MODEL-BASED TRAJECTORY CONTROL OF PRESSURE SWING ADSORPTION PLANTS

M. Bitzer K. Graichen M. Zeitz

Institut für Systemdynamik und Regelungstechnik, Universität Stuttgart, Pfaffenwaldring 9, 70550 Stuttgart, Germany

E-mail: {bitzer, graichen, zeitz}@isr.uni-stuttgart.de

Abstract: Pressure swing adsorption (PSA) plants consist of several fixed-bed adsorbers and are operated as cyclic multi-step processes. PSA processes are used for the separation and purification of gas mixtures. Based on a rigorous distributed parameter model of the considered 2-bed PSA plant, a process control scheme is derived which is composed of a nonlinear feedforward control and a linear feedback control. For the design of the feedforward control, a numerical approach for the inversion of the rigorous plant model is presented. The designed trajectory control scheme is evaluated by use of the PSA plant simulation model.

Keywords: multi-step process, periodic process operation, distributed parameter system, adsorption process, nonlinear travelling concentration waves, numerical model inversion, feedforward control, feedback control.

1. INTRODUCTION

Pressure swing adsorption (PSA) is a standard process technique for the separation of gas mixtures (Ruthven *et al.*, 1994). The plants consist in general of several fixed-bed adsorbers and are operated as cyclic multi-step processes, i.e. the connections between the different adsorbers are changed by the switching of valves at the transition from one cycle step to the next. Thereby, a periodic operation is realized for the adsorption process.

In this contribution, a 2-bed pressure swing adsorption plant for the production of oxygen from air is considered. Its flowsheet is shown in Figure 1. Each fixed-bed adsorber is described by a nonlinear model with distributed parameters (Unger, 1999). The implementation of a rigorous PSA model within e.g. the simulation environment DIVA (Köhler *et al.*, 2001) enables its dynamical analysis and the evaluation of new control schemes.

A characteristic feature of PSA plants concerns the occurrence of nonlinear travelling concentration waves which are alternating their propagation direction as a consequence of the periodic process operation. In accordance with the cyclic coupling of the fixed-bed adsorbers, the occurring waves travel back and forth within the two adsorber beds and are thereby changing their shape, see Figure 1. The cycle time as well as the duration of the cycle steps do considerably affect the product concentration, because they determine the extent of breakthrough of a concentration front at the product end of the adsorber beds. The cycle time is therefore considered to be the manipulating variable of the process.

The appropriate operation of the PSA plant requires the solution of two control tasks in order to guarantee a desired purity of the product, i.e. the average concentration in the oxygen tank, see Figure 1. These control tasks comprise the stabilization of operating points as well as the trajectory control for set-point changes. The main

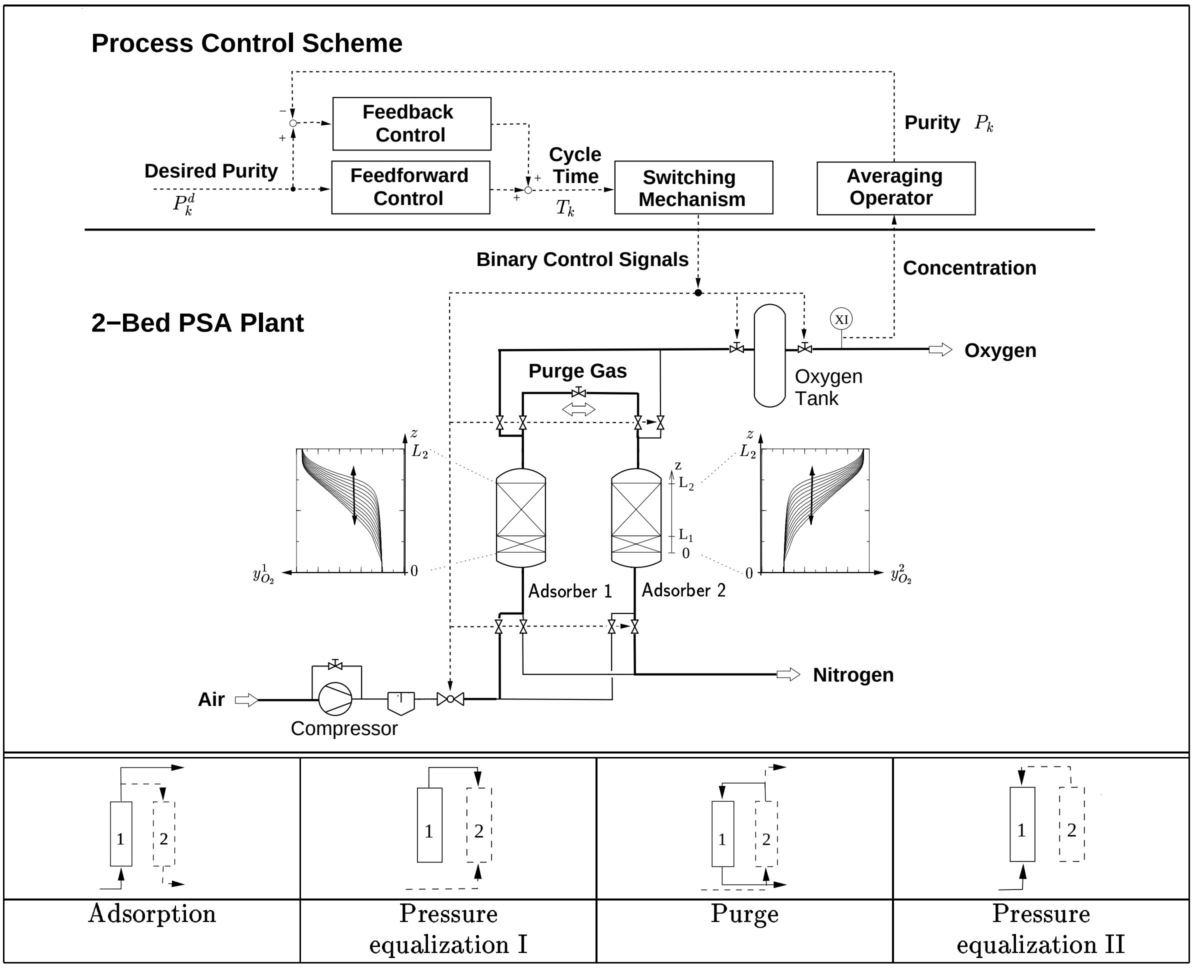

Fig. 1. Flowsheet of a 2-bed pressure swing adsorption plant for oxygen production from air with travelling oxygen concentration waves $y^i_{O_2}(z,t)$, $i \in \{1,2\}$ in both beds (middle), the coupling schemes for the adsorbers during a 4-step cycle (bottom), and the proposed process control scheme (top).

topic of this contribution is the trajectory control of the product purity. Therefore, a process control scheme is presented which consists of a feedforward control and a feedback control, see Figure 1.

The paper is organized as follows: in the next section, the model of the 2-bed pressure swing adsorption plant for the production of oxygen from air is briefly introduced and the occurring control design problem is specified. Then, an approach for the numerical model inversion used for the determination of the feedforward control is explained, the design of the feedback control is discussed, and the whole process control scheme is presented. Finally, the efficiency of the whole control concept is demonstrated by simulations with the rigorous PSA model.

2. TWO-BED PRESSURE SWING ADSORPTION PLANT

The considered 2-bed PSA plant, Figure 1, is used for the oxygen production from air for medical purposes. The produced oxygen is stored in a tank from which it is taken off by the consumer. The operation cycle consists of four steps: adsorption, pressure equalization I, purge, and pressure equalization II. The related four coupling schemes of the two adsorbers are depicted at the bottom of Figure 1.

2.1 *Nonlinear PSA plant model*

Each adsorber consists of a series connection of a prelayer and an adsorption layer with space ranges $0 \le z \le L_1$ and $L_1 \le z \le L_2$ respectively, see Figure 1. The adsorption layer model[1] considers air as a binary mixture of oxygen and nitrogen, and emanates from two phases, i.e. a gaseous and an adsorbed phase. The prelayer adsorbs moisture, which is neglected, and is therefore modeled as a gaseous phase only.

The distributed parameter model for the adsorption layer of each adsorber, $i \in \{1,2\}$ consists of six quasilinear partial differential algebraic equations for the pressure $p^i(z,t)$, oxygen mole fraction

[1] The detailed model as well as simulation results can be found in (Unger, 1999) and are also given in (Bitzer and Zeitz, 2002; Bitzer *et al.*, 2002).

Model of **adsorption layer** for each adsorber, $i \in \{1,2\}$:

$$\text{PDAE:} \quad B\left(\boldsymbol{x}^i\right)\frac{\partial \boldsymbol{x}^i}{\partial t} = A\left(\boldsymbol{x}^i\right)\frac{\partial \boldsymbol{x}^i}{\partial z} + \boldsymbol{f}\left(\boldsymbol{x}^i\right) \quad z \in \Omega^i,\ t > 0$$

$$\text{BC:} \quad \boldsymbol{0} = \boldsymbol{\varphi}^j\left(\boldsymbol{x}^i, \boldsymbol{v}^i\right) \quad z \in \Gamma^i,\ t \in \vartheta_k^j$$

$$\text{IC:} \quad \boldsymbol{x}^i(z,0) = \boldsymbol{x}_0^i(z) \quad z \in \bar{\Omega}^i$$

with state vector $\boldsymbol{x}^i = \left[p^i, y^i_{O_2}, q^i_{O_2}, q^i_{N_2}, T^i, \dot{n}^i\right]^T$,
boundary input vector $\boldsymbol{v}^i = \left[y^i_{O_2,in}, T^i_{in}, \dot{n}^i_{in}\right]^T$,
intervals $\Omega^i = (L_1, L_2)$, $\Gamma^i = \{L_1, L_2\}$, $\bar{\Omega}^i = \Omega^i \cup \Gamma^i$,
time interval $\vartheta_k^j = (t_k^j, t_k^{j+1}]$,
and cycle time $T_k = \sum_{j=1}^4 \Delta t_k^j$ with $\Delta t_k^j = t_k^{j+1} - t_k^j$.
(The BCs depend on the connections between the adsorbers during the j^{th} cycle step of the k^{th} cycle, see Figures 1 and 2.)

A similar model of 4 PDAEs with BCs and ICs is given for the **prelayer**.

Model of **oxygen tank**:

$$\text{ODE:} \quad B^t\left(\boldsymbol{x}^t\right)\frac{d\boldsymbol{x}^t}{dt} = \boldsymbol{f}^t\left(\boldsymbol{x}^t, \boldsymbol{x}^i(L,t), \dot{n}^t_{out}(t)\right) \quad t > 0$$

$$\text{IC:} \quad \boldsymbol{x}^t(0) = \boldsymbol{x}_0^t$$

with state vector $\boldsymbol{x}^t = \left[p^t, y^t_{O_2}, T^t\right]^T$.

Table 1. Model of 2-bed PSA plant.

$y^i_{O_2}(z,t)$ in the gaseous phase, adsorbed amounts $q^i_k(z,t)$, $k \in \{O_2, N_2\}$, temperature $T^i(z,t)$, and molar flux $\dot{n}^i(z,t)$. The states depend on one space coordinate z and on time t.

The model of an adsorption layer can be written in vector notation (Bitzer and Zeitz, 2002) of partial differential algebraic equations (PDAEs), boundary conditions (BCs), and initial conditions (ICs) as shown in Table 1. A similar model for the prelayer is obtained by neglecting the respective terms and equations for the adsorbed amounts q^i_k, $k \in \{O_2, N_2\}$ and consists therefore of four PDAEs and respective BCs and ICs. The model of the product tank is given by three ordinary differential equations (ODEs) for the pressure $p^t(t)$, the oxygen mole fraction $y^t_{O_2}(t)$, and the temperature $T^t(t)$ (see Table 1). The output molar flow rate $\dot{n}^t_{out}(t)$ is a time-variant operational parameter which can be adjusted. For the simulation of the PSA plant model, the simulation environment DIVA (Köhler *et al.*, 2001) is used. Thereby, the model equations are spatially discretized according to the method of lines approach.

2.2 *Cyclic operation and control problem*

Each PSA plant is operated according to a specific cycle which determines the periodic operation mode of the plant. The respective operation mode represents the specific structural cou-

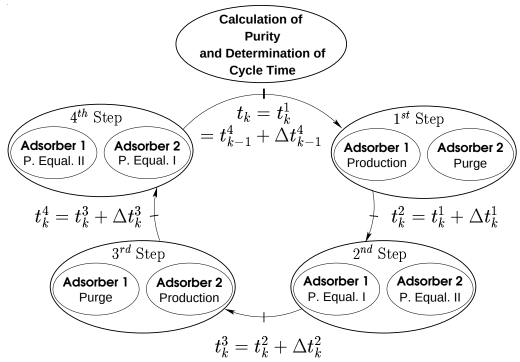

Fig. 2. Scheme of the cyclic 4-step operation of the considered 2-bed PSA plant.

plings which are associated to each step. As a consequence, the two adsorbers are operated in a phase shifted manner in order to attain a quasi-continuous production (see Figure 2). Thereby, the cycle time $T_k = \Delta t_k^1 + \Delta t_k^2 + \Delta t_k^3 + \Delta t_k^4$ is the manipulating variable of the process[2]. The controlled variable is the time-averaged purity P_k of the product, i.e. $P_{k+1} = \bar{n}_{O_2,out}/\bar{n}_{out}$ with $\bar{n}_{O_2,out} = \frac{1}{T_k}\int_{t_k}^{t_k+T_k} y^t_{O_2}\dot{n}^t_{out}\,dt$ and $\bar{n}_{out} = \frac{1}{T_k}\int_{t_k}^{t_k+T_k} \dot{n}^t_{out}\,dt$.

PSA plants can be classified as hybrid distributed parameter systems (van der Schaft and Schumacher, 2000) with a time varying cycle time T_k, which is used as the manipulating variable. These properties have to be considered in course of the design of the process control.

3. TRAJECTORY CONTROL SCHEME

The cycle time T_k (or respectively the duration Δt_k of the cycle step times) is in general a rather unconventional manipulating variable in controller design. However, it is a natural choice for PSA plants considering their hybrid process nature. In this context, it is emphasized that 'the area of hybrid systems is still in its infancy' (van der Schaft and Schumacher, 2000). It has to be considered that such a manipulating variable is subject to constraints since a minimum amount of time is physically required for each step. An upper bound is also mandatory due to the cyclic operation of the plant itself. Bemporad and Morari (1999) suggest for instance a model predictive control framework in order to control hybrid lumped parameter systems which are modeled by linear dynamic equations and linear inequalities. Such an optimization based approach is currently too complicated for the PSA plant due to the high order of the rigorous simulation model and the related real-time problems.

[2] The cycle time T_k can be changed by Δt_k^1 and Δt_k^3, because Δt_k^2 and Δt_k^4 depend on the duration of the actual pressure equalization between the two adsorbers.

Presently, PSA plants are operated based on heuristics and the process knowledge of human operators. The proposed process control scheme comprises a feedforward control and a feedback control. The feedforward control automatizes the settings of a human operator and the feedback control is used in order to compensate disturbances and model uncertainties. The feedforward control is set up by numerically inverting the input/output (I/O) behavior of the detailed plant model [3]. The design of a feedforward control by an inverse I/O model adapts the ideas known from flatness based control applied to trajectory control of a CSTR (Rothfuß *et al.*, 1996).

In the following, the focus is first put on the cyclic and time-discrete nature of the plant, which serves for the explanation and derivation of the model inversion strategy for the design of the feedforward control. Then, the feedback control design is presented.

3.1 *Derivation of feedforward control*

Current approaches for the controller design for distributed parameter systems require the derivation of a simplified design model which captures the dominant system dynamics, see e.g. (Christofides, 2001). The cyclic operation is an intrinsic property of the process. Therefore it is certainly a shared feature of any reduced-order model which intends to approximate the PSA plant together with its cyclic and variable structure. From Figure 2, it becomes evident that the cyclic operation of the PSA plant is naturally defining Poincaré maps

$$\boldsymbol{x}_{k+1} = \boldsymbol{g}\left(\boldsymbol{x}_k, T_k\right), \quad P_{k+1} = h\left(\boldsymbol{x}_k, T_k\right) \qquad (1)$$

of the internal state $\boldsymbol{x}_k := \boldsymbol{x}(t_k)$ and the purity P_k of such a lumped reduced-order design model. This means that the state $\boldsymbol{x}_{k+1}$ and the purity P_{k+1} at the end of the k^{th} cycle depend on both the initial state $\boldsymbol{x}_k$ at the beginning of that cycle and on the cycle time T_k, which becomes an explicit variable. The iterative maps $\boldsymbol{g}(\cdot)$ and $h(\cdot)$ reflect the fundamental solution of the considered model. Their analytical calculation is therefore only possible in exceptional cases. Since the cycle time T_k is the manipulated and the purity P_k the controlled variable, these iterative maps are a time-discrete representation of the I/O behavior of the plant. PSA plants are in general operated at a periodic set-point [4] P^d, i.e. with $T_k = T^d = const.$, such that $P_k = P^d = h(\boldsymbol{x}^*, T^d)$ and $\boldsymbol{x}_k = \boldsymbol{x}^* = \boldsymbol{g}(\boldsymbol{x}^*, T^d)$. In order to perform set-point changes $P^{d,1} \rightarrow P^{d,2}$, it is necessary to follow a predetermined trajectory [5] P_k^d, $k = 0, 1, \ldots, N$ with $P_0^d = P^{d,1}$ and $P_N^d = P^{d,2}$. The I/O relation (1) is needed in order to determine the feedforward cycle time T_k^d in dependence of such a desired trajectory P_k^d. Generally speaking, the global I/O behavior of (1) needs to be inverted, i.e. $T_k^d = h^{-1}(\boldsymbol{x}_k, P_{k+1}^d)$. Such an inverse I/O relation cannot be calculated analytically, but it is identical to the solution of

$$0 = P_{k+1}^d - h(\boldsymbol{x}_k, T_k^d)\,. \qquad (2)$$

This represents an end-value problem: the cycle time T_k^d is adjusted at the beginning of each cycle while the associated purity $P_{k+1} = h(\boldsymbol{x}_k, T_k^d)$ is obtained only at the end of that cycle. This end-value problem can be calculated numerically by applying the shooting method and by using the simulation model in Table 1. The entire feedforward control sequence T_k^d, $k = 0, 1, \ldots, N$ is then calculated in a repetitive way starting from the periodic set-point $P^{d,1}$ with $\boldsymbol{x}_0 = \boldsymbol{x}^{*,1}$.

However, depending on the desired trajectory P_k^d, $k = 0, 1, \ldots, N$ and the controllability of the PSA plant, a solution T_k^d of (2) is not guaranteed. It is therefore required that the PSA plant dynamics is taken into account and that the desired trajectory is sufficiently smooth such that the plant is able to follow it. Even for very smooth desired trajectories, there may still be an individual cycle and respective desired purity increment $\Delta P_{k+1}^d = P_{k+1}^d - P_k^d$, for which no solution T_k^d for (2) exists. I.e., if there's only a single cycle during the set-point change for which no solution exists, the algorithm is not robust and a replanning of the trajectory is necessary. Therefore, in order to relax this problem, the described algorithm is reformulated. Thereby, the future dynamics is also taken into account: a moving shooting horizon [6] of $N_H > 1$ cycles is chosen. Figure 3 illustrates this situation for a horizon of $N_H = 3$ cycles. This leads to the following zero-value problem

$$0 = P_{k+N_H}^d - \bar{h}(\boldsymbol{x}_k, T_k^d, T_{k+1}^d, \ldots, T_{k+N_H-1}^d) \quad (3)$$

of N_H variables instead of (2). The function $\bar{h}(\cdot)$ is calculated by applying (1) repeatedly. In order

[3] In a previous work, cf. (Bitzer *et al.*, 2002), a simplified model which coarsly approximates the I/O behavior of the PSA plant was used for the design of a feedforward control. The proposed strategy for the numerical inversion of the rigorous plant model allows a more precise calculation of the feedforward cycle time, especially since it is also possible to consider further important effects which were not included in the simple model previously used (e.g. a time varying output molar flow rate $\dot{n}_{out}^t$).

[4] A periodic set-point is also denoted as a so-called cyclic steady state (CSS), which means that the conditions at the end of each cycle are identical to those at its start. A numerical approach for the determination and the optimization of the CSS of periodic adsorption processes was presented by Nilchan and Pantelides (1998).

[5] The plant dynamics has to be taken into account for the planning of such a desired trajectory P_k^d, i.e. the trajectory has to be planned such that the plant is able to follow it.

[6] Similarly to model predictive control where a moving prediction horizon is used.

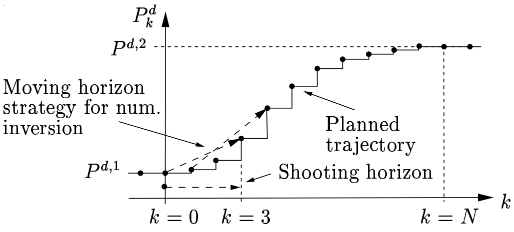

Fig. 3. Moving shooting horizon for the determination of the feedforward cycle time T_k^d and the increment ΔT_k^d.

to simplify (3), the feedforward cycle times T_k^d are chosen as $T_{k+j}^d = T_{k-1}^d + \frac{j+1}{N_H}\Delta T_k^d$, $j = 0, 1, \ldots, N_H - 1$ leading to the zero-value problem

$$0 = P_{k+N_H}^d - \tilde{h}(\boldsymbol{x}_k, \Delta T_k^d) \tag{4}$$

for the single variable ΔT_k^d. Equation (4) is repetitively solved for ΔT_k^d as described above. The feedforward cycle time for the k^{th} cycle is chosen as $T_k^d = T_{k-1}^d + \frac{1}{N_H}\Delta T_k^d$ and the T_{k+j}^d, $j \geq 1$ are rejected. When both the desired trajectory and the shooting horizon N_H are reasonably chosen, then $h(\boldsymbol{x}_k, T_k^d) \approx P_{k+1}^d$, even though (4) is solved instead of (2). The proposed strategy therefore allows the robust numerical inversion of the detailed plant model (cf. Table 1) and the calculation [7] of a feedforward control sequence T_k^d for a transient set-point change.

3.2 *Feedback control*

In open-loop, the purity P_k is influenced due to model errors and disturbances. Therefore, a feedback control is necessary for the stabilization and robust performance of desired trajectories during set-point changes. Transferring this process control scheme to the PSA plant leads to the control block diagram shown in Figure 4.

The feedforward injection of the calculated nominal feedforward cycle time T_k^d is similar to the concept of exact feedforward linearization of flat systems (Hagenmeyer, 2003). Within the vicinity of a desired trajectory $(\boldsymbol{x}_k^d, T_k^d, P_k^d)$, the tracking error e_k of the plant can be stabilized against disturbances by a linear control law [8] $\boldsymbol{r}_{k+1} = A_c\,\boldsymbol{r}_k + \boldsymbol{b}_c\,e_k$ with the tracking error $e_k = P_k^d - P_k$ as input and the output $\Delta T_k^c = \boldsymbol{c}_c^T\,\boldsymbol{r}_k + d_c\,e_k$. The straightforward design of a PID controller by use of a simplified I/O model is discussed in (Bitzer *et al.*, 2002).

[7] Currently, the feedforward control sequence needs to be calculated offline due to the large order of the simulation model. Using the simplified model given in (Bitzer *et al.*, 2002), very good starting values for the shooting method are available and only a low number of iterations steps are necessary for each cycle.

[8] Hagenmeyer (2003) proved that the tracking error of flat and feedforward linearized systems can be stabilized by a PID like control. A prerequisite is a sufficiently smooth desired trajectory. For the PSA plant, an analytical proof is not possible due to the complex model. But, an abundant number of simulation studies showed that the I/O dynamics of the considered PSA plant is rather moderate and also stable such that it can even be locally approximated by a linear discrete model. Simulated step responses are e.g. given in (Bitzer *et al.*, 2002). Based on these considerations, the assumption that the plant can be locally stabilized by a linear controller is reasonable.

4. SIMULATION RESULTS

The validation of the proposed control concept is done by simulation studies using the rigorous simulation model. In Figure 5, the open-loop control of a set-point change scenario for the purity and a simultaneous variation of the output molar flow rate $\dot{n}_{out}^t$ is shown. It can be seen that the purity P_k pursues the desired trajectory P_k^d with an almost negligible tracking error e_k. The feedforward cycle time T_k^d is calculated by numerically inverting the detailed plant model according to (4).

The influence of a step-disturbance occurring in the output molar flow rate is shown in Figure 6 for the same set-point change scenario as in Figure 5. The simulation shows the open- as well as the closed-loop case. In the closed-loop case, the desired trajectory P_k^d is stabilized by a PID controller which was derived in (Bitzer *et al.*, 2002).

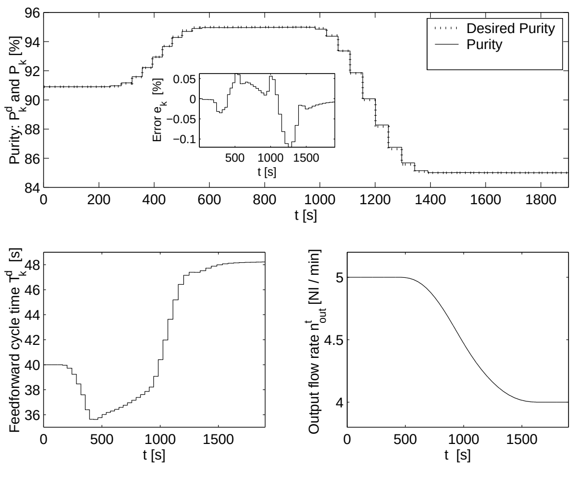

Fig. 5. Simulation of the open-loop trajectory control with a respective feedforward control sequence T_k^d calculated with a shooting horizon of $N_H = 2$. A time-variant output molar flow rate $\dot{n}_{out}^t$ is also considered.

5. CONCLUSIONS

A trajectory control scheme developed for a 2-bed PSA plant has been presented. For the feed-

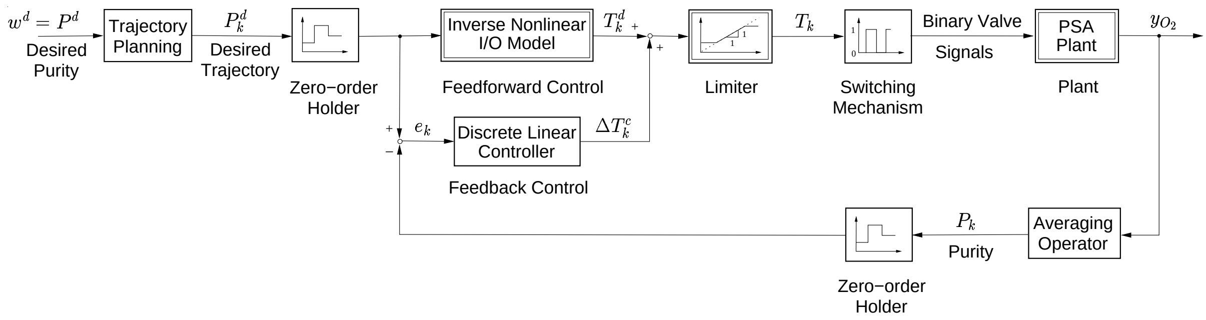

Fig. 4. Block diagram of the feedforward and feedback control for the purity P_k of the PSA plant.

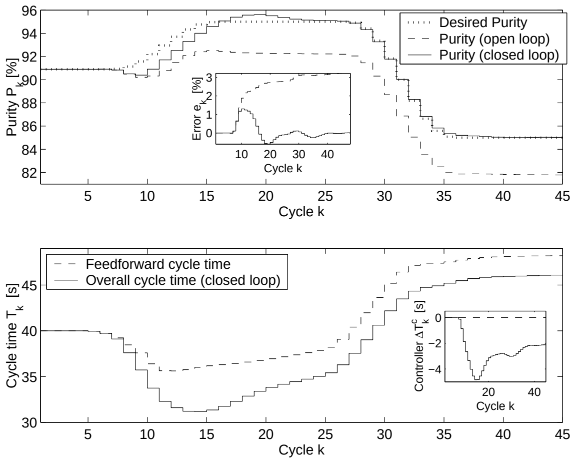

Fig. 6. Simulation of the set-point change scenario previously shown in Figure 5 subject to a step-disturbance $\Delta \dot{n}_{out}^t = +0.5\,\mathrm{Nl/min}$ superimposed to the nominal output molar flow rate and occurring at the end of the 5^{th} cycle. The open- and closed-loop case are both shown.

forward control design, a strategy for the numerical model inversion and the calculation of the inverse transient I/O behavior of the plant has been proposed. Simulation studies showed that the desired trajectory is well stabilized by a linear PID controller which is designed in a first step.

Future research will be focused on the derivation of more sophisticated reduced-order models which consider the structural changes of the process and which provide a precise representation of the internal plant dynamics. These reduced-order models will then allow real-time calculations and depending on the reduced model also the application of advanced analytical methods for the process control design.

Further issues for future research are the experimental validation (Bitzer *et al.*, 2002) of the process control concept as well as its extension to other cyclic multi-step processes, e.g. a 3-bed PSA plant (Unger, 1999).

ACKNOWLEDGEMENTS

The authors gratefully acknowledge the cooperation with Prof. G. Eigenberger, W. Lengerer, and M. Stegmaier of the *Institut für Chemische Verfahrenstechnik.* This research project is supported within *Sonderforschungsbereich 412* by *Deutsche Forschungsgesellschaft (DFG).*

6. REFERENCES

Bemporad, A. and M. Morari (1999). Control of systems integrating logic, dynamics, and constraints. *Automatica* **35**, 407–427.

Bitzer, M. and M. Zeitz (2002). Design of a nonlinear distributed parameter observer for a pressure swing adsorption plant. *Journal of Process Control* **12**(4), 533–543.

Bitzer, M., W. Lengerer, M. Stegmaier, G. Eigenberger and M. Zeitz (2002). Process control of a 2-bed pressure swing adsorption plant and laboratory experiment. In: *CHISA 2002, 15th International Congress of Chemical and Process Engineering (CD-ROM).* Prague/Czech Republic, August 25-29, 2002. Paper No. 833 (Also available at: http://www.isr.uni-stuttgart.de/~bitzer/).

Christofides, P. D. (2001). Control of nonlinear distributed process systems: recent developments and challenges. *AIChE* **47**(3), 514–518.

Hagenmeyer, V. (2003). *Robust Nonlinear Tracking Control Based on Differential Flatness.* Fortschritt–Berichte Nr. 8/978. VDI-Verlag, Düsseldorf.

Köhler, R., K. D. Mohl, H. Schramm, M. Zeitz, A. Kienle, M. Mangold, E. Stein and E. D. Gilles (2001). Method of lines within the simulation environment DIVA for chemical processes. In: *Adaptive Method of Lines* (A. Vande Wouwer, P. Saucez and W. Schiesser, Eds.). pp. 367–402. CRC Press. Boca Raton/USA.

Nilchan, S. and C. C. Pantelides (1998). On the optimisation of periodic adsorption processes. *Adsorption* **4**, 113–147.

Rothfuß, R., J. Rudolph and M. Zeitz (1996). Flatness based control of a nonlinear chemical reactor model. *Automatica* **32**, 1433–1439.

Ruthven, D. M., S. Farooq and K. S. Knaebel (1994). *Pressure Swing Adsorption.* VCH Publishers. New York, Weinheim, Cambridge.

Unger, J. (1999). *Druckwechseladsorption zur Gastrennung - Modellierung, Simulation und Prozeßdynamik.* Fortschritt–Berichte Nr. 3/602. VDI-Verlag, Düsseldorf.

van der Schaft, A. and H. Schumacher (2000). *An Introduction to Hybrid Dynamical Systems.* Lecture Notes in control and information sciences; 251. Springer. London, Berlin, Heidelberg, New York.