Proceedings of the 11th International Symposium on
Computer Applications in Biotechnology (CAB 2010),
Leuven, Belgium, July 7-9, 2010
Julio R. Banga, Philippe Bogaerts, Jan Van Impe,
Denis Dochain, Ilse Smets (Eds.)

Integration of model-predictive scheduling, dynamic real-time optimization and output tracking for a wastewater treatment process ⋆

David Elixmann, Jan Busch ⋆⋆, Wolfgang Marquardt

AVT-Process Systems Engineering, RWTH Aachen University, 52056 Aachen, Germany (e-mail: {david.elixmann, wolfgang.marquardt} @avt.rwth-aachen.de)

Abstract: A hierarchical control architecture for the integration of scheduling decisions, dynamic real-time optimization and tracking control is proposed. It is shown how the discrete-continuous problem of simultaneous scheduling and trajectory optimization on a receding horizon can be integrated within the upper control layer of a two-layer architecture. On the upper layer, the optimal plant strategy defined by a sequence of control objectives and optimal control moves is computed on a long time horizon. The lower control layer consists of a state observer and a fast-acting tracking controller which operates on a short time horizon. The properties of this architecture are illustrated by a case study in which a wastewater treatment plant is operated under the influence of external disturbances. Conflicting operational objectives may be valid, depending on the state of the plant and the expected disturbances. By calculating an optimal sequence of operational strategies and control moves on the receding horizon, economically optimal operation of the plant can be achieved.

Keywords: hierarchical control, scheduling, model predictive control, optimal control, state estimation, wastewater treatment, dynamic real-time optimization, membrane bioreactor

1. INTRODUCTION

Traditionally, control methods have focused on achieving stable process operation, using fast-acting controllers to reject disturbances and maintain the controlled variables close to their setpoints. Linear MPC algorithms are being used for this purpose in the process industries (Qin and Badgwell, 2003).

Online optimization methods such as *real-time optimization* (RTO) and its extension to transient operation, *dynamic real-time optimization* (DRTO), have expanded the scope of process control beyond disturbance rejection, to include economic optimization of process operation (Helbig et al., 2000). This drives the process to its economical optimum while regarding operational constraints. However, due to the computational effort in solving the related nonlinear, dynamic and constrained optimization problems, a re-computation of the optimal solution on the time scale of the fastest disturbances is very demanding and may not be feasible. Time-scale separation concepts are being employed as an alternative, resulting in hierarchical architectures (Tatjewski, 2008).

Control architectures designed for RTO or DRTO usually include distinct units on hierarchical levels. On an upper control layer, economically optimal steady-state setpoints or setpoint trajectories are computed by solving the (D)RTO optimization problem. On a lower layer, fast-acting controllers are employed to track these trajectories and to reject disturbances.

Recent contributions by Busch et al. (2007) and Prata et al. (2008) have introduced the concept of *dynamic predictive scheduling* (DPS) in the context of DRTO. Scheduling here refers to the planning of an economically optimal sequence of production campaigns or operational strategies on a prediction horizon. The term *operational strategy* denotes here the choice of an objective function, the specific process variable to be considered as degrees of freedom, the choice of bounds on the process variables in the optimization problem, and possibly also the choice of the process model itself.

DPS is an extension of DRTO integrating discrete decisions *and* optimal control on a receding horizon: The upper control layer optimization problem integrates the choice of the operational strategy and the calculation of control moves to realize optimal transitions between the operational strategies or production campaigns. This way, the decision on the objective, the degrees of freedom, and on the constraints to impose on the solution becomes part of the optimization problem itself. The resulting mathematical problem is a mixed-integer dynamic optimization (MIDO) problem which must be solved by appropriate methods.

⋆ We thank the German research foundation (DFG) for the financial support in the project "Optimization-based process control of chemical processes" (grant MA 1188/27-1).

⋆⋆Present address: Bayer Technology Services GmbH, 51368 Leverkusen, Germany (e-mail: jan.busch@bayertechnology.com)

Busch et al. (2007) applied this method to the optimal operation of a wastewater treatment plant. In this case the scheduling task is concerned with the planning of a sequence of control strategies that would minimize (in the order of importance) energy cost, buffer tank holdup and pollutant emissions. Each of these control objectives requires its own operational strategy. Flores-Tlacuahuac and Grossmann (2006) and Prata et al. (2008) investigated optimal polymer production problems, where an optimal production schedule with transition periods for the continuous production of polymer grades had to be determined for given quality specifications and production rates. They considered quality specifications and due dates for different polymer grades as well as economic costs caused by the transition between polymer grades. Flores-Tlacuahuac and Grossmann discretized the dynamic equations describing the grade transitions, and solved the MIDO problem using mixed-integer nonlinear programming. Prata et al. on the other hand apply a solution method proposed by Oldenburg et al. (2003), using a discretization based on single and multiple shooting. All three works have dealt with the open-loop problem only. For further examples, the reader is referred to the recent overview by Harjunkoski et al. (2009).

In this work, we consider the closed loop problem of an optimal operation of a wastewater treatment plant model. A hierarchical control architecture involving a DPS on the upper control layer, as shown in Figure 1, is proposed. The operation of the plant is disturbed by fluctuations of the wastewater feed rate and of the pollutant feed concentrations. Nominal operation of the plant is disturbed and recalculation of the plant schedule is performed.

2. WASTEWATER TREATMENT PROCESS

The type of wastewater treatment plant considered is depicted schematically in Fig. 2. The plant consists of a buffer tank of 3000 m^3 capacity, a denitrification basin and a nitrification basin with a submerged membrane filter unit. The purpose of the process is to degrade the pollutants in the wastewater, i.e. to reduce their concentrations through biochemical reactions. In the denitrification and nitrification basins (both with a volume of 1350

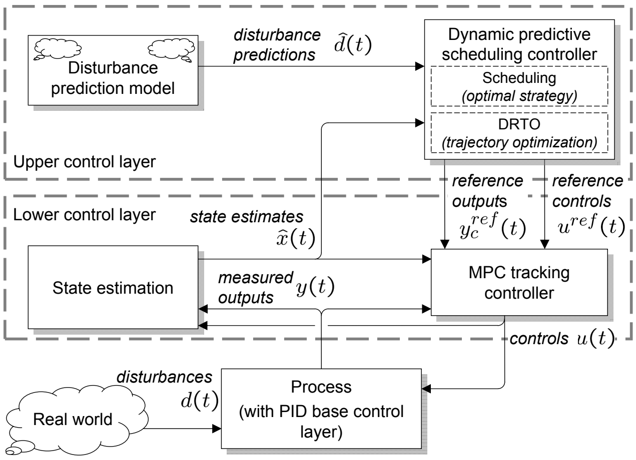

Fig. 1. Schematic of the realized process control architecture

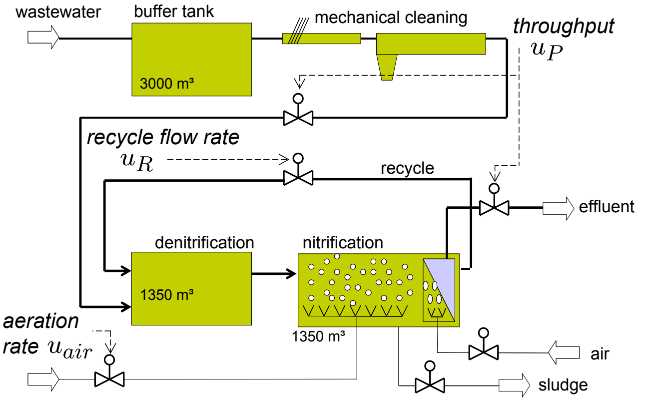

Fig. 2. Schematic flowsheet of the wastewater treatment plant

m^3), biomass is suspended in water at a concentration of several grams per liter. The denitrification basin is kept at anaerobic conditions, while in the nitrification basin aerobic conditions are established by means of intensive air injection (aeration).

Clear water is separated from the biomass-water suspension (the “activated sludge”) in the nitrification basin by means of a membrane filter, and is drawn off in the effluent. The activated sludge is recirculated to the denitrification tank. Since there is ongoing biomass growth in both basins, excess sludge is drawn off to stabilize the biomass concentration.

The process is modeled by a continuous-time differential-algebraic model consisting of mass balances for all substances in all tanks and rate equations for the biochemical reactions. The biological reactions are modeled according to the *Activated Sludge Model No. 3* by Gujer et al. (1999). This model is derived from biochemical understanding of the process and is usually regarded as the state-of-the-art for modeling municipal waste water treatment processes. All tanks are modeled as ideally mixed vessels. It is assumed that no biochemical reactions take place in the buffer tank. The oxygen transfer rate into the nitrification basin is assumed to be controllable by the aeration rate u_{air}. Also, the membrane filter is assumed to retain all suspended matter in the nitrification basin, while soluble matter passes the membrane unhindered. The complete index-1 process model consists of 55 differential equations and 246 algebraic equations.

2.1 Control problem

Due to varying feed flow rates and pollutant concentrations, the wastewater treatment process is always transient and does not settle into a steady state. Both the feed flow rate and the concentrations of major pollutants follow daily, weekly and yearly patterns influenced by human domestic activities, industrial activities, weather conditions and other environmental factors. The main pollutants are organic substrate, nitrate and ammonium. Their degradation depends on the residence time in the biological basins, and the availability of oxygen and organic substrate.

Nitrate is degraded in the denitrification basin at low oxygen concentrations, while ammonium is degraded in the nitrification basin at high oxygen concentrations. Since nitrate is also produced as a byproduct of the nitrification reaction, setting the recycle too low will give high nitrate content in the effluent. However since oxygen can be carried over from the nitrification back to the denitrification, process operation must at the same time prevent a destabilization of the process by excessive recycling or aeration.

The manipulated variables (Fig. 2) are

- plant throughput flow rate u_P,
- recycle flow rate u_R, and
- aeration intensity u_{air} in the nitrification basin.

The controlled variables are

- buffer tank holdup,
- ammonium concentration in the effluent, and
- nitrate concentration in the effluent.

2.2 Operational strategies for the wastewater plant

Stable operation of the plant means reducing effluent pollutant concentrations as much as possible and stabilizing the buffer tank holdup at a low level, while keeping the power consumption below a critical level u_{air}^{crit}. This corresponds to keeping power consumption within utility contract levels, which is a real concern in many industrial operations.

However, the operational strategies that are needed to fulfill these objectives simultaneously are in conflict with one another: To reduce the effluent concentrations as low as possible, the plant needs to operate at a low throughput rate, high recycle rate and medium aeration intensity, resulting in a high residence time and consequently the highest possible elimination of pollutants. On the other hand, when the feed rate to the plant is large or the buffer tank holdup close to its maximum, the throughput flow rate has to be set high, the recycle rate low, and the aeration to the upper tolerable limit to ensure that ammonium and nitrate can still be eliminated, despite a low residence time in the biological basins. Lastly, when the pollutant concentration in the wastewater cannot be reduced below effluent limits using only the critical aeration, the aeration is increased beyond u_{air}^{crit} causing contract costs. The control objective is then to keep the excess power consumption as low as possible while still reaching the effluent limits. This is achieved by setting the throughput as low as possible while balancing aeration and recycle flow. Ammonium has to be degraded fully in the nitrification basin, but without carrying too much oxygen over into the denitrification basin.

In order to manage these conflicts, the DPS method is applied such that the best operational strategy can be determined by solving the discrete-continuous optimization problem. A hierarchy of control objectives is defined as follows, from the highest (1) to the lowest priority (4):

(1) *Off-spec strategy:* If ammonium and/or nitrate effluent concentrations are beyond the allowed effluent limits, then reduce ammonium and nitrate effluent concentrations below the limit as quickly as possible.
(2) *Economic strategy:* If ammonium and nitrate concentrations cannot be reduced below a given limit using less than a critical aeration intensity u_{air}^{crit}, then reduce the square of the excess energy consumption $\Delta u = (u_{air} - u_{air}^{crit})^2$.
(3) *Flexibility strategy:* If aeration can be set below the critical limit; and if ammonium and nitrate effluents can be reduced below their effluent limits, then reduce the buffer tank holdup to its lower limit as quickly as possible.
(4) *Ecological strategy:* If the buffer tank holdup is at its lower level, if aeration can be set below the critical level, and if the nitrate effluent can be reduced below its effluent limit, then reduce the ammonium effluent to the lowest possible value.

2.3 Simulation scenario

The optimal trajectories are calculated on a receding horizon of three days, based on a prediction of the feed rate and the feed concentrations, which are assumed to be available to the DPS controller. This includes the prediction of a rain event that causes the feed volume to the plant to peak on day 5. Fig. 3(a) shows the predicted and actually realized feed rates, while Fig. 3(b) shows the ammonium and nitrate concentrations realized in the plant simulation. The concentrations are adapted from typical municipal wastewater compositions, with CSB between 600 and 800 g/m^{3}and total nitrogen between 30 and 60 g/m^3. The actual feed rate realized in the plant simulation will differ slightly, by having the rain event take place 4 hours later than anticipated, lasting 12 hours longer but causing 10% less total rainfall. Also, the simulation includes an unpredicted pollution event which causes a peak in the ammonium and nitrate concentrations on day 2.

3. HIERARCHICAL CONTROL ARCHITECTURE

Motivated by the control problem outlined in the previous section, the properties of the control architecture in Fig. 1 can be explained in more detail. The plant is operating under the influence of some external disturbances d. Measured outputs y and y_c are available, with y_c being the subset of controlled variables. On the upper control layer, the plant disturbances (feed rate and feed concentrations)

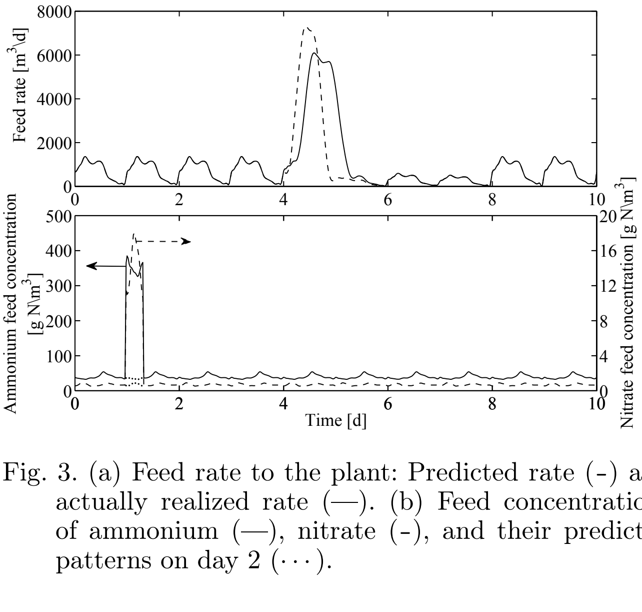

Fig. 3. (a) Feed rate to the plant: Predicted rate (-) and actually realized rate (—). (b) Feed concentrations of ammonium (—), nitrate (-), and their predicted patterns on day 2 (· · ·).

are predicted by the disturbance prediction model $\hat{d}$. A sequence of operational strategies and optimal transitions have to be found which lead to ecological and economic plant operation on the control horizon. The DPS controller performs this task by a solution of the associated discrete-continuous optimization problem, using the current state estimate $\hat{x}$ as initial value vector. The (open-loop) problem formulation is described by Busch et al. (2007) and will not be repeated here.

The optimal control moves and the predicted outputs computed by the DPS algorithm are passed to the MPC tracking controller as reference control trajectories $u^{ref}(t)$ and reference output trajectories $y_c^{ref}(t)$. The tracking controller keeps the controlled outputs y_c close to the reference trajectories, using an input-output model derived from a linearization of the process model around the current state estimate $\hat{x}$. The tracking controller operates in delta-mode, adding its control moves to the reference $u^{ref}(t)$.

All modules on the upper and lower layers were implemented in Matlab for this study. The process is simulated in gPROMS (PSE Ltd., 2004). The DPS problem is solved in the dynamic optimization software DyOS (AVT.PT, 2009).

3.1 DPS controller

The optimal control problem is formulated as a multi-stage, mixed-integer dynamic optimization problem which is solved at every time t_k on the receding horizon $[t_k, t_k + T_h]$, i.e.

$$\min_{u_{jk}, Y_{jk}, t^f_{jk}} \sum_{j=1}^{N_{st}} \phi_j \left(Y_{jk}, x_j(t^f_{jk}), u(t^f_{jk}), d(t^f_{kj}) \right) , \tag{1a}$$

$$\text{s.t.} \quad \dot{x}_j = f_j(Y_{jk}, x_j, u_{jk}, d) , \tag{1b}$$

$$0 \geq g(Y_{jk}, x_j, u_{jk}, d) , \tag{1c}$$

$$0 = h(Y_{jk}, x_j(t^f_{jk}), u_{jk}(t^f_{jk}), d(t^f_{jk})) , \tag{1d}$$

$$x_1(t_k) = \hat{x}_k , \tag{1e}$$

$$d(t) = \hat{d}_k(t) , \tag{1f}$$

$$0 = \Gamma(x_j, x_{j+1}) , \tag{1g}$$

$$0 = \Omega(Y_{1k}, \ldots, Y_{N_{st}k}) , \tag{1h}$$

with u_{jk} the control vector applied on stage j at time t_k, Y_{jk} the integer-valued strategy choice and t^f_{jk} the end time of stage j at time t_k, N_{st} the number of stages, ϕ_j the objective function on stage j, x_j the differential variables on stage j and $\hat{x}_k$ their most current estimate, g the path constraints, h the endpoint constraints, $d(t)$ the time-varying disturbances and $\hat{d}_k(t)$ their predictions at time t_k, Γ the transition conditions between the stages and Ω the conditions that the strategy sequence $\{Y_{1k}, \ldots, Y_{Nstk}\}$ must fulfill. The details of the related open-loop formulation are given by Busch et al. (2007).

Problem (1a) is solved using a MIDO strategy which combines a variant of the outer-approximation method tailored to dynamic optimization (Oldenburg et al., 2003) with the adaptive control vector discretization method developed by Schlegel et al. (2005). The reference trajectories are recalculated for updated process state variables and new disturbance predictions at the start of every day, i.e. at time zero and then every 24 hours. For this case study, it is assumed that disturbance predictions are made available once per day, for example from weather forecasts or monitoring of the sewer network.

3.2 MPC tracking controller

A linear time-variant MPC algorithm is used to track the reference inputs and outputs u^{ref} and y_c^{ref} on the lower control layer. A quadratic objective function is formulated,

$$\min_{\delta u} \quad \phi = \frac{1}{2}\delta y_c^T Q \delta y_c + \frac{1}{2}\delta u^T R \delta u + \frac{1}{2}\Delta u^T S \Delta u , \tag{2a}$$

$$\delta y_c = y_c^{ref} - y_c , \tag{2b}$$

$$\delta u = u^{ref} - u , \tag{2c}$$

$$\Delta u = \delta u(t_i) - \delta u(t_{i-1}) , \tag{2d}$$

with Q, R and S positive definite weighting matrices. δy_c and δu are vectors of the deviations at discrete times on the prediction horizon between the plant outputs y_c and their time-varying references y_c^{ref}, and between the control inputs u and their time-varying reference trajectories u^{ref}, respectively. The rate of change Δu from time t_{i-1} to the current time t_i is weighted against δy_c and δu to prevent excessive control movement. The sampling time of MPC is set to one hour.

3.3 State estimation algorithm

In previous work, Busch et al. (2009) investigate state estimation methods for wastewater treatment processes. Since DRTO is inherently a state feedback control method and thus dependant on the estimation of unmeasured states from plant outputs, the effect of faulty state estimation has to be investigated as well. In wastewater treatment processes, estimating the unmeasured states is generally not an easy task since many model states are only indirectly observable by lumped measurements like the total chemical oxygen demand, the total nitrogen concentration or the total amount of suspended biomass. For this study, the sensor placement determining the output variables y was chosen such that the simulated linear system was observable at all times, using available measurements of ammonium, nitrate, oxygen, pH, total suspended solids and total chemical oxygen demand. This is similar to the approach taken by Busch et al. (2009) where an optimization-based method for sensor placement in wastewater treatment plants is proposed. This sensor placement strategy does not guarantee observability of the nonlinear system, though it yields a reasonable sensor configuration resulting in satisfactory estimation performance. A constrained EKF algorithm (Gesthuisen et al., 2001) is implemented to prevent negative concentration estimates.

4. CONTROL PERFORMANCE

In open-loop, each of the disturbances described in Section 2.3 would lead to highly undesirable results, such as significant violation of the ammonia effluent limits following the feed concentration disturbance on day 2, and an overflow of the buffer tank following the rain event on day 5. Perfect control performance would instead reject the feed concentration disturbance in the shortest amount of time possible, and handle the rain event by using the buffer capacity for intermediate storage of the wastewater feed. The operational strategies should be planned accordingly. At optimal control performance, ecological operation (strategy 4) should also be pursued for the maximum time feasible.

4.1 Scheduling of operational strategies

Fig. 4 shows the controlled and the manipulated variables. The strategies chosen by the dynamic predictive scheduler are shown by the shaded areas. As can be seen, the optimal strategy on the first and second day is the flexibility strategy (3). During this time the buffer tank holdup is reduced from 30% to 20% of its maximum capacity (3000 m^3), permitting a switch to the ecological strategy (4) at the earliest possible time. With the recalculation of the strategies at the beginning of day 2, the ammonium concentrations are detected to be beyond the bound of 1 gN/m^3. As a result the plant switches briefly to the off-spec strategy (1). Following the strategy prioritization described in Section 2.2, the off-spec strategy (which permits intensive use of aeration and high throughput) is applied only for the shortest possible amount of time, followed by the flexibility strategy and then again the ecological strategy. Control moves are computed to give the fastest possible transition from the off-spec strategy back to the ecological strategy. The ecological strategy is pursued from day 2 to day 5, and the ammonium concentration is reduced from 1 gN/m^3 to 0.4 gN/m^3. This is achieved by a throughput of less than 1000 m^3/d, and a recycle flow rate of 100 m^3/d. On day 5 the rain event takes place, requiring a switch first to the economical strategy (2) and then to strategy 3. The buffer tank holdup rises quickly towards the upper limit of 3000 m^3. The ammonium effluent concentration is maintained near its limit of 1 gN/m^3 by adjusting the aeration rate and recycle flow rate accordingly. On day 8, the buffer tank holdup is found to be below the minimum value of 300 m^3. The off-spec strategy (1) is applied again, and the plant is temporarily operated at a lowered throughout flow rate of 200 m^3/d.

4.2 Reference tracking

Reference tracking performance is depicted in Fig. 5. The reference trajectories consist of the setpoints for the input and output variables that are passed from the DPS to the MPC on the lower control layer. The actually realized input trajectories in Fig. 5(a)-(c) are the control values that were computed by the MPC in order to force the output values Fig. 5(d)-(f) towards their reference trajectories. It can be seen in Fig. 5(b)-(d) that the MPC controller is particularly active on day 1, 5 and 6 when the recycle rate is adjusted to compensate for the offset between the expected and measured ammonium concentration.

In Fig. 5(d-e) the effects of the feed concentration disturbance on day 2 can be seen. From the reference trajectories it is expected that neither nitrate nor ammonium should break through, and that the aeration rate should remain at 550 1/d throughout day 1 and 2. It can be seen that the ammonium concentration could be tracked fairly accurately on day 1 and 2, while the nitrate concentration was higher than expected from the reference trajectory (dashed line in subfigure (e)). This is caused by the tuning of the tracking controller, which was set to prefer accurate tracking of the ammonium concentration over the nitrate concentration. During the rain event the references could be tracked more accurately, as can be seen on day 5 and 6 where no comparable concentration spikes occur. Here,

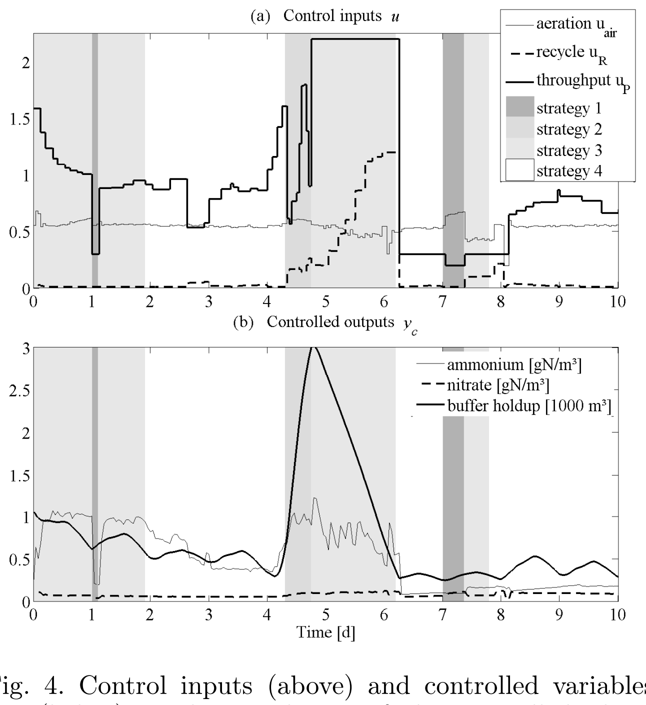

Fig. 4. Control inputs (above) and controlled variables (below) in the simulation of the controlled plant. The shaded areas show where different strategies were applied.

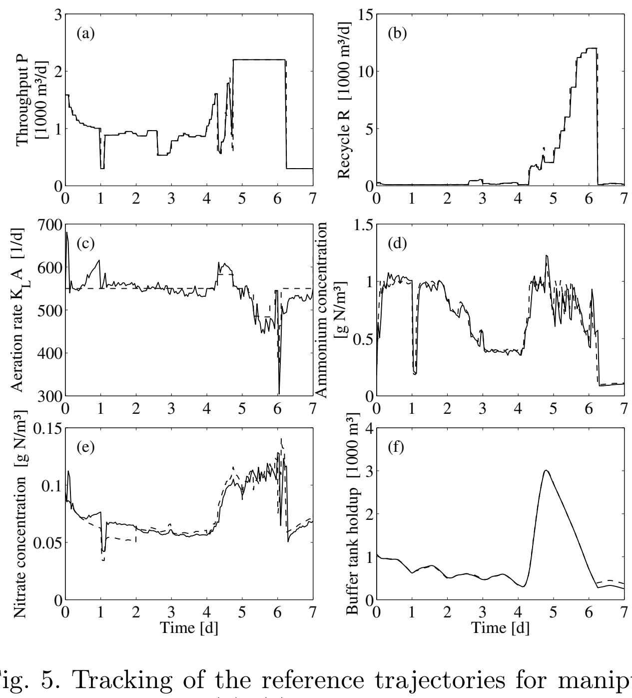

Fig. 5. Tracking of the reference trajectories for manipulated variables (a)–(c) and controlled output variables (d)–(f): Reference trajectories (-) and actually realized trajectories (—)

too, an offset between expected and measured ammonium concentration is visible (Fig. 5(d), time 4 to 5).

4.3 State estimation

The performance of the state estimation can be assessed from Fig. 6 where the estimates and the true values of selected process states are shown. All estimates were initialized at time zero at 120% of their true values. The covariance matrix was initialized with values corresponding to 5% process noise for all concentration estimates. In total 33 concentrations were estimated. With the exception of inert substances such as the soluble inerts in the buffer tank (Fig. 6(a)) and in the denitrification basin (Fig. 6(c)) the estimation performance is generally satisfying, as estimates follow and eventually converge to their true values. However it is likely that the offset between expected and measured effluent concentrations, as explained in Section 4.2, is caused by the inaccurate state estimation at time zero and time 4 in some of the measured states. However with all states showing some estimation error and none (except the inert substances) showing particularly bad estimation, it is impossible to exactly tell which states caused the offsets.

5. CONCLUSION

A hierarchical control architecture for integrated predictive scheduling, DRTO and tracking control of a wastewater treatment plant is presented. A simulation study shows the interdependency of the different control layers. It is shown how operational strategies are planned on a moving horizon, anticipating changes in operating conditions such as a surge in the feed volume. An unpredicted disturbance caused by a pollution event can be reasonably controlled by the MPC tracking controller and a recalculation of the reference trajectories. The model states can be estimated with good accuracy, allowing for accurate reference trajectories. Besides improved controller tuning, future work will aim at developing a control framework that can be applied to the operation of real wastewater treatment plants. As a next step, the DPS and MPC control setup will be tested by applying more protracted disturbances to the plant simulation. The effect of model inaccuracies, which were neglected in this study, will be examined. Also, delta-mode MPC which was used for tracking control may be replaced by a control algorithm more suited for DRTO, such as neighboring extremal updates (Würth et al., 2009).

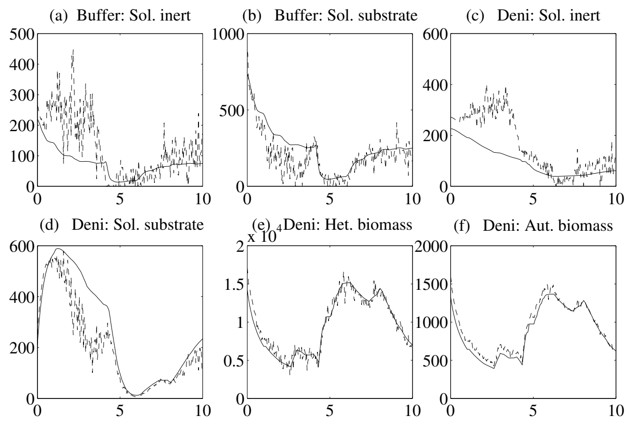

Fig. 6. Performance of the state estimation for selected states. Solid lines: Real states, dashed lines: Estimated states. All states are given in $gCOD/m^3$.

REFERENCES

AVT.PT Process Systems Engineering (2009). *DyOS User's Guide, release 2.3.* RWTH Aachen University, Germany.

Busch, J., Oldenburg, J., Santos, M., Cruse, A., and Marquardt, W. (2007). Dynamic predictive scheduling of operational strategies for continuous processes using mixed-logic dynamic optimization. *Comput. Chem. Eng.*, 31(5-6), 574–587.

Busch, J., Kühl, P., Schlöder, J.P., Bock, H.G., and Marquardt, W. (2009). State estimation for large-scale wastewater treatment plants. In *ADCHEM09 Symposium on advanced control of chemical processes, July 11–15, 2009.*

Flores-Tlacuahuac, A. and Grossmann, I.E. (2006). Simultaneous cyclic scheduling and control of a multiproduct CSTR. *Ind. Eng. Chem. Res.*, 45, 6698–6712.

Gesthuisen, R., Klatt, K.U., and Engell, S. (2001). Optimization-based state estimation – a comparative study for the batch polycondensation of polyethyleneterephthalate. In *Preprints of European Control Conference, Porto, Portugal*, 1062—-1067.

Gujer, W., Henze, M., Mino, T., and van Loosdrecht, M. (1999). Activated Sludge Model No. 3. *Wat. Sci. Tech.*, 39(1), 183–193.

Harjunkoski, I., Nyström, R., and Horch, A. (2009). Integration of scheduling and control–theory or practice? *Comput. Chem. Eng.*, 33(12), 1909 – 1918.

Helbig, A., Abel, O., and Marquardt, W. (2000). Structural concepts for optimization based control of transient processes. In F. Allgöwer and A. Zheng (eds.), *NMPC - Assessment and Future Directions, Ascona, Switzerland, 3.-5.6.1998.*

Oldenburg, J., Marquardt, W., Heinz, D., and Leineweber, D.B. (2003). Mixed-logic dynamic optimization applied to batch distillation process design. *AIChE J.*, 49(11), 2900–2917.

Prata, A., Oldenburg, J., Kroll, A., and Marquardt, W. (2008). Integrated scheduling and dynamic optimization of grade transitions for a continuous polymerization reactor. *Comput. Chem. Eng.*, 32(3), 463–476.

PSE Ltd., London, UK (2004). *gPROMS 3.0.4 Introductory User Guide.*

Qin, S.J. and Badgwell, T.A. (2003). A survey of industrial model predictive control technology. *Control Eng. Pract.*, 11, 733–764.

Schlegel, M., Stockmann, K., Binder, T., and Marquardt, W. (2005). Dynamic optimization using adaptive control vector parameterization. *Comput. Chem. Eng.*, 29(8), 1731–1751.

Tatjewski, P. (2008). Advanced control and on-line process optimization in multilayer structures. *Annu. Rev. Control*, 32(1), 71 – 85.

Würth, L., Hannemann, R., and Marquardt, W. (2009). Neighboring-extremal updates for nonlinear model-predictive control and dynamic real-time optimization. *J. Process Cont.*, 19, 1277—1288.