MODELLING AND STATE OBSERVATION OF SIMULATED MOVING BED PROCESSES

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Abstract

State observation of distributed parameter systems pose the problem of coping with the infinite state dimension of the process models. In addition to this difficulty, the dynamics of Simulated Moving Bed (SMB) processes is described by partial differential equations which are governed by switching initial conditions or switching boundary conditions, respectively. Furthermore, due to the setup of SMB plants only limited measurement information of the process behaviour is available. To overcome these difficulties, a model of the wave fronts of the SMB concentration profiles is derived which comprises a linear time–variant discrete–time state–space model describing the form, position and propagation of the wave fronts. A new approach to the solution of the state observation problem is proposed which is based on this model. Simulations of a closed–loop controlled SMB process are presented to show the applicability of the developed observer in the surrounding of the stationary operating point.

1 Introduction

The Simulated Moving Bed (SMB) technique is a continuous chromatographic separation principle for binary mixtures based on the counterflow between the solvent and adsorbent. The counterflow is simulated by stepwise moving the inlet and outlet ports on a circle of separation columns in the direction of the solvent flow. The states of SMB units are the distributed time-varying concentrations $c_A(t,z)$ and $c_B(t,z)$ of the mixture components A and B. The distributed states have the form of bell curves which move in a certain distance relative to each other through the circle of separation columns. Because both purely discrete and purely continuous signals occur on an SMB process, the system has hybrid dynamical behaviour [3].

In the recent years, closed-loop control of SMB processes has received considerable attention [1], [4], [6]. The control problem is difficult to solve because of the complexity of the process and the limited measurement information. In SMB units, a concentration measurement is only possible between the separation columns. Furthermore, measurement units providing precise values of the single concentrations are very expensive. A possible solution is to apply single column analytic chromatography. However, due to the batch nature of the technique, only discrete–time measurements are possible. The problem posed by this restriction with respect to process modelling and state observation is addressed in this paper: An SMB process is considered in the stationary state. It is assumed that the dynamical behaviour of $c_A(t,z)$ and $c_B(t,z)$ can be described by means of the convection–diffusion equation. Only selected measurements $c_A(t_m,z_m)$ and $c_B(t_m,z_m)$ at discrete times t_m and positions z_m are available. The task is to determine the shape, the position and the propagation velocity of $c_A(t,z)$ and $c_B(t,z)$.

This task is considered as an observation problem. Note, that only the wave fronts of the concentration curves $c_A(t,z)$ and $c_B(t,z)$ are of interest for SMB control purposes. Approximating $c_A(t,z)$ and $c_B(t,z)$ with the solutions of the true counterflow (True Moving Bed, TMB) process model based on the convection–diffusion equation shows, that the wave fronts of $c_A(t,z)$ and $c_B(t,z)$ belong to a certain class of curves. The shape, position and spatial shift of this class is described by three parameters.

Interpreting these parameters as state variables, a simple linear discrete–time state–space model of the wave front dynamics can be derived. From the model output the measurements $c_A(t_m,z_m)$ and $c_B(t_m,z_m)$ can be determined. It turns out that a measurement time which is varying with respect to the port switching time has to be applied to achieve observability of the model. A new approach to the derivation of an observer based on the model of the wave fronts is presented.

This paper is structured as follows. Section 2 gives a brief description of the TMB and the SMB principle. The state observation problem is formulated in Section 3. In Section 4 an approach to TMB and SMB modelling is proposed. Section 5 addresses wave front modelling. In Section 6 the new observer for the wave fronts is derived. Section 7 presents simulation results.

2 Simulated Moving Bed principle

2.1 True Moving Bed process

Continuous chromatographic separation requires a counterflow between the adsorbent and the solvent. The True Moving Bed (TMB) principle realises a true counterflow in one separation column (Fig. 1). A two component mixture is fed continuously to the middle of the column. Because of the stronger adsorption tendency the component A is carried in the direction of the adsorbent. The component B which has the lower adsorption tendency, is carried in the direction of the solvent. Therefore, solvent streams with high purity of the single components can be recovered in an adequate distance from the feed inlet port. The four spatial intervals between the inlet and outlet ports are called the sections of the TMB process. In the stationary state, the concentrations $c_A(z)$ and $c_B(z)$ in the solvent are time-invariant.

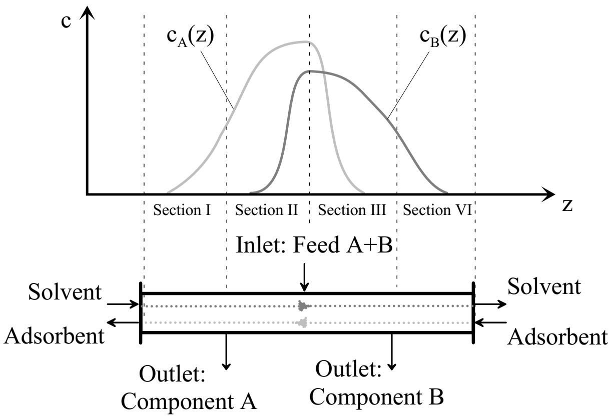

Fig. 1: True Moving Bed principle

2.2 Simulated Moving Bed process

On a technical scale, the transport of the adsorbent cannot be realised. Therefore, the counterflow is simulated by keeping the adsorbent in a fixed bed and moving the inlet and outlet ports instead (Fig. 2 a)). To realise the movement of the ports the separation column is connected to a circle and is divided into at least four interconnected columns. The inlet and outlet ports are located between the columns and switched to the next position at discrete times $t = kT_{sw}$, where k is the switching period and T_{sw} is the switching time interval (Fig. 2 b)). The solvent inlet is called the desorbent, the circulating solvent flow is called the recycling stream. The spatial ranges between the inlet and outlet ports are called the sections of the SMB process. Obviously, the SMB process has hybrid dynamical behaviour.

The process behaviour is represented by the concentration profiles $c_A(t, z)$ and $c_B(t, z)$ (Fig. 3). In the stationary state the profiles propagate periodically through the separation columns. The form of the profiles of an SMB process has similarities with those of a TMB process [4], [5]. Each of the concentration profiles have two wave fronts. Therefore, in a binary mixture separation of an SMB process, four wave fronts $c_1(t, z)$, $c_2(t, z)$, $c_3(t, z)$ and $c_4(t, z)$ are considered (cf. Fig. 3).

For closed-loop SMB control a model of the four wave fronts is necessary. SMB control then means to adjust the operation parameters such that the wave fronts take the desired form and movement. The operation parameters are the solvent mass flows $\dot{m}_j$ in the SMB sections $j = I, II, III, IV$, and the switching time interval T_{sw}. Reliable on–line concentration measurements on SMB plants are obtained applying analytic chromatography. A solvent probe is withdrawn at $t = t_m$ at

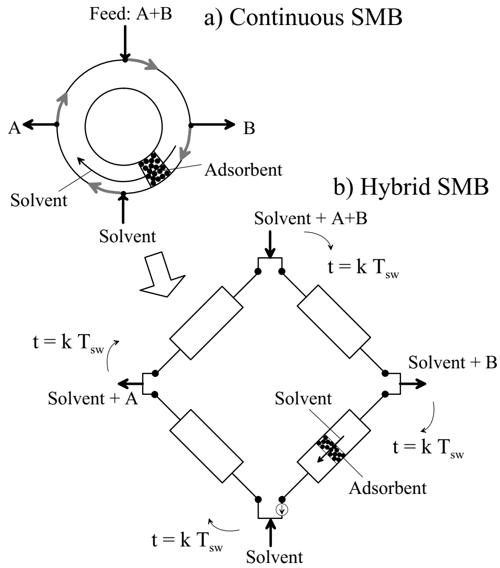

Fig. 2: Simulated Moving Bed principle

a given measurement position z_m (Fig. 3). The analysis provides an accurate value of $c_A(t_m, z_m)$ and $c_B(t_m, z_m)$. The frequency of measurement repetition depends on the setup of the analysis unit. In the following, it is assumed that during one switching period one measurement is available per SMB section.

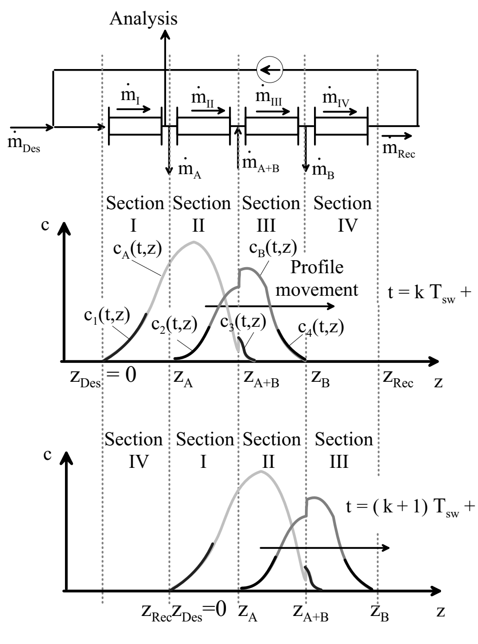

Fig. 3: Concentration profile and wave front propagation in SMB plants

3 SMB state observation problem

Given is an SMB process with synchronously switched ports in the stationary state, a physical model based on the convection-diffusion equation for the description of $c_A(t, z)$

and $c_B(t,z)$, and a measurement setup, which provides one discrete-time measurement of the concentrations per SMB section and per period k.

Problem 3.1 *Determine the form, position and movement of the wave fronts $c_1(t,z)$, $c_2(t,z)$, $c_3(t,z)$ and $c_4(t,z)$.*

The solution to Problem 3.1 is to derive a dynamical model of the wave fronts which allows to apply an observer of the model states based on the discrete–time concentration measurements.

4 SMB process modelling

4.1 Phenomenological view

In the general case, the concentration profiles in an SMB process are described by the functions

$$\begin{array}{l} c_A = c_A(t,z) \\ c_B = c_B(t,z) \quad . \end{array} \tag{1}$$

Suppose that the origin of the spatial coordinate z is tied to $z_{Des} = 0$ such that with each switching of the desorbent/recycling port the coordinate system is also switched (cf. Fig. 3). Then, the global time t can be replaced by the local time counter $\tau \in [0, T_{sw}]$, $\frac{d\tau}{dt} = 1$, which is reinitialised to 0 at each port switching instant. Applied to Eq. (1) one obtains

$$\begin{array}{rcl} c_A &=& c_A(\tau,z,k) \\ c_B &=& c_B(\tau,z,k) \, . \end{array}$$

In the stationary state, the periodic behaviour of the SMB process results in a time–invariant form of the profiles at selected times $\tau' \in [0, T_{sw}]$ for all k:

$$\begin{array}{l} c_A(\tau',z,k) = c'_A(z) \\ c_B(\tau',z,k) = c'_B(z) \quad . \end{array} \tag{2}$$

With the assumption that the shape of the concentration profiles $c_A(\tau,z,k)$ and $c_B(\tau,z,k)$ for all $\tau \in [0, T_{sw}]$ can be approximated by one concentration profile $c'_A(z)$ or $c'_B(z)$, respectively, the application of a continuous spatial shift to Eq. (2) leads to an approximate description of the complete concentration profiles in the stationary state, where v is the propagation velocity of the profiles:

$$\begin{array}{l} c_A(\tau,z,k) \approx c'_A(z - v\cdot\tau) \\ c_B(\tau,z,k) \approx c'_B(z - v\cdot\tau) \quad . \end{array} \tag{3}$$

4.2 TMB modelling

TMB modelling leads to the following form of the convection–diffusion equation:

$$\begin{array}{rcl} \frac{\partial c_{A,j}}{\partial t} &=& F'_A \left(-v_{A,j} \frac{\partial c_{A,j}}{\partial z} + D \frac{\partial^2 c_{A,j}}{\partial z^2} \right) \\ \frac{\partial c_{B,j}}{\partial t} &=& F'_B \left(-v_{B,j} \frac{\partial c_{B,j}}{\partial z} + D \frac{\partial^2 c_{B,j}}{\partial z^2} \right) \quad . \end{array} \tag{4}$$

For linear adsorption the factors F'_A and F'_B are constant, which is assumed for further model derivation. The TMB sections are specified by $j = I, II, III, IV$. $v_{A,j}$ and $v_{B,j}$ are the relative solvent flow velocities

$$\begin{array}{rcl} v_{A,j} &=& u_j - F\,H_A\,u_s \\ v_{B,j} &=& u_j - F\,H_B\,u_s \quad , \end{array} \tag{5}$$

with the solvent and the adsorbent flow velocity u_j and u_s. H_A and H_B are the Henry–constants and F is the phase relation of the fixed bed adsorbent. $u_j \neq u_j(z)$ is assumed to be constant in each TMB section.

The initial condition for Eq. (4) is given by $c_{0,A}(z) = c_A(0,z)$ and $c_{0,B}(z) = c_B(0,z)$. In the stationary state $\frac{\partial c_{A,j}}{\partial t} = 0$ and $\frac{\partial c_{B,j}}{\partial t} = 0$ holds and Eq. (4) is an ordinary differential equation with respect to z. The solution is

$$\begin{array}{rcl} c_{A,j}(z) &=& a_{A,j}\,\mathrm{e}^{b_{A,j}\,z} + d_{A,j} \\ c_{B,j}(z) &=& a_{B,j}\,\mathrm{e}^{b_{B,j}\,z} + d_{B,j} \quad , \end{array} \tag{6}$$

with the parameters $a_\star$, $b_\star$ and $d_\star$ ($\star$ is a placeholder for the component index A or B and the TMB section j, respectively). Considering physical boundary conditions, $a_\star$, $b_\star$ and $d_\star$ can be estimated for each section and component [2]. Fig. 4 shows an example of a solution (6). The four wave fronts are visible.

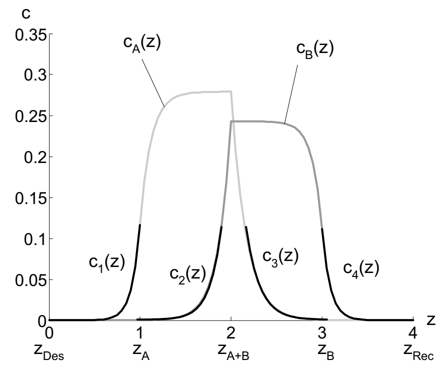

Fig. 4: Steady state TMB model solution

4.3 SMB modelling

For modelling of a two component SMB separation with $c_A(t,z)$ and $c_B(t,z)$ the convection–diffusion equation is given in the following form for each SMB section $j = I, II, III, IV$:

$$\begin{array}{rcl} \frac{\partial c_{A,j}}{\partial t} &=& F'_A \left(-u_j \frac{\partial c_{A,j}}{\partial z} + D \frac{\partial^2 c_{A,j}}{\partial z^2} \right) \\ \frac{\partial c_{B,j}}{\partial t} &=& F'_B \left(-u_j \frac{\partial c_{B,j}}{\partial z} + D \frac{\partial^2 c_{B,j}}{\partial z^2} \right) \quad . \end{array} \tag{7}$$

Due to the hybrid character of the SMB process, the stationary solution of Eq. (7) is periodic in time and space. The derivation of an analytical solution is very complex. Because the SMB process is a discretised implementation of the TMB process, the SMB model solution is approximated using Eq. (6). Applying the spatial shift $-v_c\,\tau$ one obtains

$$\begin{array}{rcl} c_{A,j}(\tau,z,k) &=& a_{A,j}\,\mathrm{e}^{b_{A,j}\,(z - v_c\,\tau)} + d_{A,j} \\ c_{B,j}(\tau,z,k) &=& a_{B,j}\,\mathrm{e}^{b_{B,j}\,(z - v_c\,\tau)} + d_{B,j} \, , \end{array} \tag{8}$$

with $\tau \in [0, T_{sw}]$ and the switching coordinate system z. In the stationary operation of the SMB process the parameters $a_\star$, $b_\star$, $d_\star$ and v_c are constant for all k and the propagation velocity v_c of both profiles is $v_c = u_s = \frac{L}{T_{sw}}$, where L is the normalised length of one column.

5 Wave front modelling

For the control of SMB units only the wave fronts of the concentration profiles are of interest. A mathematical model, which provides the description of $c_i(\tau, z, k)$ with respect to the form, position and movement is called the *wave model* of the wave front i.

5.1 Wave model derivation

Eq. (8) can be applied to obtain an approximate model of the wave fronts:

$$\begin{aligned} c_1(\tau, z, k) &= a_{A,I}\, \mathrm{e}^{b_{A,I}\,(z - v_c\,\tau)} + d_{A,I} \\ c_2(\tau, z, k) &= a_{B,II}\, \mathrm{e}^{b_{B,II}\,(z - v_c\,\tau)} + d_{B,II} \\ c_3(\tau, z, k) &= a_{A,III}\, \mathrm{e}^{b_{A,III}\,(z - v_c\,\tau)} + d_{A,III} \\ c_4(\tau, z, k) &= a_{B,IV}\, \mathrm{e}^{b_{B,IV}\,(z - v_c\,\tau)} + d_{B,IV} \end{aligned} \tag{9}$$

Obviously, each wave front $i = 1, 2, 3, 4$ is described by the same class of curves. Therefore, for further model derivation only one equation is used. In the transient state of the SMB process, the propagation velocity of the wave fronts might be different, i.e. $v_c = v_{c,i}$. Changing the indices of the parameters $a_\star$, $b_\star$ and $d_\star$ to $\star = i = 1, 2, 3, 4$ one obtains

$$c_i(\tau, z, k) = a_i\, \mathrm{e}^{b_i\,(z - v_c\,\tau)} + d_i\,. \tag{10}$$

Eq. (10) describes one wave front over the length of $z \in [0, L]$ and the time span of $\tau \in [0, T_{sw}]$ for each switching period k. For each wave front, one coordinate system is introduced which moves with the switching of the ports (Fig. 5).

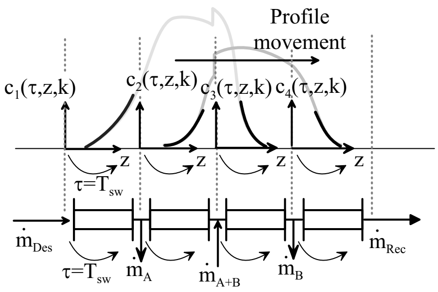

Fig. 5: Wave front coordinate systems

d_i is a constant concentration offset, which can be neglected. Applying the transformation $a_i = \mathrm{e}^{-b_i\, z_{0,i}}$ to Eq. (10) one obtains

$$c_i(\tau, z, k) = \mathrm{e}^{b_i\,(z - (v_{c,i}\,\tau + z_{0,i}))}\,. \tag{11}$$

The parameters b_i, $v_{c,i}$ and $z_{0,i}$ in Eq. (11) have a physical meaning. b_i specifies the form, $v_{c,i}$ the propagation velocity and $z_{0,i}$ the spatial offset at $\tau = 0$. In the stationary SMB operation b_i, $v_{c,i}$ and $z_{0,i}$ are supposed to be time–invariant. If Eq. (11) is used to describe the transient SMB behaviour it is assumed that the parameters b_i, $v_{c,i}$ and $z_{0,i}$ are constant during one switching period k, but perform a stepwise change after each port switching:

$$b_i = b_i(k) \;\; v_{c,i} = v_{c,i}(k) \;\; z_{0,i} = z_{0,i}(k)\,. \tag{12}$$

Because the wave model (11) has the same structure for each SMB wave front, the index i is omitted in the following. If a wave front propagates from one SMB section into the next, which e.g. is the case for the wave front $c_1(\tau, z, k)$ if there is one only column in section I, the propagation velocity of parts of the wave front changes because of the different solvent mass flows in the SMB sections. However, with respect to the spatial offset z_0, it is assumed that v_c is not a function of z. Therefore, $z_0(k+1)$ only depends on $z_0(k)$, $v_c(k)$ and T_{sw}:

$$z_0(k+1) = z_0(k) + v_c(k)\,T_{sw} - L\,. \tag{13}$$

The following factorisation is applied to derive new parameters $x_1(k)$, $x_2(k)$ and $x_3(k)$ which are interpreted as the *state variables* of the wave model:

$$\begin{aligned} x_1(k) &= b(k) \\ x_2(k) &= -b(k)\,v_c(k) \\ x_3(k) &= -b(k)\,z_0(k) \quad . \end{aligned} \tag{14}$$

For the dynamics of $\boldsymbol{x}(k) = (x_1(k) \quad x_2(k) \quad x_3(k))^T$ one obtains

$$\boldsymbol{x}(k+1) = \underbrace{\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ L & T_{sw} & 1 \end{pmatrix}}_{\boldsymbol{A}} \boldsymbol{x}(k)\,. \tag{15}$$

Eq. (15) is called the *state equation* of the wave model which in this case is an autonomous linear discrete–time state equation. The wave front $c(\tau, z, k) := \mu(\boldsymbol{x}(k), \tau, z)$, $\tau \in [0, T_{sw}]$, $z \in [0, L]$, is determined applying

$$\mu(\boldsymbol{x}(k), \tau, z) = \mathrm{e}^{x_1(k)\cdot z + x_2(k)\cdot \tau + x_3(k)}\,, \tag{16}$$

which directly follows from Eq. (11), (12) and (14). The output of the wave model is defined by

$$y(k) = g(\mu(\boldsymbol{x}(k), \tau_m(k), z_m)) \tag{17}$$

where $\tau_m(k) \in [0, T_{sw}]$ is the measurement time and z_m is the measurement position. Eq. (17) is called the *output equation* of the wave model. For the presented wave model the natural logarithm $g(\cdot) = \ln(\cdot)$ is chosen. Then, Eq. (17) transformes to

$$y(k) = \underbrace{(z_m \quad \tau_m(k) \quad 1)}_{\boldsymbol{C}'(k)}\, \boldsymbol{x}(k)\,. \tag{18}$$

The output $y_p(k)$ of an SMB plant wave front is determined by the application of g to the concentration measurement $c_p(\tau_m(k), z_m, k)$:

$$y_p(k) = g(c_{p,k}(\tau_m(k), z_m, k))\,. \tag{19}$$

6 Wave front observation

6.1 Observation problem

Problem 3.1 can be formulated uniquely for each wave front in terms of the derived wave model: An SMB wave front in the stationary regime with the state $\boldsymbol{x}(k)$ and the measurements $c_p(\tau_m(k), z_m, k)$, is given. Furthermore, a wave model with the states $\hat{\boldsymbol{x}}(k)$ and the output $\hat{y}(k)$ as well as the functions g and μ are given.

Problem 6.1 *Determine $\hat{\boldsymbol{x}}(k)$ such that $\|\boldsymbol{x}(k) - \hat{\boldsymbol{x}}(k)\| \to 0$ for $k \to \infty$ by an observer f : $\hat{\boldsymbol{x}}(k+1) = f(\hat{\boldsymbol{x}}(k), e(k))$, where $e(k) = y(k) - \hat{y}(k)$.*

Fig. 6 illustrates the problem.

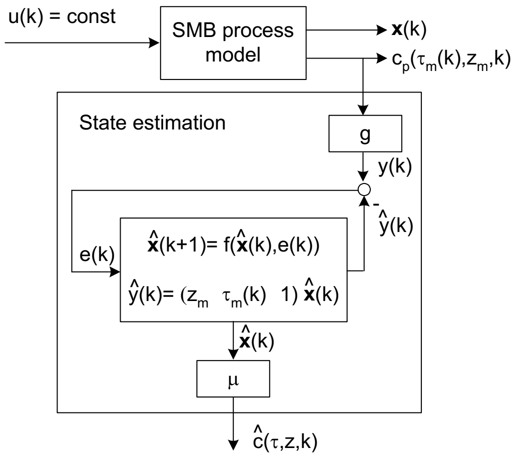

Fig. 6: Wave front observation problem

The following stationary wave front behaviour is assumed:

$$\begin{aligned} \boldsymbol{x}(k+1) &= (x_{1,0} \;\; x_{2,0} \;\; x_{3,0})^T \\ y(k) &= z_m\, x_{1,0} + \tau_m(k)\, x_{2,0} + x_{3,0}\,. \end{aligned} \tag{20}$$

The wave model is obtained from Eqs. (15) and (18):

$$\hat{\boldsymbol{x}}(k+1) = \boldsymbol{A}\, \hat{\boldsymbol{x}}(k) \tag{21}$$

$$\hat{y}(k) = \boldsymbol{c}'(k)\, \hat{\boldsymbol{x}}(k)\,, \tag{22}$$

with the model state $\hat{\boldsymbol{x}}(k) = (\hat{x}_1(k) \;\; \hat{x}_2(k) \;\; \hat{x}_3(k))^T$. In a first approach it is assumed that $\tau_m(k) = \tau_m =$ const. Then, $\boldsymbol{c}'(k) = \boldsymbol{c}' =$ const. However, it can easily be checked that the rank of the observability matrix $\boldsymbol{S}_B$ with

$$\boldsymbol{S}_B = \begin{pmatrix} \boldsymbol{c}' \\ \boldsymbol{c}'\;\boldsymbol{A} \\ \boldsymbol{c}'\;\boldsymbol{A}^2 \end{pmatrix} \tag{23}$$

is $\mathrm{rank}(\boldsymbol{S}_B) = 2$. This means that for a solution of the observation problem additional measurements are necessary. To achieve this the measurement time is varied at every switching period k, e.g. by choosing

$$\tau_m(k) \in \{\tau_{m1}, \tau_{m2}\} \;\wedge\; \tau_m(k) \neq \tau_m(k-1)\,. \tag{24}$$

Then the output equation (22) is time–variant. The observability check based on the observability matrix $\boldsymbol{S}_B(k)$ for linear time–variant systems with

$$\boldsymbol{S}_B(k) = \begin{pmatrix} \boldsymbol{c}'(k) \\ \boldsymbol{c}'(k+1)\,\boldsymbol{A}(k) \\ \boldsymbol{c}'(k+2)\,\boldsymbol{A}(k+1)\,\boldsymbol{A}(k) \\ \vdots \\ \boldsymbol{c}'(k+n-1)\;\boldsymbol{A}(k+n-2)\,\ldots\,\boldsymbol{A}(k) \end{pmatrix},$$

where n is the state dimension of the system, shows that $\mathrm{rank}(\boldsymbol{S}_B(k)) = 3$. This means, that the considered wave model becomes observable if Eq. (24) is applied.

6.2 Wave model for the observer

The result that $\mathrm{rank}(\boldsymbol{S}_B) = 2$ for $\tau_m =$const can be interpreted such that the observation problem can be solved if one of the states $x_1(k)$, $x_2(k)$ or $x_3(k)$, respectively, is known exactly. Considering Eq. (20) the state $\hat{x}_2(k)$ can be determined in the stationary state if two successive measurements $y(k-1)$ and $y(k)$, which are recorded at the different measurement times $\tau_m(k) \neq \tau_m(k-1)$, are available:

$$\begin{aligned} y(k-1) &= z_m\, x_{1,0} + \tau_m(k-1)\, x_{2,0} + x_{3,0} \\ y(k) &= z_m\, x_{1,0} + \tau_m(k)\, x_{2,0} + x_{3,0} \\ \Rightarrow \;\; x_{2,0} &= \frac{y(k) - y(k-1)}{\tau_m(k) - \tau_m(k-1)}\,. \end{aligned} \tag{25}$$

If an observer includes Eq. (25) to determine the state $x_2(k)$ at each step k the observation problem can be solved. The following derivation of the observer f is proposed:

First, Eq. (25) is applied to determine $\hat{x}_2$:

$$\hat{x}_2(k+1) = (1-k_2)\,\hat{x}_2(k) + k_2\,\frac{y(k) - y(k-1)}{\tau_m(k) - \tau_m(k-1)}\,, \tag{26}$$

where k_2 is a design parameter with $0 \leq k_2 \leq 1$. To avoid an alternating behaviour of $e(k)$, a sliding mean with horizon 1 of is introduced:

$$e(k) := \frac{1}{2}\left((y(k) - \hat{y}(k)) + (y(k-1) - \hat{y}(k-1))\right)\,. \tag{27}$$

Second, the classical error injection is applied for the correction of $\hat{x}_1(k)$ and $\hat{x}_2(k)$, which leads to the observer f with

$$f\!:\begin{cases} \hat{x}_1(k+1) = \hat{x}_1(k) + k_1\, e(k) \\ \hat{x}_2(k+1) = (1-k_2)\,\hat{x}_2(k) + k_2\,\frac{y(k)-y(k-1)}{\tau_m(k)-\tau_m(k-1)} \\ \hat{x}_3(k+1) = L\,\hat{x}_1(k) + T_{sw}\,\hat{x}_2(k) + \hat{x}_3(k) + k_3\, e(k) \end{cases} \tag{28}$$

k_1, k_2 and k_3 are the design parameters of the observer.

6.3 Observer design

The design of k_1, k_2 and k_3 is based on the analysis of the observer state dynamics. A model of the dynamics of $\hat{\boldsymbol{x}}(k)$ can be derived using Eqs. (20), (22), (27) and (28). For the analysis a new state $\boldsymbol{\zeta}(k)$ has to be introduced:

$$\boldsymbol{\zeta}(k) = \begin{pmatrix} \zeta_1(k) \\ \zeta_2(k) \\ \zeta_3(k) \\ \zeta_4(k) \\ \zeta_5(k) \\ \zeta_6(k) \end{pmatrix} = \begin{pmatrix} \hat{x}_1(k) \\ \hat{x}_1(k-1) \\ \hat{x}_2(k) \\ \hat{x}_2(k-1) \\ \hat{x}_3(k) \\ \hat{x}_3(k-1) \end{pmatrix}.$$

The stationary and dynamical properties of the observer (28) are determined by the dynamics of $\boldsymbol{\zeta}(k)$:

$$\boldsymbol{\zeta}(k+1) = \boldsymbol{H}(k)\,\boldsymbol{\zeta}(k) + \boldsymbol{e}\,, \tag{29}$$

where $\boldsymbol{H}(k)$ is a function of T_{sw}, L, $\tau_m(k)$, $\tau_m(k-1)$ and k_1, k_2 and k_3. $\boldsymbol{e}$ depends on k_1, k_2 and k_3, and on $x_{1,0}$, $x_{2,0}$ and $x_{3,0}$. In the stationary regime with $\boldsymbol{\zeta}(k+1) = \boldsymbol{\zeta}(k)$ the observer states are equal to the process states:

$$\hat{x}_1 = x_{1,0}\,, \;\; \hat{x}_2 = x_{2,0}\,, \;\; \hat{x}_3 = x_{3,0}\,.$$

The dynamical behaviour is determined by the Eigenvalues of $\boldsymbol{H}(k)$. The Eigenvalues do not depend on k and can be placed by a suitable choice of the k_1, k_2 and k_3. [2]

7 Simulation results

The wave front observer was tested with a simulation of a closed–loop controlled eight column SMB plant. Two columns per SMB section and the separation of cis- and trans–phytol in supercritical carbon dioxide with a nonlinear adsorption behaviour were considered [2]. During the startup of the unloaded plant the state observation was started with $\hat{\boldsymbol{x}}(0) = \mathbf{0}$ at $k = 17$.

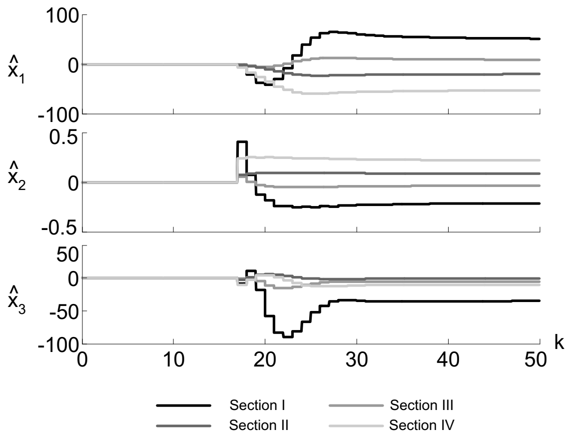

Fig. 7: Transient observer state behaviour

Fig. 7 shows the trajectories of the observer states for each SMB section. The steady observer state is reached at about $k = 30$. The convergence behaviour of the observer states is visible. Slow transitions of the SMB process are tracked by the wave front observers. The wave front concentrations $\hat{c}_i(T_{sw}, z, k)$, $i = 1, 2, 3, 4$, were supplied to discrete–time PI–controllers with the sampling time T_{sw} to control the solvent flows $\dot{m}_j$ in the SMB sections j such that the outlet concentrations reach a given setpoint.

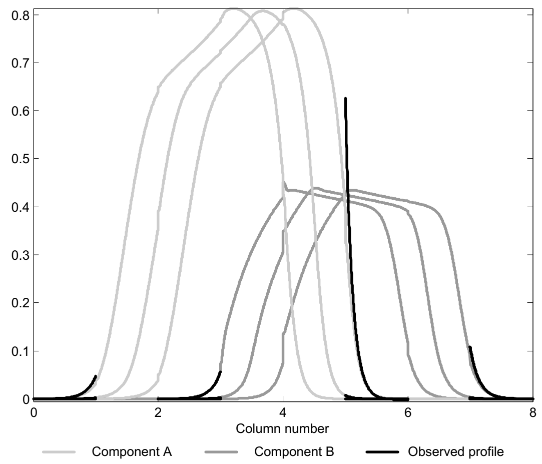

Fig. 8: Snapshots of concentration profi les

Fig. 8 shows steady state concentration profile snapshots at $\tau = 0$, $\frac{1}{2}T_{sw}$, T_{sw} of one switching period k. Fig. 9 is a zoom of Fig. 8. Despite of the nonlinear adsorption and the compressible solvent, a good agreement of $\hat{c}_i(\tau, z)$ and $c_i(\tau, z)$ is achieved for two reasons. On the one hand, the high number of columns results in a good agreement between the TMB and the SMB. On the other hand, wave fronts have low concentrations, which leads to linear adsorption in this part of the concentration profiles.

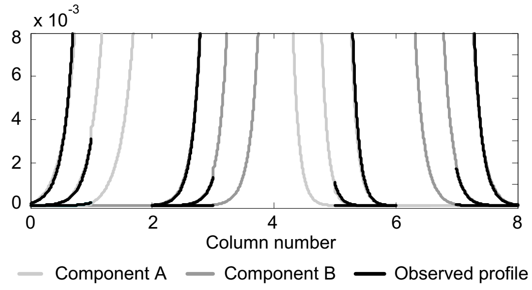

Fig. 9: Zoom of the concentration profi les

8 Conclusion and outlook

This paper deals with the derivation of a simplified SMB model. It was shown, that under the assumption of a good approximation of the SMB by the TMB and the consideration of the convection-diffusion equation as a physical plant model, the wave fronts of the concentration profiles in an SMB plant in the stationary state belong to special class of curves. By interpreting the parameters of the curves as states, a linear discrete-time model of the wave front state dynamics could be derived suitable for the observation of the SMB wave fronts. To achieve observability of all states, the measurement time is varied in each switching period. A new approach to the derivation of a wave model observer was presented.

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