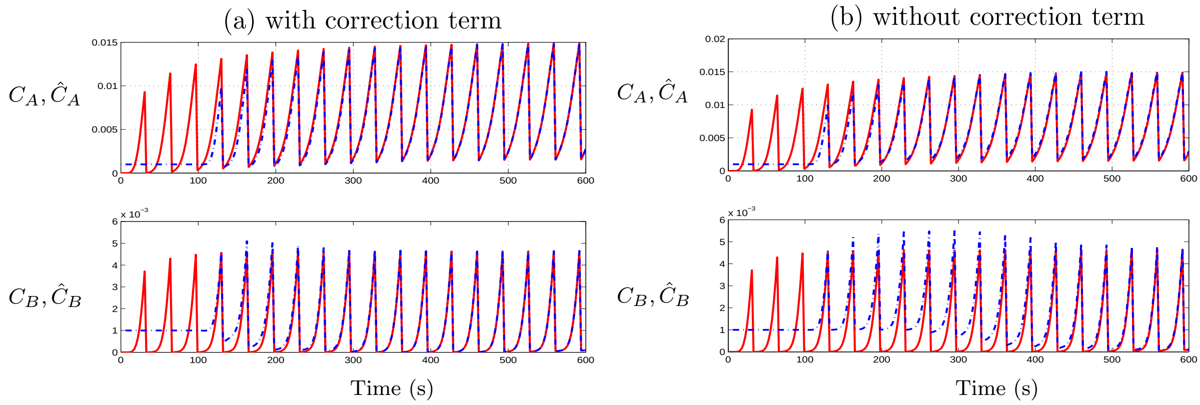


Fig. 4. Convergence of the observer for a point located at middle of section III of the SMB for components A (top) and B (bottom). Continuous line (real states), dashed line (estimated states). (Conditions: no measurement noise, no model errors, **(a) correction term included in the observer. (b) Correction term is not included**).

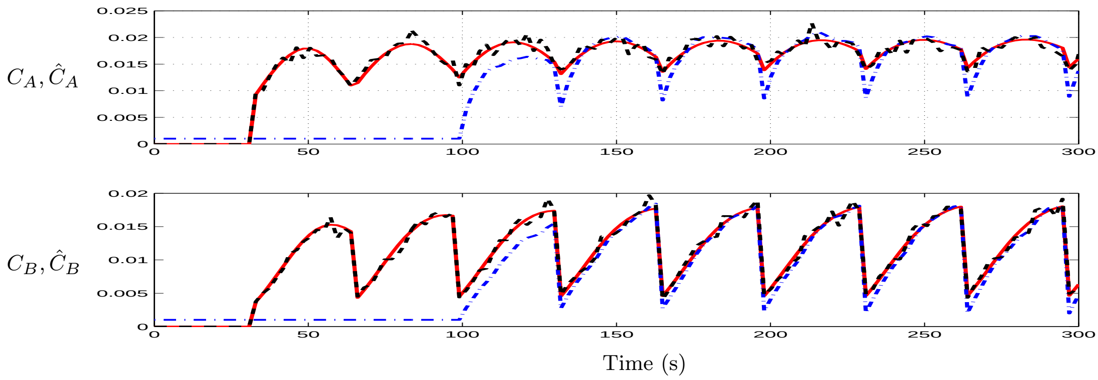


Fig. 5. Convergence of the observer for the feed point of the SMB for components A (top) and B (bottom). Continuous line (real states), dashed-point line (estimated states), dashed line (measurements). (Conditions: measurement normal noise ($\sigma = 0.25$), model errors on the equilibrium constants $K_i$ and $N_i$ (5%), the flow rates (±5%) and the feed concentration (±5%), **correction term included in the observer**

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