15th Triennial World Congress, Barcelona, Spain

# A HYBRID AUTOMATON REPRESENTATION OF SIMULATED MOVING BED PROCESSES

**Tobias Kleinert** [*] **Jan Lunze** [**]

[*] *Institut of Control Engineering, Technical University Hamburg - Harburg, Hamburg, Germany, email: kleinert@tu-harburg.de*
[**] *Institute of Automation and Computer Control, Ruhr University Bochum, Bochum, Germany, email: lunze@esr.ruhr-uni-bochum.de*

Abstract: Simulated Moving Bed (SMB) chromatographic separation processes show typical hybrid phenomena: discrete state jumps and switching dynamics. The SMB principle and two modelling approaches based on hybrid automaton are presented and discussed within the context of hybrid systems theory. It is shown, how these models are affected by open-loop and closed-loop control. *Copyright ©2002 IFAC*

Keywords: Simulated Moving Bed, Chromatographic Separation, Hybrid Automaton, Systems Analysis, Process Control

## 1. INTRODUCTION

Hybrid systems are of increasing interest in modern system theory. A system is called hybrid, if it contains coexisting continuous-variable and discrete-event subsystems, and if neither a purely continuous nor a purely discrete model can be used to describe the dynamic behaviour with sufficient detail. Typical phenomena encountered in hybrid systems are switches of the dynamics and state jumps in the continuous subsystem.
This paper investigates chromatographic separation processes in the context of hybrid systems theory. These processes are widely used for the large scale separation and purification of chemical mixtures. To simulate the counterflow between solvent and fixed adsorbent, the Simulated Moving Bed (SMB) principle combines the continuous-variable separation process with discrete changes of inlet and outlet positions in a circle of separation columns. Thus, the abrupt change of the dynamic behaviour by a discrete action is a characteristic issue of this process.

Two approaches are common in chemical process modelling to cope with the problem of representing the switching dynamics of such processes, namely the use of a fixed or a moving coordinate system, respectively. Both approaches are used here to derive models based on the theory of hybrid automata. Two interesting results can be verified: First, the choice of representation determines, whether the system shows state jumps or switching dynamics. Second, the structure of the discrete-event subsystem is prescribed by the SMB principle. Therefore, the performance of the whole system is set up by design and configuration of the continuous-variable subsystem. The paper discusses, how the model representation is affected if closed loop process control is applied.

Recent research dealing with the system theoretical analysis and the closed-loop control of SMB separation processes is described in (Klatt *et al.*, 2000), (Kloppenburg, 2000) and (Schramm *et al.*, 2001). A common modelling approach is the approximation of the SMB process with the True Moving Bed process, which assumes a true countercurrent, and the optimisation of the separation process based on simulations, respectively. Here, a new approach based on hybrid systems methods is proposed and evaluated.

The focus of this work is the hybrid modelling of the SMB process. The SMB principle and its continuous and discrete dynamics are presented. The modelling concepts are described and compared with respect to hybrid phenomena. Simulation results are shown and the closed-loop control is briefly discussed.

## 2. SIMULATED MOVING BED PRINCIPLE

Chromatographic separation is based on the different retention behaviour of several spices towards an adsorptive, porous solid. If carried by a suitable solvent through the solid, two spices can be separated from each other, if the adsorptive mass exchange of one of the spices dominates the exchange of the other spice. Therefore, the resulting propagation velocity of the concentration peak is lower and the distance between the two concentration peaks of the spices increases, which leads to the separation.

For a continuous separation a counterflow between the solid and the solvent is necessary. Fig. 1 shows such a setup of the fictitious True Moving Bed (TMB) separation process. The mixture of the two components $A$ and $B$ are fed continuously to the middle of the separation column. The stronger adsorbed component is mainly carried with the solid and the less adsorbed one is carried with the solvent. As a result, the profiles of the solvent concentrations $c_A$ and $c_B$ in the column show areas where the solvent carries only one of these two components. There, pure components can be recovered.

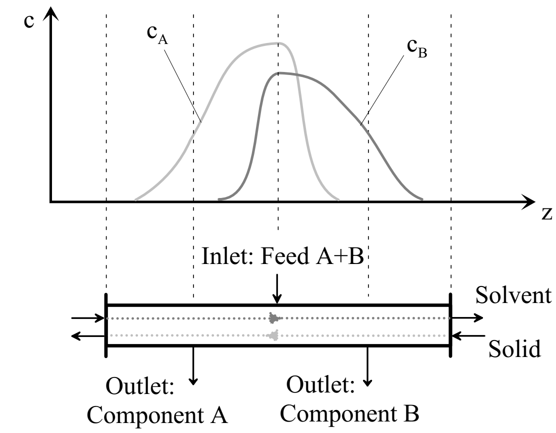


Fig. 1. Fictitious True Moving Bed separation process

The TMB principle cannot be technically applied because it necessitates the movement of the solid through the separation column. If the inlet and outlet ports are moved instead of the solid, the relative movement between solvent, ports and fixed solid results in the same counterflow as in the TMB process. For the technical realisation, the column has to form a circle, in which the solvent flow is established. The ports are moved around this circle in the direction of the solvent flow (Fig. 2). The result is a *simulation* of the countercurrent of the TMB process.

To realise the movement of the ports and the solvent circulation, the column is divided into at least four single columns. The ports and the pump for the solvent circulation are positioned between the

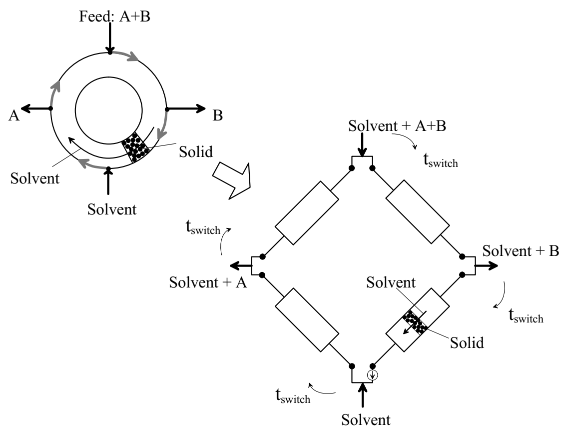


Fig. 2. Simulated Moving Bed principle

columns and are switched at equidistant, discrete times $t_0 = n \cdot t_{switch}$, $n = 1, 2, 3, \dots$, to move the port position. This is realised with multiport valves, which allow to connect one port to different inputs and outputs by changing the valve position $VP$.

The step from continuous to discrete port movement can be interpreted as a temporal and spatial discretisation. The result is a plant setup that can be realised in a technical scale. The principle is called the **S**imulated **M**oving **B**ed or SMB technique. Note, that the larger the number of columns, the closer is the approximation of the TMB process by the SMB process.

## 3. PROCESS CHARACTERISTICS

### 3.1 *Concentration distribution*

If set up properly, concentration profiles similar to the TMB process can be realised by an SMB process. That means that pure solved components $A$ and $B$ can be recovered at the outlet ports. As the solid is fixed, the concentration profiles move through the columns in the direction of the solvent flow. If plotted over the spatial coordinate $z$, the concentration profiles shown in Fig. 3 are obtained, which change over time. At $t = nt_{switch} + \delta t$, where $\delta t$ is an infinitesimal time step, the profiles have the form shown in the left diagram. Until the next port switch a movement along the $z$-axis takes place. Before the right front of $c_A$ reaches the outlet at the position $z_B$, the next switch must be initiated. For complete separation, the remaining three fronts have to fulfil similar criteria. Especially the last front between $z_B$ and $z_{Rec}$ has to be adsorbed completely such that the recycling stream, which is fed back to the inlet at $z_{Des}$, consists of pure solvent.

Currently, the process is usually driven under open-loop control with a set $p$ of constant process parameters. The parameters are the mass flows $\dot{m}_I$ to $\dot{m}_{IV}$ between the ports, the feed concentration $c_{Fe,A,B}$, and the time period $t_{switch}$ between two switching events. With the parameter vector $p$, the form and movement of the concentration profiles are determined. Thus, for

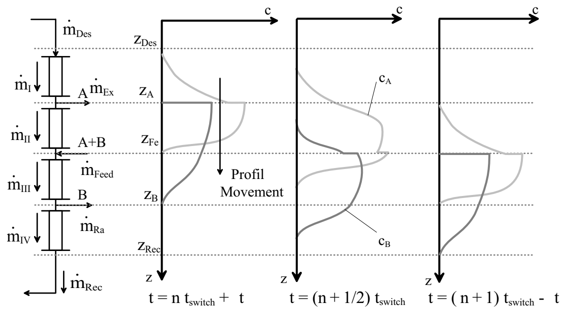


Fig. 3. Profile movement between the switching events

a proper setup of $p$, the cyclic steady state of the process results in a complete separation of the mixture.

For the survey of the outlet composition the measurement of the concentration is necessary. Two setups are possible. On the one hand, continuous measurements in the outlet streams at $z_A$ and $z_B$, on the other hand, temporally discrete measurements at times $t_{meas} = t_0 + \delta t_{meas}$ , with $\delta t_{meas} \in [0, t_{switch})$ , between the columns at coordinates $z_{meas}$ can be performed (Kloppenburg, 2000).

### 3.2 *Continuous dynamics*

First principle modelling allows to derive the description of the mass exchange dynamics. Depending on the depth of mass transport and mass exchange modelling, more or less general models can be derived (Spieker, 2000). Here, the equilibrium dispersive model (Eq. (3)) is used to describe the general effects of the concentration evolution. Accordingly, for the description of the continuous dynamics, a partition of $z$ into the intervals

$$\begin{aligned} I_I &= [z_{Des}, z_A) \\ I_{II} &= [z_A, z_{Fe}) \\ I_{III} &= [z_{Fe}, z_B) \\ I_{IV} &= [z_B, z_{Rec}) \end{aligned} \tag{1}$$

is suitable (compare Fig. 3). Based on the process descriptions given in Section 3.1, the continuous state variable $x$ and the output $y$ can be defined as follows:

$$\begin{aligned} x(t,z) &= \begin{pmatrix} c_A(t,z) \\ c_B(t,z) \end{pmatrix} \\ y(t,z) &= x(t_{meas}, z_{meas}) \,. \end{aligned} \tag{2}$$

A further continuous state is the time counter $\zeta$.

The state equation derived from the equilibrium dispersive model is

$$\frac{\partial x}{\partial t} = Q(x) \left( -v \frac{\partial x}{\partial z} + D_d \frac{\partial^2 x}{\partial z^2} \right) . \tag{3}$$

Eq. (3) describes the propagation of a spatial wave. The equation contains the first temporal state derivative on the left side and the first and second spatial state derivative on the right side, where $-v \frac{\partial x}{\partial z}$ is the convective and $D_d \frac{\partial^2 x}{\partial z^2}$ the dispersive mass transport. $Q(x)$ is a nonlinear function

$$Q(x) = \begin{pmatrix} Q_1(x_1) \\ Q_2(x_2) \end{pmatrix} , \tag{4}$$

which describes the adsorption behaviour, and $D_d$ is a constant parameter. The solvent flow velocity $v = v(z)$ is assumed to be constant between the inlet and outlet ports and thus is a piecewise constant function of $z$:

$$\begin{aligned} z \in I_I &\Rightarrow v(z) = v_I \\ z \in I_{II} &\Rightarrow v(z) = v_{II} \\ z \in I_{III} &\Rightarrow v(z) = v_{III} \\ z \in I_{IV} &\Rightarrow v(z) = v_{IV} \end{aligned} \tag{5}$$

The dynamics of $x$ depend on the right hand terms of Eq. (3). Thus, due to (5) the dynamics change in $I_i$, with $i = I, II, III, IV$.

If an initial condition and two boundary conditions are given, a unique solution for the evolution of $x$ in time and space exists. The initial condition at $t = t_0$ is given by

$$x(t_0, z) = x_0(z) \,. \tag{6}$$

Two boundary conditions are given for the coordinates $z_{in,i}$ and $z_{out,i}$:

$$\begin{aligned} 1.\quad \left.\frac{\partial x}{\partial z}\right|_{z_{in,i}} &= \frac{v(z)}{D} \cdot \left( x(t, z_{in,i}) - c_{in}(t)|_{z_{in,i}} \right) \\ 2.\quad \left.\frac{\partial x}{\partial z}\right|_{z_{out,i}} &= 0 \end{aligned} \tag{7}$$

The interconnection of the columns and the port positions are taken into account by the first boundary condition. The input concentration of the column at the positions $z_{in,i}$ is

$$c_{in}(t)|_{z_{in,i}} = \left. \begin{pmatrix} c_{in,A}(t) \\ c_{in,B}(t) \end{pmatrix} \right|_{z_{in,i}} . \tag{8}$$

Special positions are $z_{Des}$, where $c_{in} = 0$, and $z_{in,III}$, where $c_{in}$ depends on the outlet concentration at $z_{out,II}$ and on the feed concentration. Eq. (1) to (8) give the complete representation of the equilibrium dispersive model. Based on this equations the continuous state $x$ and the output $y$ of the SMB process can be computed.

### 3.3 *Discrete dynamics*

Switching the port position $VP$ means an abrupt change of the continuous dynamics. It is a discrete event $E_{switch}$, which is initiated if certain conditions are fulfilled by some continuous states. Thus, the discrete state $l$ is a function of $E_{switch}$:

$$l = l(E_{switch}) \tag{9}$$

## 4. PROCESS MODELLING

Obviously, an SMB process contains continuous and discrete dynamics, which should be represented by a

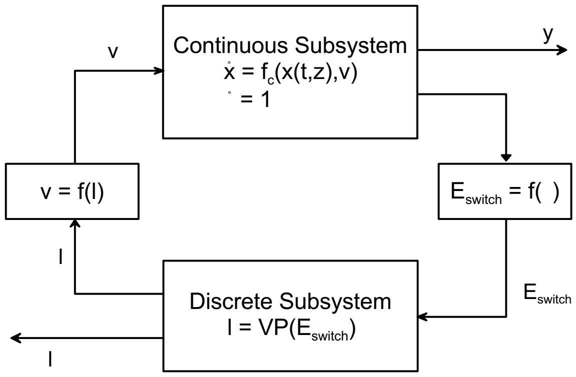


Fig. 4. Hybrid system structure

continuous or a discrete subsystem, respectively. The continuous subsystem includes the mass exchange and a clock. The discrete subsystem consists of the valves which position the inlets and outlets. The discrete subsystem affects the continuous part by a change of $v$ (Eq. (5)). Note, that due to the first boundary condition in Eq. 7, no state jump occurs at $z = z_{Fe}$. The discrete subsystem reacts on switching events $E_{switch}$ triggered by the time counter $\zeta$.

The system is represented in Fig. 4. It is an autonomous hybrid dynamical system with the discrete output $l$ and the output $y$ of the continuous subsystem.

### 4.1 *Hybrid automata*

The considerations made so far show, that a hybrid model is suitable to represent the SMB process. For this task a hybrid automaton is chosen.

A hybrid automaton (Alur *et al.*, 1993) can be viewed as a generalisation of the timed automaton, in which the behaviour of continuous variables is represented in each automaton state by a set of differential equations. Thus, a hybrid automaton $A = \{X, D, \mu_1, \mu_2, \mu_3\}$ consists of five elements:

(1) The set $X \in \mathrm{R}^n$ of the continuous $n$-dimensional state $x$.
(2) The set $D$ of discrete states $l$ (locations).
(3) A labelling function $\mu_1$ that assigns to each location $l$ possible dynamics of $x$.
(4) A labelling function $\mu_2$ assigning to each location $l$ an exception set $\mu_2(l) \subseteq X$. As long as $x \in X \backslash \mu_2(l)$ holds, a transition of the location $l$ is not possible.
(5) A labelling function $\mu_3$ that assigns to each pair $e \in D$ a transition relation $\mu_3(e) \subseteq X^2$ . For $l, l' \in D$ and $\sigma, \sigma' \in X$ the state $(\sigma', l')$ is called the successor state of $(\sigma, l)$, if $(\sigma, \sigma') \in \mu_3(l, l')$ .

Initial states are $x_0$ and $l_0$. In the automaton graph, each location $l$ is represented by a node, which is labelled by $\mu_1$ and $\{X \backslash \mu_2\}$. Possible transitions are represented as edges of the graph which are labelled with the transition relation $\mu_3$. Transition relations which assign successor states to the actual state like $x := x$ and $l := l$ are not included.

### 4.2 *Subsystem representation*

To simplify the representation of the continuous-variable subsystem, Eq. (3) is written as

$$\dot{x} = f_c(x, l)\,, \tag{10}$$

where $\dot{x}$ denotes the partial temporal state derivative, $x = x(t, z)$ the continuous state defined in Eq. (2) and $l$ the actual location, indicating the valve position. Eq. (10) is supposed to give a complete description of the state $x$ in $I_i$ and thus includes the dynamic specification (5) and the boundary condition (7) and (8). The temporal derivative of the time counter $\zeta$ is 1. Thus, if the continuous state variables are lumped in the variable

$$\kappa(t, z) = \begin{pmatrix} x(t, z) \\ \zeta(t) \end{pmatrix},$$

$\mu_1$ can be defined as

$$\dot{\kappa} = \mu_1(x, \zeta, l) = \begin{pmatrix} f_c(x, l) \\ 1 \end{pmatrix}.$$

Because the representation of the discrete-event subsystem depends on the choice of the modelling concept, it is described in the following sections.

## 5. PROCESS MODELLING BASED ON A FIXED COORDINATE SYSTEM

The 'natural' point of view concerning the inlet and outlet port positions and their movement is fixing the origin $z_0 = 0$ of the spatial coordinate system at one column interconnection. Then, for a four column SMB plant with the column length of $L$, four different valve positions are possible (Fig. 5).

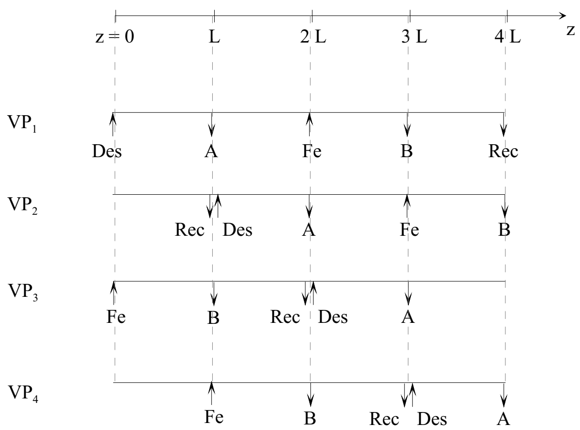


Fig. 5. Port positions in a four column SMB plant

The vector $z_p = (z_{Des}, z_A, z_{Fe}, z_B, z_{Rec})^T$ specifies the combinations of the valve positions:

$$\begin{aligned} z_{p,1} &= (0, L, 2L, 3L, 4L)^T \\ z_{p,2} &= (L, 2L, 3L, 4L, 0)^T \\ z_{p,3} &= (2L, 3L, 4L, 0, L)^T \\ z_{p,4} &= (3L, 4L, 0, L, 2L)^T \end{aligned}$$

Thus, the set $D$ consists of four discrete states $l$:

$$D : l \in \{VP_1, VP_2, VP_3, VP_4\}$$

The mapping $\Psi : l \mapsto \Psi(l)$ is defined by:

$$\Psi : z_p = z_{p,i} \Rightarrow l = VP_i\,, \quad \text{for } i \in \{1,2,3,4\}$$

Thus, each state $l$ can be associated with the corresponding representation of the continuous dynamics specified by Eq. 10.

If $\zeta$ enters the exception set

$$\mu_2(l) = \{\zeta | \zeta \geq t_{switch}\} \tag{11}$$

a transition $(l, l')$ takes place. $\zeta$ is reset and the valve position is switched. The dynamics $\mu_1$ change, whereas the continuous state $x$ remains the same ($x := x$). The automaton graph of the system is given in Fig. 6.

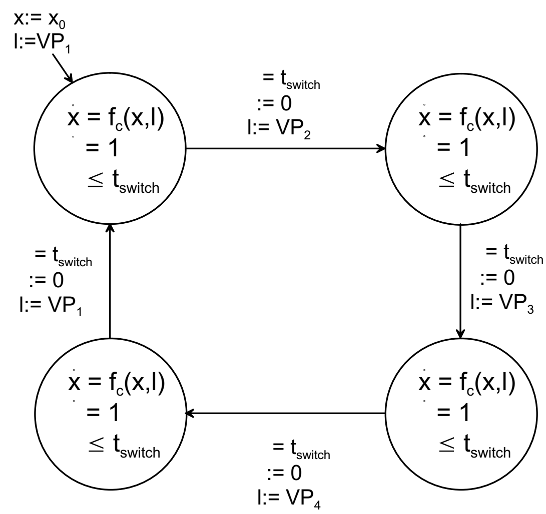


Fig. 6. Fixed coordinate system representation

## 6. PROCESS MODELLING BASED ON A MOVING COORDINATE SYSTEM

A further choice of the spatial representation is a moving coordinate system $z$. If the origin $z_0 = 0$ of the spatial coordinate is set to

$$z_{Des} := z_0\,,$$

the set of discrete states has only one component: $D : l \in \{VP_1\}$. If $\zeta$ enters the exception set (11) at $t = t_0$, the coordinate $z_0$ is reset to the position of the solvent input $z_{Des}$. However, this modelling concept results in a state jump $(\sigma, \sigma')$ initiated by the discrete action $E_{switch}$:

$$\begin{aligned} 0 \leq z < 3L &\;\Rightarrow\; x'(t_0, z) := x(t_0, z + L) \\ 3L \leq z < 4L &\;\Rightarrow\; x'(t_0, z) := x(t_0, z - 3L) \end{aligned} \tag{12}$$

$x'$ labels the successor state. Note, that Eq. (12) applies to a four column SMB plant only. The graphical representation of this modelling concept is shown in Fig. 7.

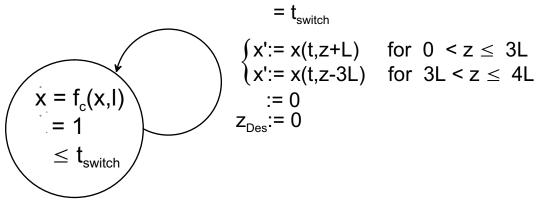


Fig. 7. Moving coordinate system representation

## 7. COMPARISON

Section 5 and 6 show the application of the proposed modelling approaches of an open-loop controlled four column SMB plant. Both approaches can be extended to a setup with a higher number of columns. Further more, the hybrid automaton modelling concept can be extended to a more general representation as proposed e.g. in (v. d. Schaft and Schuhmacher, 2000), to include the output variables of the subsystems. However, only under the assumption that all ports are switched simultaneously, the representation remains symmetric. Then, with each of the two modelling approaches one of the discussed hybrid systems phenomena can be verified: Switching dynamics or state jumps, respectively. The state jump results from the fictitious view of a moving observer, who realises the port switch as a spatial shift of the continuous state $x$.

The proposed modelling approaches enable the application of methods form hybrid systems theory to the analysis and control of the SMB process. In general, process simulation and system analysis can be performed. Further on, control actions and conditions for a control action for open-loop and close-loop control can be derived.

## 8. SIMULATION RESULTS

A dynamic process simulation was implemented allowing single port switching and dynamic variation of the process parameter $p$. See (Kleinert, 2002) for further detail. Fig. 8 shows the steady state concentration profile movement between two switching events. The figure shows an incomplete separation under nonlinear conditions. For the implementation of the nonlinear function $Q(x)$ in Eq. (4) data published in (Lübbert *et al.*, 2001) were used.

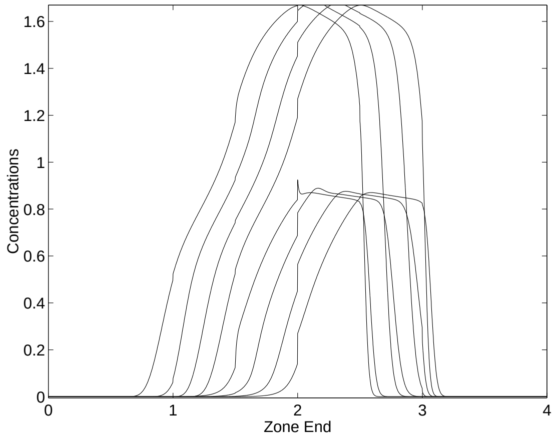


Fig. 8. Simulation results

## 9. SUPERVISORY CONTROL

The so called triangle theory published in (Storti *et al.*, 1993) offers a method for the estimation of the process parameters $p$ of an SMB process. The procedure leads to the reduction of complexity, which itself leads to the simple model representation proposed in Sect. 5 and 6. As already mentioned, the models include the design of the continuous subsystem with respect to the restrictions resulting from given discrete subsystem.

Due to immeasurable disturbances the adsorptive behaviour changes, which can lead to incomplete separation. Closed-loop supervisory setpoint control aims to guarantee pure product recovery. With respect to the hybrid automaton representation, the detection of a product pollution tendency means the replacement of (11) by an exception set for the continuous state $x = x(t,z)$ , namely

$$\mu_2(l) = \{x | x > x_{set}\}, \tag{13}$$

where $x_{set}$ yet is to define. Thus, a realisation without a time counter $\zeta$ is possible (Fig. 9). If is detected that (13) holds, suitable process parameter of $p$ have to be adapted. The concepts of the triangle theory give a good guideline for the choice of the manipulated variable. However, the main problem exists in the estimation of the concentration due to the limited measurement information (Sect. 3.1, (Klatt *et al.*, 2000), (Kloppenburg, 2000)). The synthesis of a closed-loop control is subject to future research work.

## 10. CONCLUSION

In this contribution, the hybrid automaton representation is applied to two different modelling concepts of the open-loop controlled Simulated Moving Bed separation process. The interaction between the continuous and the discrete subsystem had been represented in a clear form. Two interesting phenomena could be verified: For each of the modelling concepts, the process shows either switching dynamics or state

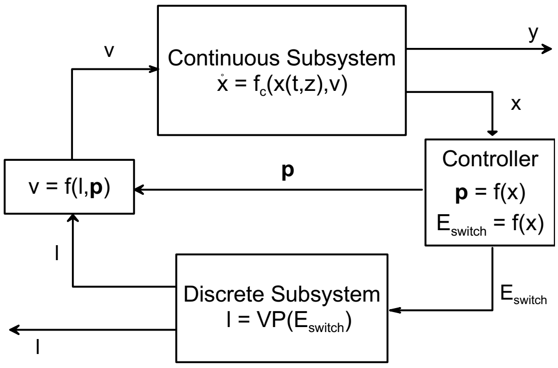


Fig. 9. Supervisory control of the SMB process

jumps, which are typical hybrid system phenomena. Further, on it was shown that because the discrete subsystem is determined by the process principle, the performance of the process has to be set up by the design of the continuous subsystem. The choice of the hybrid system representation allows the application of hybrid systems methods to the SMB process.

## 11. REFERENCES


Alur, R., C. Courcoubetis, T. Henzinger and P. Ho (1993). *Hybrid Automata: An algorithmic approach to the specification and verification of hybrid systems*. Vol. 736 of *Lecture Notes in Computer Science*. Springer–Verlag, Berlin.

Klatt, K., F. Hanisch, G. Dünnebier and S. Engell (2000). Model-based optimization and control of chromatographic processes. In: *Proceedings of PSE2000, Keystone, Col., USA*.

Kleinert, T. (2002). Theoretical modelling and dynamic simulation of simulated counterflow chromatographic separations. Research report. Arbeitsbereich Regelungstechnik,TU Hamburg-Harburg.

Kloppenburg, E. (2000). Modellbasierte Prozessführung von Chromatographieprozessen mit simuliertem Gegenstrom. PhD thesis. Stuttgart.

Lübbert, M., M. Johannsen and G. Brunner (2001). Adsorption from supercritical mixtures of carbon dioxide and modifiers. In: *2. International Meeting on High Pressure Chemical Engineering*.

Schramm, H., S. Grünner, A. Kienle and E. Gilles (2001). Control of moving bed chromatographic processes. In: *Proceedings of the European Control Confenrence 2001*.

Spieker, A. M. (2000). Modellierung, Simulation und Optimierung der präparativen Flüssigchromatographie. PhD thesis. Stuttgart.

Storti, G., M. Mazzotti, M. Morbidelli and S. Carra (1993). Robust design of binary countercurrent adsorption separaion processes. *American Institute of Chemical Engineers Journal (AIChE)*.

v. d. Schaft, A. and H. Schuhmacher (2000). *An Introduction to Hybrid Dynamical Systems*. Springer Verlag London.