MODEL SIMULATION FOR IMPROVED OPERATION AND CONTROL OF WASTEWATER TREATMENT PLANTS

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INTRODUCTION

In the current operation of wastewater treatment plants one finds that automation, while introduced in the late sixties (Buhr et al., 1974), can still be considered minimal. Few plants are equipped with more than some elementary sensing elements and control loops, mostly concerning flow metering and control. Since the early seventies, when a major leap forward was made by the widespread introduction of dissolved oxygen control, little progress has been made.

It is, however, worthwhile to confront this with the potential benefits of the use of dynamic models and control systems as put forth by Andrews (1974) some 20 years ago:

Performance:	Maintaining plant efficiency closer to its maximum by improved operation;
Productivity:	Increasing the amount of waste that can be treated per unit process capacity;
Reliability:	Decreasing the frequency of gross process failures with concomitant wastewater bypassing;
Stability:	While appearingly highly stable processes, occasional upsets may have important consequences that could be avoided by increased process control;
Personnel:	Run plants with less skilled personnel or decrease time devoted to plant management;
Operation:	Reducing chemical and energy consumption;
Start-up:	The procedure for start-up of new treatment plants can be shortened;
Guidelines:	Dynamic models can be used to make up procedures/control charts for manual operation that summarise the obtained experience from model simulations;
Dynamic Operation:	Improving performance by taking advantage of process dynamics
Variable Efficiency:	Integrating the dynamics of the receiving waters within the control of the treatment plant so as to match the assimilative capacity of the receiving waters;

Clearly, this list of potential benefits of the use of models and control systems still holds. However, the increased public awareness as reflected in more stringent regulations, has considerably increased the requirements imposed on treatment plants compared to the time this list was compiled. Not only the organic carbon pollution of a wastewater must now be eliminated, but to this has been added the removal of nutrients (nitrogen and phosphorous). With biological nutrient removal being the most economic way of treatment in most cases, rather complex process configurations have resulted. The numerous interactions that occur among the different unit processes and the fact that the biological potential is taken to its limits make that nutrient removal plants are rather vulnerable to external disturbances or erroneous manipulations. Hence, the increased complexity due to this process integration has become a major driving force for the introduction of models, advanced instrumentation and control systems.

The need to make the best use of previous investments by upgrading existing plants for handling increased loads or extension with nutrient removal capability is another incentive for increased use of mathematical models. Still, in many cases, the alternative upgrade path via additional reactor volumes is still preferred notwithstanding the considerably higher capital investments. The lack of full-scale demonstrations of the potential of advanced instrumentation, control and automation is clearly one of the main reasons of the hesitation to take this route (Spanjers et al., 1998a). Hence, designers remain rather conservative, maintaining large safety margins in the plant designs (Olsson, 1993). At the same time, however, no attention is paid to the inclusion of sufficient flexibility and controllability into the plants which will be, as it is for current plants, a set-back for future upgrades (Olsson & Jeppsson, 1994).

Another effect of the changes in legislation concerns the decisions made with respect to surface or groundwater use in industrial processes. The imposed limitations are such that total recycling of process water has become an issue in certain industries, e.g. textile industry. Hence, the wastewater treatment becomes part of the production process and consequently, quality control of the effluent becomes much more important since failure of the treatment process may lead to important production losses. Control of the treatment plant therefore becomes a bare necessity. Note that this development means that wastewater treatment is finally no longer regarded as a non-profit process.

AIM OF THE CONTRIBUTION

The paper aims to give a concise overview on the use of mathematical models in control systems of treatment plants. The following topics will be covered:

1) Support of mathematical models in the design of control structure
2) Model-based tuning of control schemes
3) Controllers with embedded process models
4) Software sensors
5) Model use for disturbance prediction in feedforward control
6) Time-varying effluent quality description

BUILDING BLOCKS OF A CONTROL SYSTEM

Before introducing the different application areas of mathematical models, it is good to shortly review the four building blocks on which a control system is always based (Figure 1): 1) insight in the plant operation as summarised in a proper process model; 2) sensors that provide on-line data on some of the output variables of the process and disturbances acting upon it; 3) adequate control strategies which try to minimise deviations ε from the objectives and 4) actuators which implement the controller outputs on the plant.

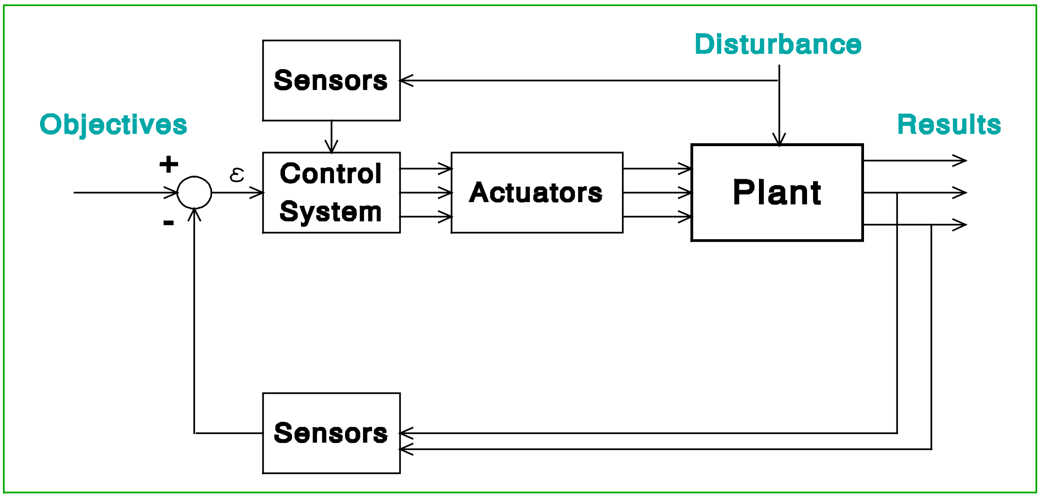

Figure 1 *The building blocks of a control system*

CONTROL SYSTEM STRUCTURES

Conventional Feedback Control

Although the process is inherently multiple input multiple output (MIMO), the different time constants of a wastewater treatment system (ranging between minutes for DO dynamics to days for the sludge composition), allows to decouple the many control actions into separate single input/single output (SISO) controllers (Olsson & Jeppsson, 1994, Steffens et al., 1997). Classic examples of SISO controllers are the on/off and PID-controllers. Although optimal control performance cannot be expected from conventional PID or on/off controllers for the timevarying, nonlinear processes considered, their widespread use in industry and the resulting familiarity with their properties and concepts for design, have made that these regulators are the most widely applied in wastewater treatment processes and this already for a long time (Andrews, 1974; Marsili-Libelli, 1989; Heinzle et al., 1993; Spanjers et al., 1998b; Olsson & Newell, 1999). The control action of a PID-control system is based on the following formula in which the time evolution of the difference *e(t)* between desired and measured behaviour is used to assign the control action *u(t)*:

$$u(t) = u_0 + K_C \left[e(t) + \frac{1}{\tau_I} \int_0^t e(t)\,dt + \tau_D \frac{de(t)}{dt} \right]$$

The three coefficients K_p, τ_I and τ_D are weights given to the proportional, integral and derivative action respectively. In order to tune the parameters of the controller, it is necessary to gain insights in the dynamics of the process. This information is typically obtained by experimentation on the real plant. However this may endanger process performance since important disturbances may be required to obtain the necessary data (Dunn et al., 1992). As an alternative one can use a reliable process model to simulate plant behaviour under a wide range of disturbances and concomitantly tune the controller (Vaccari et al., 1988; Marsili-Libelli, 1992; Heinzle et al., 1993; Spanjers et al., 1998a; Alex et al., 1999; Janssen et al., 2000). Hence, a first application of mathematical models, i.e. as a support for the tuning of control systems, is introduced here.

Optimal Feedback Control

Controller design methods have been developed which aim to devise a controller that extremises a certain criterion function *J* which typically consists of a weighted function of the tracking error *e(t)* and the efforts *u(t)* required:

$$J = \int_0^t \left[e^2(t) + \gamma u^2(t) \right] dt$$

In case a linear model adequately describes process behaviour, the classical linear quadratic (LQ) regulator theory can be used to design an optimal feedback controller (Marsili-Libelli, 1989).

For nonlinear models, linearisation around the desired operating point can be used. Fan et al. (1973) and Steyer et al. (1995) derived (approximative) optimal feedback controls of the influent flow rate on the basis of effluent substrate concentration measurements. Devisscher et al. (2000) successfully designed a LQ controller for an equalisation system in an industrial WWTP. Other LQ-examples for sludge recycle and dissolved oxygen control are reported in Marsili-Libelli (1989) and for nitrogen removal by, for instance, van Schagen et al. (1995) and Weijers et al. (1997).

When nonlinear models are the only reasonable means to describe the process dynamics, the problem becomes much more intractable. Only a few results of an analytical solution of the optimal control law have been published (d'Ans et al., 1971; Herremans et al., 1997). A solution is to approach the optimisation problem by numerical means and a number of (simulation) exercises have been performed (Sincic & Bailey, 1978; Yeung et al., 1980; Marsili-Libelli, 1982; Kabouris et al., 1992; Demuynck et al., 1994). The main problem with the resulting control strategies is that no closed-loop solution is obtained and that the optimal control solution relies on the (unrealistic) assumption of a perfect process model with fixed model structure and parameters. von Jeszensky and Dunn (1976) and Yeung et al. (1980) showed indeed that the optimal control actions depend to a large extent on the model structure. Therefore, in view of the uncertainty on the correct model and the inherent nonstationarity of the process, one should be cautious with the implementation of such control schemes. Possible means of dealing with this problem are to incorporate adaptivity in the optimal control law (Van Impe et al., 1992) or to make the controller robust against model deficiencies, either in the parameters or in the model structure (Steyer et al., 1995; Devisscher et al., 2000).

Another approach in which optimal control actions are calculated numerically is the so-called model-based predictive control approach. In this, a process model is used to predict how the system would behave under a proposed sequence of control actions $u(t)$ (Figures 2 and 3). Traditionally a linear model is used in e.g. the DMC model-based predictive control algorithm and an analytical solution of the optimal control action can be calculated (Oggunaike & Ray, 1994). This approach was adopted by Weijers et al. (1997) showing the limitations of the linear approximation of the process dynamics. When nonlinear models are used in the algorithm, a numerical search algorithm is used to compute an optimal sequence $u^{Opt}(t)$ (for the process model that is!). To reduce the effects of model mismatch, only the first action of the sequence is implemented on the process after which the optimisation exercise is reiterated. Evidently, model updating can be performed to reduce the mismatch between process behaviour and model predictions. More details can be found in te Braake et al. (1994). Applications of model based predictive control can be found in Patry and Takàcs (1995); Weijers et al. (1997); Hoen et al. (1998) and Lukasse (1999).

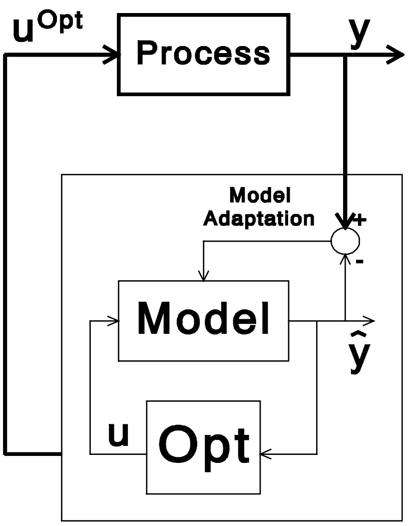

Figure 2 *Principle of MBPC*

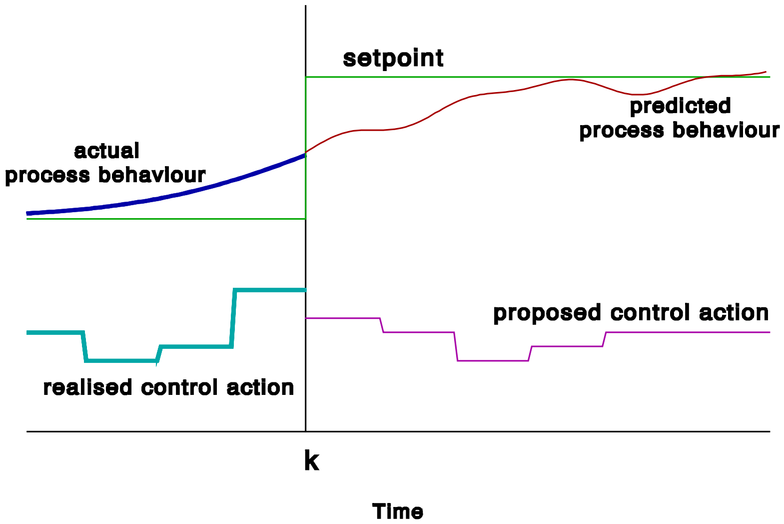

Figure 3 *Typical calculation performed by a MBPC algorithm*

MIMO control

The large span of time constants associated to the different (sub)processes allows to decouple their control to a certain extent. As mentioned above, this allows the use of SISO control schemes. It can be expected though that performance improvements can be obtained by considering the MIMO nature of the process during controller design (Weijers, 2000). Nielsen and Onnerth (1995) provided a good example of this by showing the advantage of a two-input control of a denitrification reactor: both the carbon addition and the oxygen supply were manipulated for the control of effluent nitrate. Moreover, in this work the cost/benefit was clearly proven at a full-scale WWTP.

One should be aware though that controller design problems may arise due to the increased number of feasible, alternative configurations of control loops (Stephanopoulos, 1984; Weijers, 2000). Lech et al. (1978ab) also exemplified that interactions between control loops may lead to process instability. MIMO controller design techniques therefore aim for complete elimination of the interaction between loops (Stephanopoulos, 1984). Mathematical models are extremely useful during the design phase as they allow to quickly review different possible configurations and evaluate potential instabilities. A simulation example of a decoupling MIMO control scheme for a carbon removal wastewater treatment plant can be found in Van Impe et al. (1991).

Feedforward Control

Feedback control is hampered by the fact that first a deviation of normal behaviour must surface before any corrective action is taken. In cases where large dead times exist or where the system reacts only slowly to the manipulations, the system may seriously deviate from desired behaviour. The characteristics mentioned above make wastewater treatment processes exemplary for this category of systems.

In a feedforward control scheme the knowledge on upcoming disturbances is used to the benefit of a treatment plant's operation by preparing it to cope with for instance toxic loads, important hydraulic disturbances or increased organic loading. Theoretically, complete compensation of the disturbances can be obtained provided the disturbance is measured or predicted (see further), a perfect process model exists and unlimited control authority is available. It must be clear that the current state of knowledge is far from satisfying these conditions. However, the advantages of feedforward control actions should not be discarded and a combination with feedback correction may be very beneficial. In such set-up, the feedforward part of the controller aims to anticipate for the effect of measured disturbances, while the feedback part corrects for any deviations that result from the deficiencies in process model, control limits and inadequate measurement or prediction of the disturbance(s).

Ratio control is a simple feedforward control algorithm that consists of setting a control variable proportional to the disturbance. The model used in this type of feedforward controller is therefore very simple. A classical example is the ratio control of the sludge recycle flow rate to the influent flow rate that acts as the disturbance (Brett et al., 1973; Andrews, 1974). The goal of the control action is to maintain the sludge concentration in the aeration tank and therefore the biodegradation capacity nearly constant.

In Figure 4 the dynamic behaviour of a WWTP with constant recycle flow is compared to the behaviour of a WWTP with ratio controlled recycle in case of an important rain event. Details on the simulated system can be found in Vanrolleghem et al. (1996a). One clearly observes that the variation of the heterotroph concentration in the aeration tank is considerably lower in case of the ratio controlled system. However, if one considers the concentration of thickened sludge in the underflow of the settler, one observes that the variation of the recycle flow rate disturbs the thickening process in the secondary clarifier leading to decreased settler performance. Similar observations were made by Olsson & Jeppsson (1994) who observed that the effluent quality also deteriorated under ratio controlled recycle flow.
The conclusion must be that one unit process may suffer from the optimisation of another. Hence, it is important to make an adequate trade-off, for instance using a simulation study.

In another simple feedforward control approach, the respiration rate in the aeration tank is measured. Basically, for a given K_La - air flow relationship: $K_L a = \alpha F_{in} + \beta$, the necessary air flow rate F_{in} can be calculated from the oxygen mass balance of the aeration tank (with the inlet oxygen concentration assumed to be negligible):

$$\frac{dS_O}{dt} = K_L a\left(S_O^{sat} - S_O\right) - \frac{Q}{V} S_O - r$$

leading, for a steady state desired oxygen S_O^* value to: $F_{in} = \frac{1}{\alpha}\left(\frac{\frac{Q}{V} S_O^* + r}{S_O^{sat} - S_O^*} - \beta\right)$

As with all feedforward controls the performance of such strategy depends a lot on the quality of the underlying model that predicts the effect of the disturbance. In this case the performance depends on the accurate description of the K_La-F_{in} relationship (α, β), the appropriate values of the saturation concentration (S_O^{sat}) the volume (V) and flow rates (Q_{in}, Q_{rec}) and the respiration rate (r). Finally, it must be stressed that the desired value will only be reached under steady state conditions.

Vanrolleghem et al. (1996c) studied the potential of feedforward control to protect the plant for intoxication. Using respirometric measurements, toxicity levels of the influent could be measured and it could be shown on full-scale that control actions can be taken that protect the plant for suffering from toxicity to such an extent that the effluent quality deteriorated.

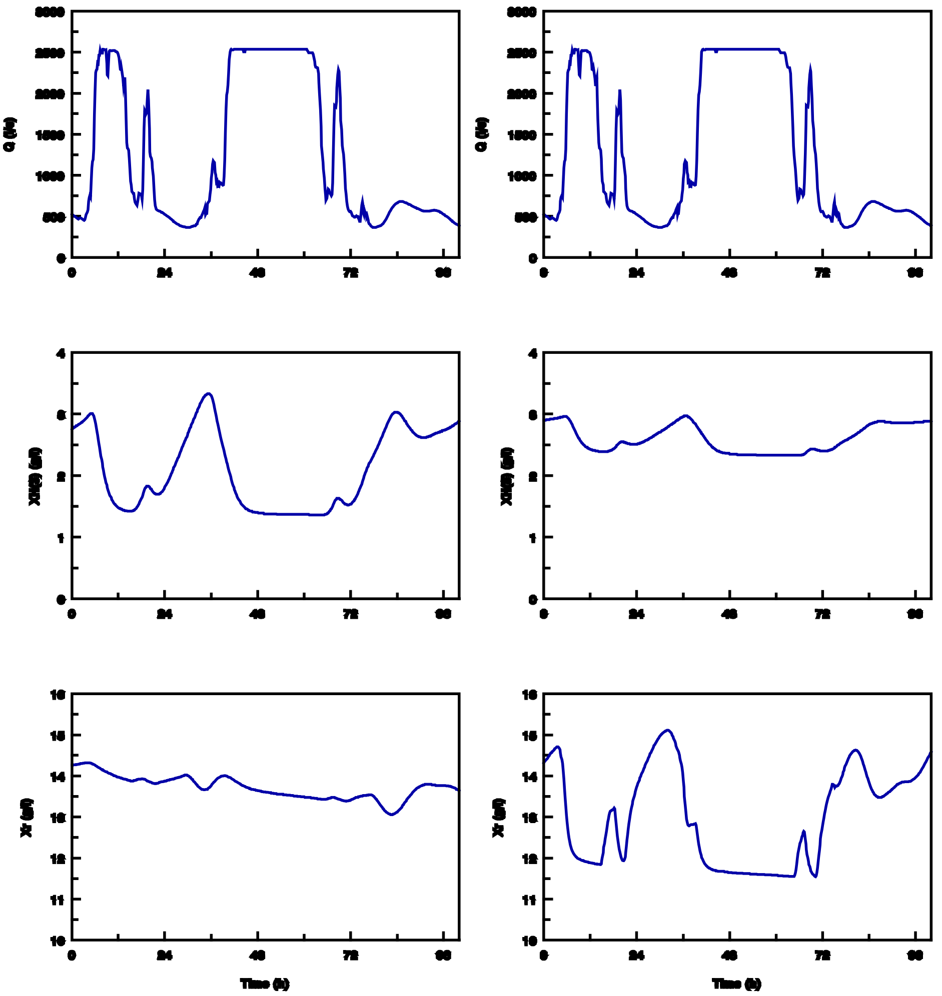

Figure 4 *Comparison of a WWTP behaviour with fixed (left) and ratio controlled (right) recycle. Influent flow (top), heterotroph concentration in aeration tank (middle) and in thickened sludge (bottom)*

Control of Nonlinear Processes

Nonlinearity is one of the features for which bioprocesses are well-known in systems' theory. It is not surprising to see new theories for the control of nonlinear systems being illustrated using bioprocesses as benchmark problems. Indeed, in biotechnology, the classical approach of linearising the nonlinear model around an operating point and applying linear theory for control design is often not acceptable due to the highly varying process conditions. This leads to new operating points where the linearised model is no longer providing a good description of process behaviour. Then, adaptation laws must be included in the controllers to accommodate for this (e.g. gain scheduling). An illustrative example of the problems induced by accepting a linearised model as part of a model based control system was given by Weijers et al. (1997).

A second design approach that deals with the bioprocess nonlinearities starts from the nonlinear model to devise a nonlinear controller which ensures that the closed-loop behaviour is linear, from which stems the term for this controller type, linearising control (Ko et al., 1982; Bastin & Dochain, 1990, Lindberg, 1997).

The design procedure is as follows. Consider a nonlinear process model with one (linear) input *u(t)* and measurements or estimates of all state variables *X(t)*:

$$\frac{dX}{dt} = f(X, u, t, \theta) + b \cdot u(t)$$

Suppose that the aim is to track a certain reference behaviour $X^*(t)$, then a control law is to be devised for manipulation of *u(t)*. To impose linear behaviour of the closed loop system, a stable linear reference model is imposed on the tracking error $e(t) = (X - X^*)$:

$$\frac{de}{dt} = -\lambda \cdot e$$

This will ensure that if an initial error *e(t=0)* will disappear according to a first order process with time constant $1/\lambda$. Rewriting this in X(t):

$$\frac{dX}{dt} = -\lambda\left(X - X^*\right) + \frac{dX^*}{dt}$$

The linearising control law is obtained by elimination of *dX/dt* between the process model and the tracking error model, yielding:

$$u = \frac{-\lambda\left(X - X^*\right) + \frac{dX^*}{dt} - f(X, u, t, \theta)}{b}$$

Note that the nonlinear process model *f* is incorporated into the control law, which makes it a nonlinear controller. The extension of linearising control towards MIMO models was presented by Dochain (1991) and applied to wastewater treatment systems in Van Impe et al. (1991) and Dochain & Perrier (1997).

Neural and Fuzzy Control

In the last decade neural networks and fuzzy logic have gained increasing attention to solve control problems characterised by ill-defined systems, for instance, the nonlinear time-varying biological wastewater treatment processes considered here. A good introduction in the field is given in te Braake et al. (1994).

Experimental data are the only source of information used to build a neural network model. An essential characteristic of the use of neural nets is the learning stage that precedes the application. During this stage, examples of desired behaviour are applied to the net and with a learning algorithm the parameters of the network model are adjusted. Once trained, neural nets can be applied for different tasks, such as process control (Miller et al., 1990; Hunt et al., 1992). For a control application, the inputs of a neural network consist of measurements of the process. A control action is then obtained as the network output. While neural control is being used in other applications and has been evaluated in biotechnological applications (Thibault & Van Breusegem, 1991; Chtourou et al., 1993), it is not as widespread implemented in wastewater treatment (Wilcox et al., 1995; Guwy et al., 1997).

In case a lot of qualitative knowledge is available (e.g. for settleability of activated sludge), fuzzy sets provide an excellent means of representing this in mathematical terms. Fuzzy control systems have been designed for the different unit processes of wastewater treatment, e.g. controlling the influent pumping rate in a sewer system (Fukano, 1993), anaerobic digestion regulation (Boscolo et al., 1993; Müller, 1997; Steyer et al., 1997), dissolved oxygen control (Kalker et al., 1997), ammonium control in a combined nitrification/denitrification reactor (Aoi et al., 1992), sludge dynamics (Marsili-Libelli, 1992; Marsili-Libelli & Gigli, 1997) and the supervision of local controllers in an activated sludge process (Couillard & Zhu, 1992; Devisscher et al., 2000).

Adaptive and Robust Control

For two reasons a need exists to adapt a control law in wastewater treatment processes. First, when the approach is taken to linearise the model of the nonlinear system under study around an operating point to design a controller, a deviation of the operating point induces the need to adjust the parameters of the control law to maintain control performance. An important example of adaptation induced by applying a linearisation of the process model can be found in the modification of the conventional PID controller, the self-tuning regulator. The adaptation of the PID parameters is essentially based on the on-line identification of a simple linear model that gives a local description of process dynamics. From this model, the optimal controller parameters are readily calculated using one or another control design criterion (Stephanopoulos, 1984). Self-tuning PID regulators are used in the adaptive control of dissolved oxygen in activated sludge plants. They were shown able to deal with changes in mass transfer efficiencies and important variations in oxygen demand (Olsson et al., 1985; Marsili-Libelli, 1990; Carlsson et al., 1994).

A second need for adaptation of the control law is due to the inherent nonstationarity of bioprocesses, e.g. adaptation of a microbial population to new wastewater composition or process conditions (e.g. temperature, see Baetens et al., 1999). Since the regulators are designed on the basis of nominal values of the process model, the need exists to adapt the controller's parameters to the new system. In the case of the linearizing control mentioned above, adaptivity is simply introduced by replacing the model parameters in the control law by their estimates obtained from an on-line parameter estimator. Applications of adaptive linearizing control have been presented for anaerobic digestion and activated sludge systems (Renard et al., 1988; Van Impe et al., 1991; Dochain & Perrier, 1997).

It is worthwhile to mention a more recent, alternative approach to deal with systems with time-varying or uncertain dynamics. In this methodology, model uncertainty is taken into account and fixed, linear time-invariant robust designs are used. A main disadvantage of these control systems is that their performance in terms of conventional performance criteria is sacrificed to ensure robustness (Gendron et al., 1993). Recently robust control theory is also applied in the field of wastewater treatment (Haarsma & Keesman, 1995; Steyer et al., 1995; Weijers, 2000).

MODEL USE IN SENSOR SYSTEMS

Sensors play a key role in control systems as they provide both information on the state of the system, the outputs from the system (which can be compared with the objectives) and the disturbances to the system for which feedforward compensation can be pursued. The aim of this section is only to review the role models play in modern "sensor systems".

Some sensors like redox (oxidation reduction potential, ORP), pH and dissolved oxygen (DO) electrodes have proven their robustness, reliability and limited demand for maintenance. Recent efforts have therefore been directed towards the extraction of as much information as possible from the primary data these sensors provide. The approach taken is to combine process knowledge (in the form of mathematical models) with these data to produce upgraded information. Such combination is called a "software sensor" (Bastin & Dochain, 1990). The data produced by these software sensors can subsequently be used in the same manner as other data to feed a control algorithm with the necessary information. In the following examples are given of such software sensing systems.

Simple Software Sensors

The ORP dynamics in batch-wise operating systems contain all information necessary to detect the disappearance of nitrate under denitrifying conditions: in Figure 5 typical patterns can be observed during the unaerated periods (where ORP decreases). These so-called "nitrate knees" reflect the disappearance from the mixed liquor of the nitrate that was formed during the preceding aerated period. Model-based methods to reliably detect such knees from the raw data were evaluated in Vanrolleghem & Coen (1995). Control based on such on-line detected nitrate knees has been applied in many instances (Wareham et al., 1993; Demuynck et al., 1994; Caulet et al., 1997).

Similar work in which specific characteristic changes in pH data series were focused upon also proved successful (Al Ghusain et al., 1994).

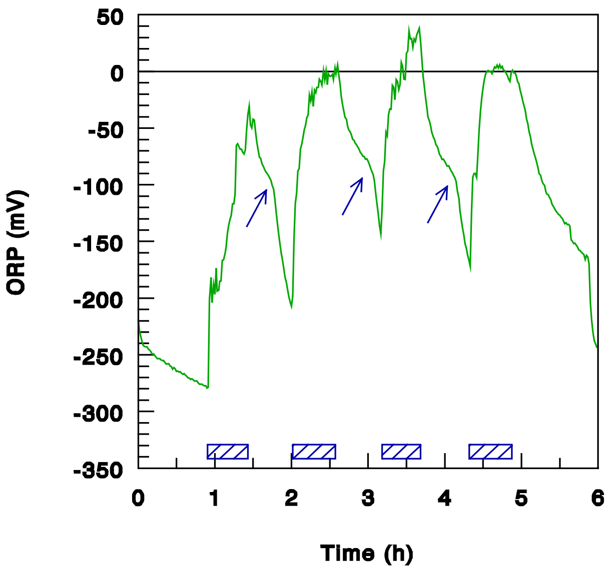

Figure 5 *ORP-data obtained from an intermittently aerated (hatched boxes) BNR plant. Nitrate knees are indicated with arrows.*

However, prior to this work on pH-profile features, an alternative way to use the monitoring of pH effects induced by biological reactions was adopted. Indeed, a difficulty related to the observation of pH changes is the buffer capacity of the liquid medium that varies with pH due to the presence of several acid-base buffer systems with pH depending buffer capacity (Stumm & Morgan, 1981). The pH variation of the liquid medium during biological reactions is thus difficult to convert into a precise number of protons that are released or consumed. The data interpretation problems caused by the pH depending buffer capacity of the liquid medium can be avoided by controlling the pH of a liquid medium at a constant pH setpoint through addition of acid and/or base. Monitoring the acid and/or base consumption rate, needed to keep the pH constant, provides the rate of proton formation or consumption due to biological reactions. This is exactly the information that is needed to monitor biological activity. It should be clear that such approach only allows to monitor processes or biological reactions that will result in a proton production or consumption.

The principle of the pH-STAT was already described in 1957, as a device that could quantify the amount of protons consumed or produced during biochemical reactions (Jacobsen *et al.*, 1957). The growing importance of wastewater treatment also resulted in the development of titrimetric sensor applications in this field. Titrimetric biosensor principles were soon developed for the nitrification process (Beccari *et al.*, 1980; Ramadori *et al.*, 1980; Aivasidis *et al.*, 1992), as an alternative to respirometry (measurement of the oxygen uptake rate, see below). In the titrimetric sensor, the stoichiometric conversion of NH_4^+ to produce 2 H^+ ($NH_4^+ + 2\ O_2 \rightarrow NO_3^- + H_2O + 2\ H^+$) is used to obtain information about the nitrification process.

A typical data-set obtained in a titrimetric sensor is depicted in Figure 6. Nitrification starts immediately after addition of the sample and continues for 25 minutes. The initial high base dosing rate is needed to quickly reach the pH setpoint. Interpreting the cumulative base addition curves can be done using a simple slope extrapolation method, assuming that nitrifying 14 mg N will produce 2 meq protons. The NH_4^+-N concentration S_{NH} (mg N/l) and the nitrification rate r (mg N/l.h) are readily calculated according to the following equations:

$$S_{NH} = \frac{2}{14} \cdot (B2 - B1)$$

$$r = \frac{2}{14} \cdot (S1 - S2) \cdot 60$$

where the intercepts B1 and B2 (obtained as illustrated in Figure 6) are expressed in meq/l units, while the slopes S1 and S2 are expressed in meq/l.min units.

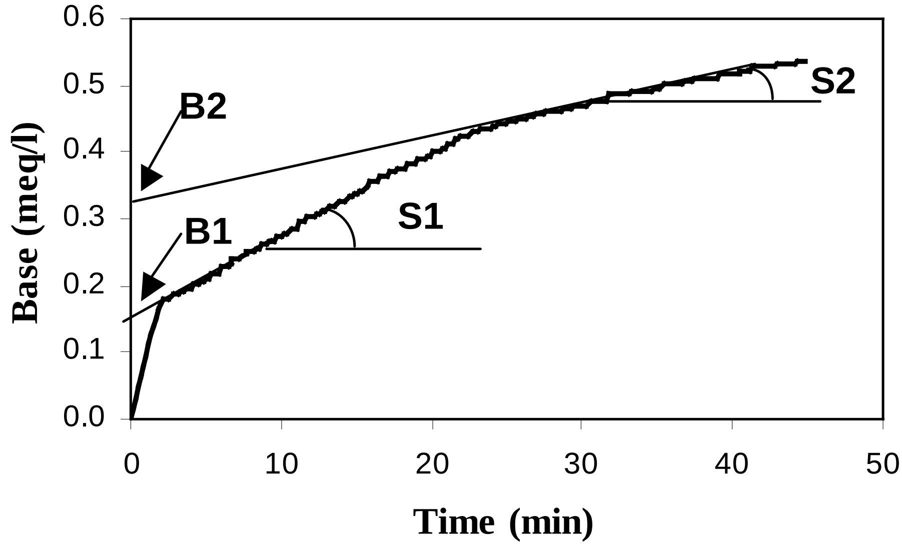

Figure 6. *Raw cumulative base addition curve obtained in a titrimetric experiment conducted with nitrifying sludge.*

Massone et al. (1995, 1998) showed that a good correlation can be obtained between the amount of ammonium added to activated sludge and the amount of ammonium measured with the titrimetric sensor. This measuring principle has been developed and applied further to the on-line measurement of the nitrification rate in activated sludge (Gernaey *et al.*, 1997), the on-line measurement of the ammonium concentration in activated sludge (Gernaey *et al.*, 1997) and even nitrifiable nitrogen (Yuan et al., 2000), the estimation of biokinetic parameters for the nitrification process, (Gernaey *et al.*, 1998, 2000; Ficara *et al.*, 2000; Petersen *et al.*, 2000a, 2000b), and the detection of toxic effects of wastewater and chemical compounds (Aivasidis *et al.*, 1992; Gernaey *et al.*, 1999; Rozzi *et al.*, 1999).

Contrary to dissolved oxygen measurements and respirometry, a pH measurement can also be used to monitor the anoxic denitrification process. Denitrification usually results in proton consumption, and this characteristic of the denitrification process is applied in titrimetric sensors. The applications include determination of volatile fatty acid concentrations (Massone et al., 1996), nitrate concentration measurement (Bogaert et al., 1997), measurement of the amount of carbon source needed to obtain full denitrification (Bogaert et al., 1997), and addition of carbon source based on measurement results provided by a titrimetric sensor (Bogaert et al., 1997; Yuan et al., 1997).

Van Vooren (2000) did not attempt to circumvent the varying buffer capacity of water samples and created an on-line sensor system in which titration curves are automatically collected and interpreted. The procedure is as follows: first, a titration curve data set is collected (Figure 7). By differentiation of the added base with respect to pH, the buffer capacity curve is obtained (Figure 8). Using mathematical models that describe the buffering of a mixture of different buffer systems, concentrations of these buffers can be calculated. The technique was successfully applied to monitor treatment plant effluents and mixed liquor samples for ammonia, bicarbonate and phosphorous contents (Van Vooren et al., 1996; Van Vooren et al., 1999). Note that, theoretically, all pollutants that are involved in acid/base reactions can be monitored (e.g. the VFA/bicarbonate alkalinity-monitor of Moosbrugger et al., 1993).

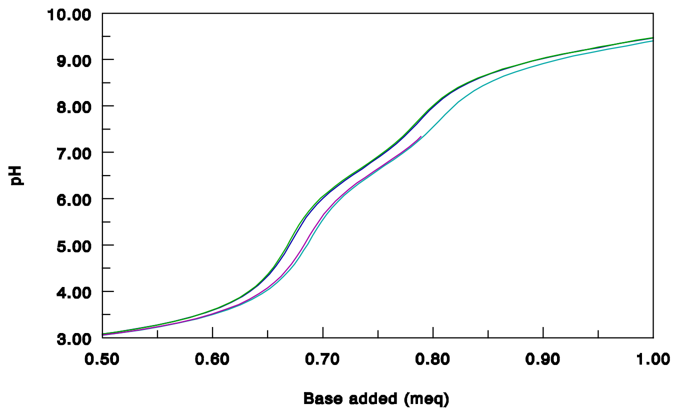

Figure 7 *Four repeat titration curves obtained for a typical treatment plant effluent.*

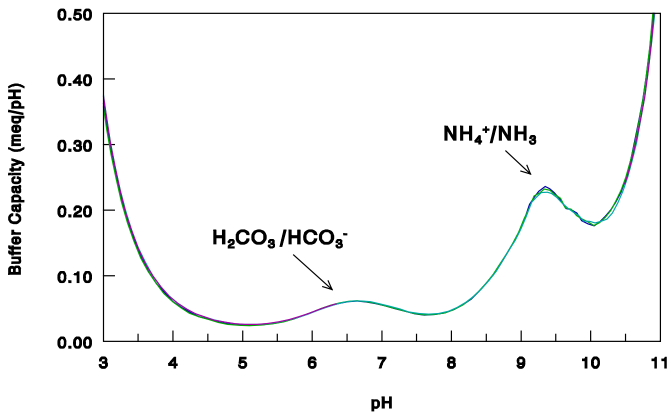

Figure 8 *Four repeat buffer capacity curves calculated from the titration curves of Figure 7.*

Dissolved oxygen probes are probably the most widely applied sensors in biological wastewater treatment plants and it is no surprise that numerous efforts have been devoted to maximise the information extracted from the raw data. Here only a simple example is given of one such software sensor used in nitrification control (Demuynck et al., 1994). With an on-off control of the aeration (aeration on if DO < 1.5 mg/l and aeration off when DO > 2.5 mg/l), a DO-profile can be obtained as in Figure 9. When the aeration is switched off, the slope of the DO-curve is equal to the oxygen uptake rate of the sludge. Therefore, the time between switching the aeration off and on is a measure of the oxygen consumption rate. In the experiment depicted in Figure 9, one clearly observes that the on/off frequency significantly drops after 90 minutes. Further evidence showed that this was the time when nitrification had completed. This information calculated (using a simple model !) can be used in nitrification control (Demuynck et al., 1994).

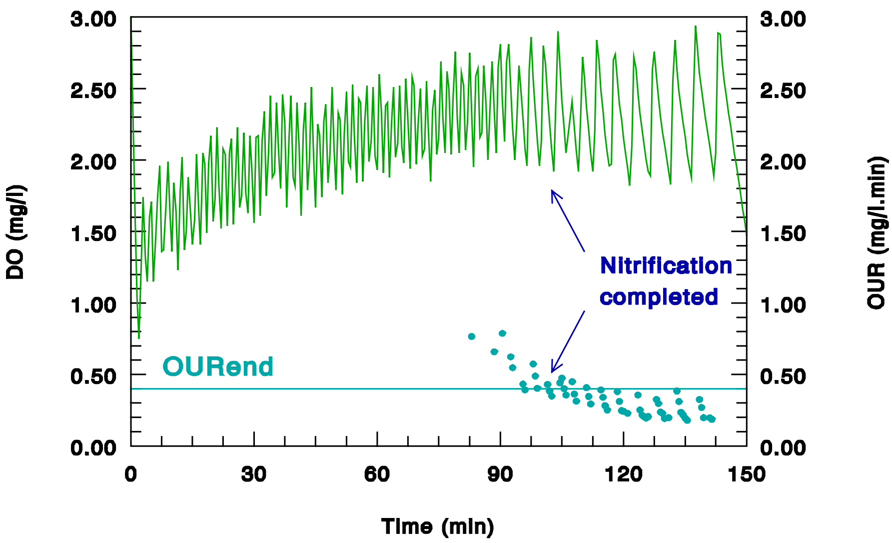

Figure 9 *DO (line) and deduced oxygen uptake rate (dots) data from a SBR for nitrogen removal. Aeration is regulated with an on/off controller (Demuynck et al., 1994).*

“Traditional” software sensors

More advanced software sensors incorporate a dynamic process model as an essential ingredient. Two types of software sensors are important, the state observers and the parameter estimators.

State observers
Starting from the (linear) state space process model:

$$\frac{dX}{dt} = AX + Bu$$
$$Y = CX$$

where *X*, the state vector, is a set of variables that are needed to describe the process behaviour, one can construct a state observer by replacing the real values by their estimates and adding a so-called "driving term" that aims to minimise the "observation error" between measured values *Y* and model predictions $\hat{Y}$:

$$\frac{d\hat{X}}{dt} = A\hat{X} + Bu + K\left(Y - \hat{Y}\right)$$
$$\hat{Y} = C\hat{X}$$

Running this observer consists of starting from an initial state estimate $\hat{X}(t = 0)$ and integrating the observer model. State estimates are then calculated on the basis of the experimental data. Remark that it is assumed that all model parameters, *A*, *B* and *C* and the input *u(t)* are known. The design of the observer now reduces to the adequate choice of the matrix *K*, known as the "gain matrix". The two approaches that have become standard, i.e. the Luenberger and Kalman observers, both start from the desire to minimize the observation error *e(t)*. The dynamics of the observation error are readily obtained by subtracting the observer equation from the process model:

$$\frac{de}{dt} = \frac{d\left(X - \hat{X}\right)}{dt} = A\left(X - \hat{X}\right) - KC\left(X - \hat{X}\right)$$
$$\frac{de}{dt} = \left[A - KC\right]e$$

The aim is now reduced to the problem of designing the gain matrix in such a way that the observation error decreases in a desirable way. Bastin and Dochain (1990) provide some support in this design problem.

Parameter estimators
As mentioned before, the time-varying nature of bioprocesses results in the need for updating the process model. As the process models in a control environment are used for on-line purposes a problem of on-line modelling results. Hence, selection of a mathematical model structure and estimation of the model parameters must be performed on-line.

In most cases (but not always, see Vanrolleghem et al., 1996c), the model structure can be assumed to remain constant and the problem may be simplified to the on-line determination of parameters. For this type of problem the second type of more advanced software sensors can be applied, i.e. the parameter estimators. A number of techniques have been proposed to incorporate the process model in the algorithm so as to improve its performance (Bastin & Dochain, 1990).

In the "observer-based parameter estimator", the observer (now with the parameters being replaced by current estimates) is used to predict the states. These state estimates are compared with the measured states. Subsequently, the observation error, reflecting the mismatch between the true parameter values and the parameter estimates, is used as the driving force in a parameter update model. In addition to the observer gain, the user must now also supply the gain matrix of the parameter updating law.

A second approach consists of rewriting the process model such that a model linear in the parameters is obtained. With a standard recursive least squares algorithm on-line parameter estimation can be performed. A number of user supplied tuning parameters must be chosen to provide an adequate convergence rate. This estimator tuning is typically done by trial and error using simulation with the process model (Bastin & Dochain, 1990).

Information Richness

On-line modelling is faced with one particular problem, i.e. the information richness in actual plant data is often insufficient to allow reliable model identification. Figure 10 illustrates this problem in case on-line model selection is required. The example may be illustrative for a well-controlled nitrifying system on which data on the nitrification rate are obtained for a limited range of substrate (0 to 4 mg NH_4^+-N/l) only. It is evident from this figure that, given the typical measurement errors, no discrimination can be made between a Monod-type saturation model and a Haldane type inhibition model. However, in case an important excursion of the substrate concentration would occur (e.g. to 15 mg NH_4^+-N/l due to a peak loading), it is important that a model-based controller applies the correct model, since only then adequate control actions can be taken.

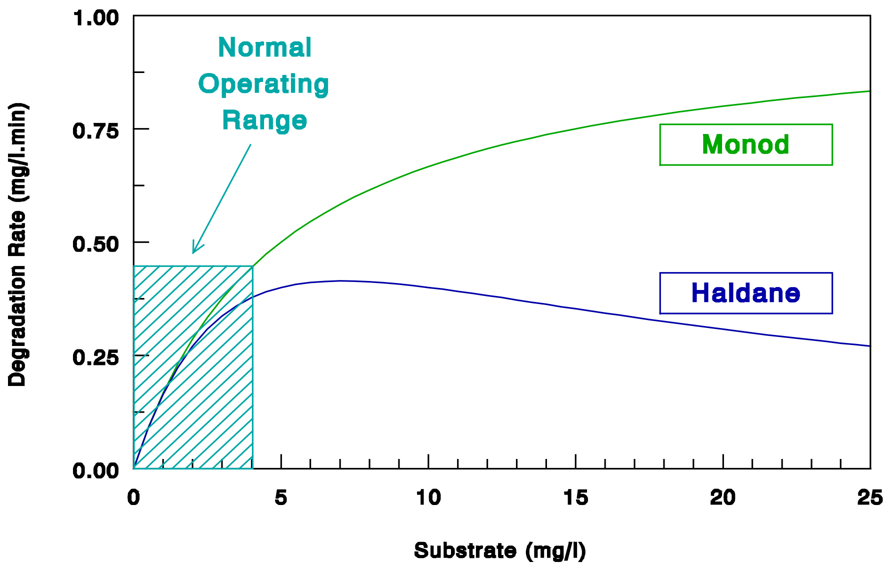

Figure 10 *Problem of on-line modelling of the substrate degradation kinetics using data from a controlled process.*

Evidently, data are required from the system for the higher concentration ranges. For certain process configurations the problem is non-existing as the operation is based on important dynamics of the important variables. Examples of such systems are alternating nutrient removal systems (Isaacs et al., 1994) or sequencing batch reactors (Demuynck et al., 1994).

Relay feedback control approach

In other, less favourable (from the information content point of view) treatment processes, a possible solution by which data can be obtained over a wider range is to loosen the control and allow for temporary deterioration of the WWTP performance, e.g. the effluent quality. Hence, a conflict arises between control performance, which should result in very smooth operation, and need for informative data for model identification, which requires sufficient variations in the measured variables. These contrasting requirements can, however, be reconciled to a certain extent if a probing or excitation signal is superimposed on the control action (Box & MacGregor, 1974; Aström & Hägglund, 1984; Partanen & Bitmead, 1993). This so-called relay feedback control approach has also been applied in adaptive control designs for the dissolved oxygen concentration and is illustrated below (Holmberg, 1982; Howell & Sodipo, 1985; Holmberg et al., 1989; Marsili-Libelli, 1990; Vanrolleghem & Verstraete, 1993).

The method starts from a model, in this case the oxygen mass balance:

$$\frac{dS_{O2}}{dt} = K_L a\left(S_{O2}^{sat} - S_{O2}\right) - OUR + \frac{Q}{V}\left(S_{O2}^{in} - S_{O2}\right)$$

in which the mass transfer coefficient K_La is known to be a function of the gas flow rate U, the temperature T and many other factors. One may however choose to only explicitly model the dependency on the gas flow rate U, e.g. $K_La=\alpha.U$. The idea of the special controller used here is to manipulate U in such a way that three goals can be met: 1) control the dissolved oxygen (S_{O2} near a particular setpoint (S^*_{O2}); 2) generate sufficiently rich data that allow reliable estimation of the actual oxygen uptake rate and 3) allow the estimation of the (possibly time-varying) mass transfer parameter α. Note that this parameter α will have to compensate for all deficiencies of the simple K_La-model used, e.g. its dependency on temperature, surfactant concentrations, ... To obtain sufficiently rich data, an excitation signal is superimposed on the (optimal) control action calculated by the adaptive controller. This induces the necessary variation of the dissolved oxygen data for accurate estimation of both parameters (Figure 11).

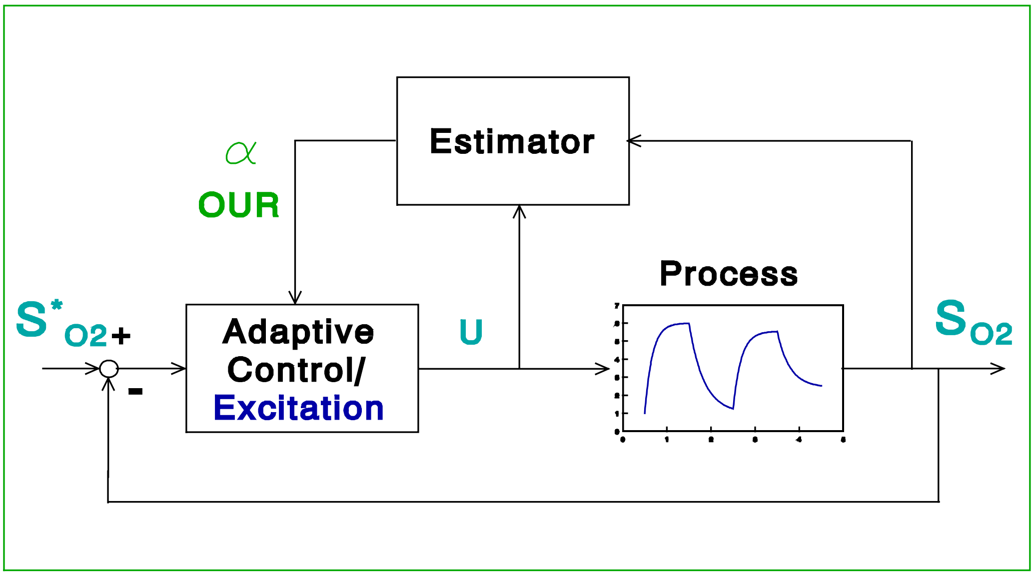

Figure 11 *Principle of the DO controller with superimposed excitation for reliable estimation of mass transfer parameters and oxygen uptake rate.*

In Figure 12 lab-scale results are summarised to illustrate the behaviour of such dedicated controller/estimator under time-varying conditions. In this case not the bioprocess is considered time-varying, but a change in the efficiency of the aeration system is evaluated. In the studied pilot scale reactor, aeration intensity is determined by the mixing intensity and the air flow rate. The dissolved oxygen control action is based on manipulation of the mixing intensity (tpm, revolutions per minute). A deliberate disturbance of the aeration intensity can therefore be achieved by changing the air flow rate from 2.5 to 4 l/min. As the K_La-model used did not consider the dependency on the air flow rate, i.e. $K_La = \alpha$.tpm, the proportionality constant α has to be varied to compensate for the increased aeration efficiency induced by the increased air flow rate.

In Figure 12, one observes that the different objectives of the dedicated controller are satisfied, i.e. the DO is controlled around 3 mg/l by manipulation of the mixing intensity. Rather than a smooth variation of the manipulated variable (tpm) one should note the superimposed oscillation and the concomitant, fast dynamics of the controlled variable (S_{O2})! The controller rapidly reacts to the increased aeration efficiency by reducing the mixing intensity and the estimator of α converges reasonably fast. A temporary disturbance of the OUR-estimation algorithm can also be deduced from Figure 12.

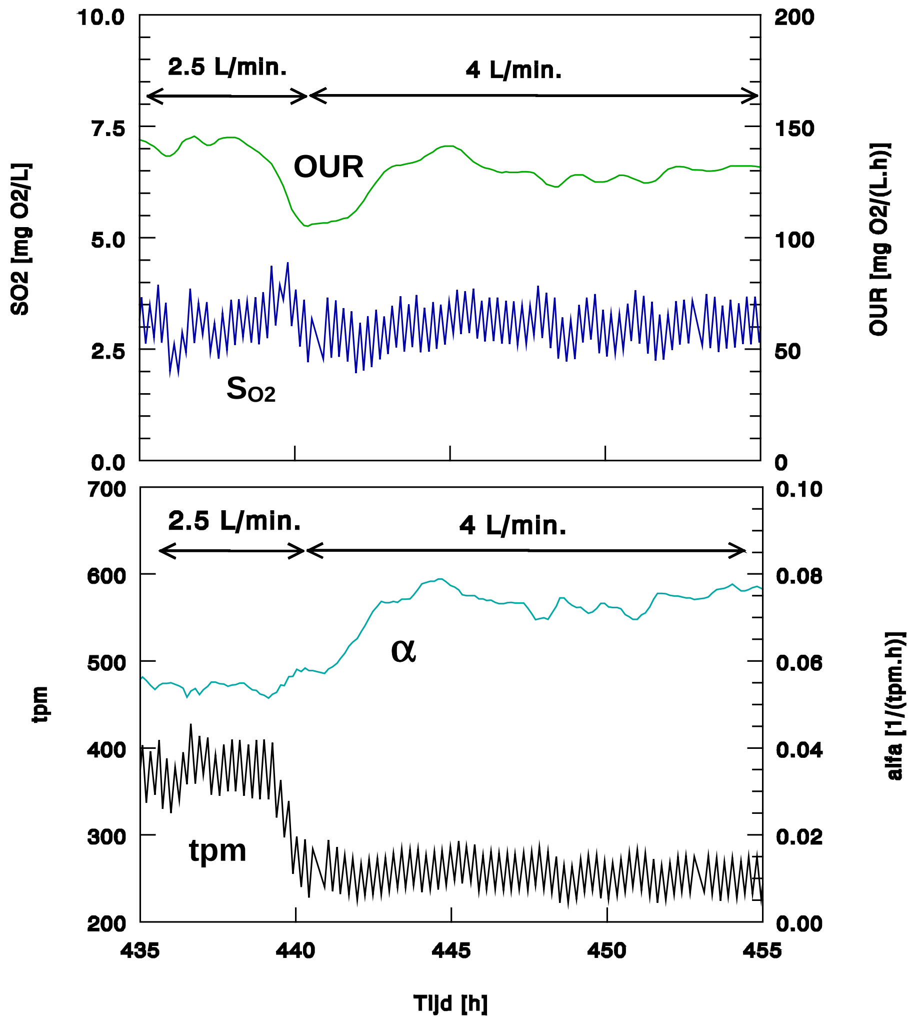

Figure 12 *Control of DO (top) by manipulation of mixing intensity(tpm, bottom) under constant OUR (estimate: top) and varying aeration efficiency (α: bottom)*

In-Sensor-Experiment approach

So-called In-Sensor-Experiments have been proposed by Vanrolleghem & Coen (1995) as an alternative solution to obtain rich information on the bioprocesses occurring in the treatment plant. The main advantage of the approach is that it is not necessary to make a difficult trade-off between the control performance and the modelling accuracy. This is achieved by separating the data generation from the control goal of a full-scale monitoring program. The method essentially consists in performing the experiments on a down-scaled version of the full-scale process that is sufficiently representative of the plant, e.g. the reactor contains activated sludge from the plant that is to be modelled on-line. In-Sensor-Experiments are performed in this down-scaled reactor that is operated in parallel to the full-scale system (Figure 13). Evidently, no restrictions exist with respect to the type of experiments that are allowed to be performed since the full-scale plant itself will not be affected by them. Consequently, the information content of the collected data can be made sufficiently large to allow for the identification of rather sophisticated process models.

In Figure 13 a sensor system is schematised with the ability to perform In-Sensor-Experiments aimed at modelling denitrification. A sample of sludge can be taken either from the nitrate or sludge recycles while wastewater samples can either be influent or a synthetic wastewater. Such synthetic wastewater can have a composition especially designed for calibration of the sensor or specific experimentation, e.g. to determine the denitrification capacity of the sludge residing in the built-in reactor. Different sensors can be installed in the device to monitor the progress of the experiment. For example, in Figure 14 a data set is presented of a system where an ORP electrode is used. The detected nitrate knee is then used for instance to deduce the denitrification potential of a carbon source. Such information could not have been obtained from a continuous flow denitrification zone because the dynamics necessary for reliable application of the ORP signal are not present in such system.

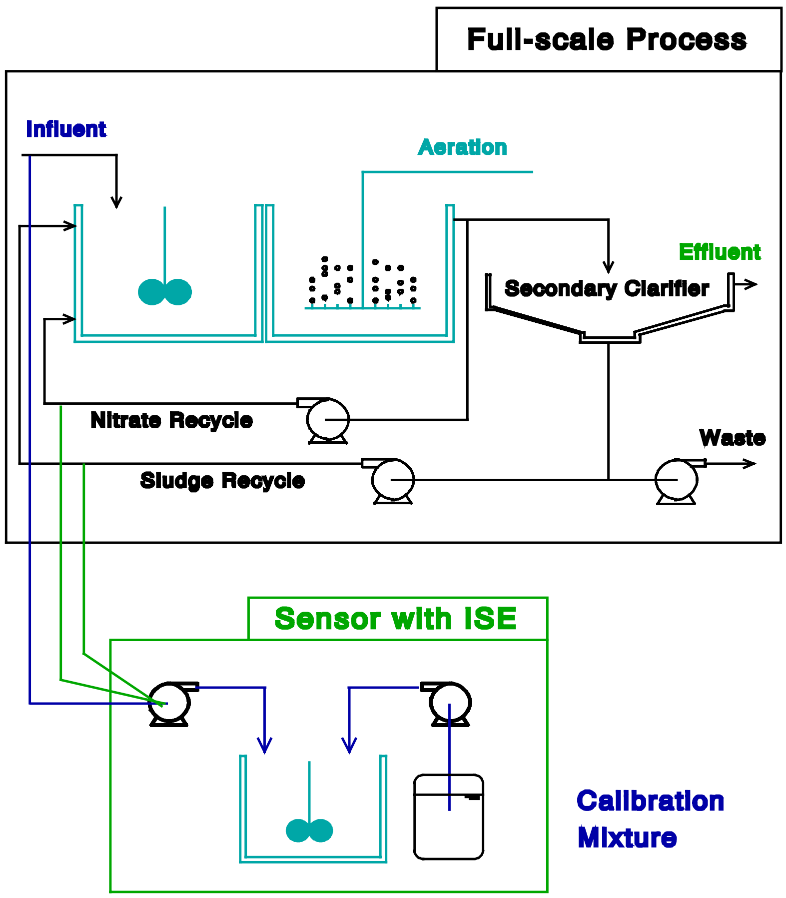

Figure 13 *Principle of In-Sensor-Experiments (ISE) for a denitrifying process.*

In Figure 15 another application of this new concept is presented. A sensor was developed in which settling experiments can be performed automatically at a treatment plant (Vanrolleghem et al., 1996d). For this unit process too a clear need for on-line modelling is felt and this device aims at providing quantitative data that can not be obtained from turbidity measurements of a well-controlled secondary clarifier. More details on this sensor system can be found in Vanrolleghem et al. (1996d), its application in on-line monitoring of a treatment plant in Vanderhasselt et al. (1999) and estimation of settling model parameters is discussed by Vanderhasselt and Vanrolleghem (1999)

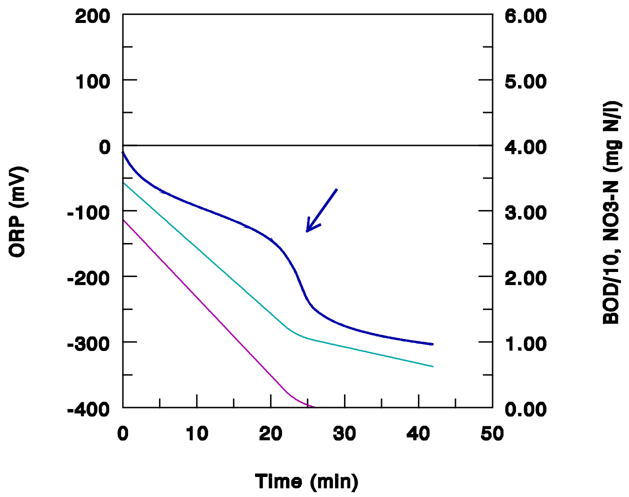

Figure 14 *Data collected from a batch In-Sensor-Experiment for denitrification modelling. ORP (full line), nitrate (-.-) and COD (--).*

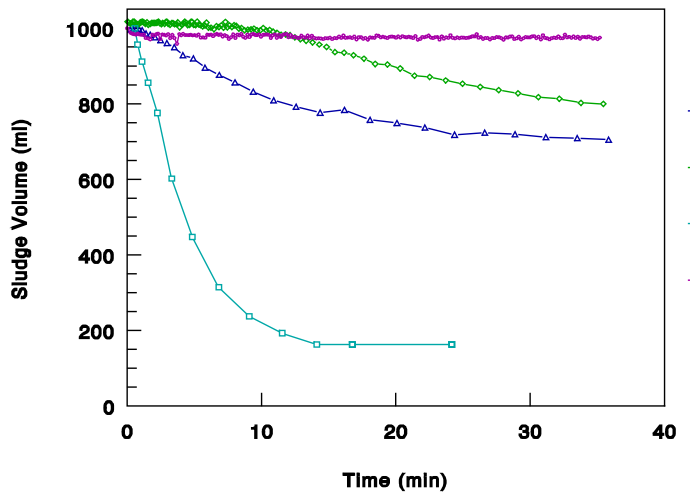

Figure 15 *Settling curves obtained for four different sludges in a settlometer performing batch In-Sensor-Experiments.*

Finally, the important efforts that have been put in the development of respirometric techniques for on-line modelling of the interaction between wastewater and activated sludge warrant some attention. A number of applications have proven their usefulness, e.g. model-based toxicity detection (Vanrolleghem et al., 1996c) or characterisation of wastewater composition in terms of particular process models (Spanjers & Vanrolleghem, 1995; Vanrolleghem et al., 1999). An important idea that was prototyped on such respirometric sensors was the application of optimal experimental design techniques to improve the quality of the data obtained from the In-Sensor-Experiments. Goals pursued were optimal experiments for model selection (Vanrolleghem & Van Daele, 1994) and parameter estimation (Vanrolleghem et al., 1995). Important was to ensure that the experimental design could be performed on-line since the time-varying and nonlinear nature of the processes studied imposes that the optimal experiment is time-varying as well. Hence, adaptivity of the In-Sensor-Experiments is needed and from this stems the term given to such sensing system, i.e. "adaptive sensor" (Vanrolleghem, 1994).

PREDICTION OF DISTURBANCES AND RECEIVING WATER CAPACITY

When one considers the wastewater treatment plant in its larger context, the attention is immediately drawn to the up- and downstream processes to which a treatment plant is connected, i.e. the sewer system (or the industrial production facility) and the receiving water body. These three subsystems take care of the collection of sanitary (or industrial) sewage and drainage of rain runoff, its transport and treatment. In recent years awareness has increased substantially that the assessment of the interactions between these subsystems is very important to evaluate the overall performance of the urban drainage system. However, according to the present state-of-the-art, sewer system and treatment plant are planned and designed as totally separate entities, each subject to a specific set of performance objectives, which are only loosely related to receiving water quality standards. Moreover, these receiving water norms are typically given as invariant maximum discharge limits, and only recently , some differentiation is being made depending on the specific planned use of the water body (fishing, drinking water production) (Rauch et al., 1998).

These last few years it is postulated that an integrated view could allow for a more efficient urban water management with lower risks of harmful effects on the receiving water and a more constant quality of the discharged water. As the time constant of actions at the level of the design of the subsystems is in the order of 10 years or more, most of the attention is currently focused on a better operation of the systems by introducing real-time control strategies. As the aim of this paper is only to discuss the control of the wastewater treatment plant, the RTC systems that are being developed for the sewage transport system or the batch scheduling for waste design in a chemical production facility are not considered here, albeit that the treatment plant is considered in the optimisation process (note that certain optimal solutions may be worse for the treatment plant compared to the situation prior to the implementation of RTC in the sewer system, see Vanrolleghem et al., 1996a).

Control of a treatment plant that integrates the sewer within the decision process is based on predictions of future flows and loads. Drainage modelling therefore becomes an integral part of such control scheme. Such a model includes two parts: 1) an inflow forecasting model that transforms measured or predicted rainfall into runoff and inflow to the collection system and 2) a sewer transport model that describes the movement of the sewage in the sewer network (Capodaglio, 1994). At this stage some schools exist on the type of models to be used for this purpose. Deterministic models have the advantage to incorporate available mechanistic knowledge on the hydraulics (and transport of solutes and particulate material, although modelling of the latter is still under debate). However, it is computationally intensive and requires the identification of an important number of parameters. To reduce computations, model reduction can be made from a highly detailed network description which is calibrated and validated for a few specific rain events to a simplified system that retains the general dynamic behaviour characteristics (Meirlaen et al., 2000). An alternative is to apply stochastic transfer function descriptions as black box models of the system, i.e. the user must not invest time to gain insight in the system and identification requires less effort. The approach aims at finding an adequate input-output mapping amongst the variables considered most important, e.g. the rainfall and the outflow and composition. This approach is solely based on time series of experimental data.

Data that typically give rise to such modelling efforts are depicted in Figure 16: a week of influent waste concentration is given for a hospital wastewater treatment plant in Gent. One clearly observes the important diurnal pattern.

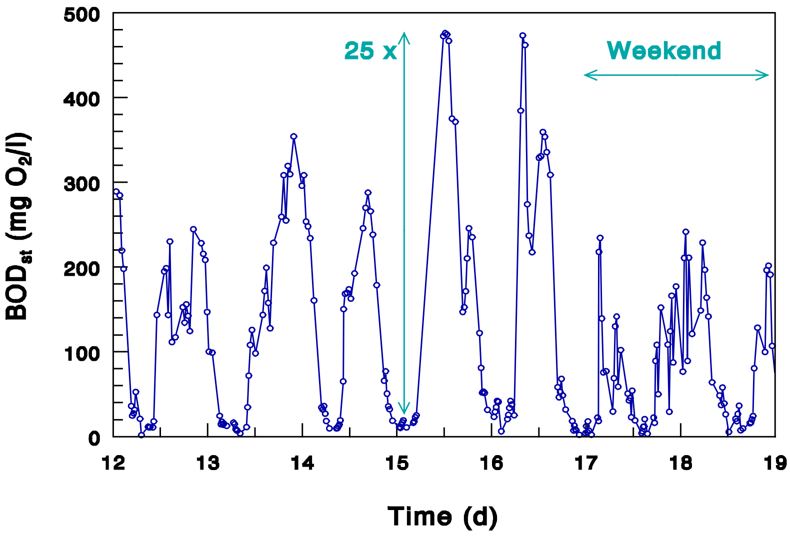

Figure 16 *Typical weekly pattern of influent waste concentration measured with a respirometer at a hospital wastewater treatment plant in Gent, Belgium.*

Moreover, in this plant the flow rate changes nearly in sync. Hence, the load variation is amplified further, the main result being that a high-strength wastewater is to be treated under a shorter hydraulic retention time. Evidently, predictions of the incoming load can be used by a feedforward controller to the advantage of the treatment plants' performance. A time series model can easily capture this diurnal pattern. In the literature several examples of time series analyses for flow and load predictions are described, with prediction horizons ranging from one-day-ahead (Berthouex et al., 1978; Capodaglio, 1994) to one-hour-ahead or even 6-minute-ahead (Tan et al., 1991).

An important application of sewer models is the prediction of flow rates after rain events as these have an important effect on the hydraulics of a treatment plant and may disturb the final settling to such an extent that sludge washout occurs. A treatment plant can be protected against such events but sufficient time is needed for the feedforward control actions (step feed, storm tank emptying) to have their desired effect. Different upstream sensor signals combined with predictive models can be used, each with a different forecasting horizon: weather radar (Aspegren et al., 1993; Pleau et al., 2000), rain gauges and flow meters in the outer parts of the sewer network. Depending on the measurement made, different models are used to map these inputs to the influent flow of the treatment plant.

As mentioned before, models are also used in the control scheme to describe the objective of a treatment plant. Ultimately, such model may be a complete description of the costs associated to a treatment facility over its lifetime (Vanrolleghem et al., 1996b; Gillot et al., 1999) and may involve many aspects (investment, operational costs, etc.). Currently, however, the model that describes the objectives is very simple, i.e. fixed standards are used that are supposed to be the translation of water quality goals. Hence, the objectives are emission-based and therefore are representative of the separated view on the different unit processes of the urban drainage system. However, a distinct move is being made towards an immission-based approach that considers the interaction between combined sewer overflows from the sewer system, diffuse pollution, purified wastewater discharge and receiving water quality (Harremoës et al., 1993; Vanrolleghem et al., 1996a, Schilling et al., 1997). Clearly, the models used to describe the objectives of the wastewater treatment plant now become much more comprehensive. Typically these models involve a good description of the hydraulics of the receiving water. Main factors to which attention is drawn for the definition of the objectives are oxygen depletion, ammonia toxicity and eutrophication with the resulting algal blooms.

Secondary factors that have to be taken into account are the temperature, the transport of sediments, nitrate and phosphate levels, light input and dynamics of higher trophic levels including fish (Beck & Reda, 1994).

In Figure 17 simulation results are given for one year of dissolved oxygen levels in a river (Vanrolleghem et al., 1996a). It is evident that oxygen depletion occurs for periods of substantial length. A closer inspection of the data learns that these critical periods do not coincide with what apparently are the main CSO discharges. On the contrary, a sequence of small overflow events in summertime when the river flow rate is at its minimum causes the long dissolved oxygen depletion periods that are detrimental for the ecological quality of the river system.

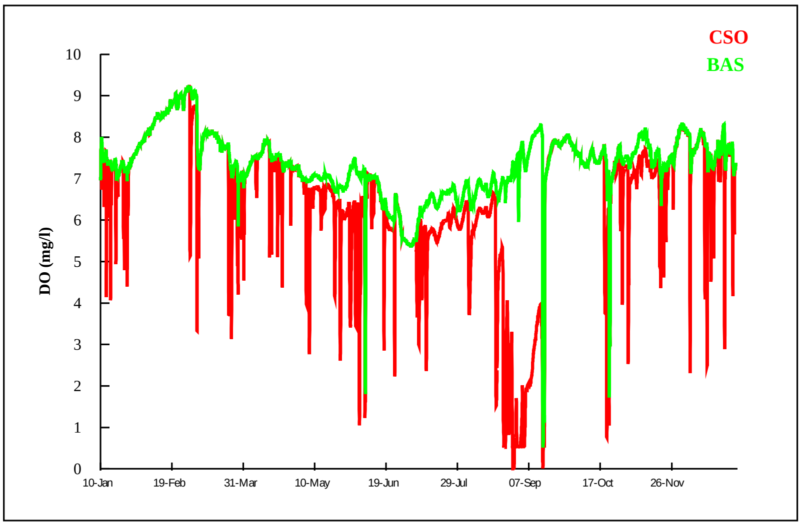

Figure 17 *Example of a one year simulation of the DO levels in a river to which CSO and wastewater discharges occur (dark line and thin line depict two sewer designs).*

CONCLUSIONS

The main message of this contribution is that models are ubiquitous in WWTP control. In the control system itself, models are involved in

-> Support for design of the control structure
-> Support for controller tuning
-> Model-based control algorithms

In the monitoring system, mathematical models play an increasing role as part of

-> Software sensors

Closely related to the monitoring system application, prediction of upcoming disturbances is also heavily depending on mathematical descriptions of the

-> Sewer system
-> Scheduling of industrial processes

Finally, it was indicated that future definitions of control objectives for wastewater treatment plants will increasingly rely on an integrated view on the immissions to the receiving water and models will play a dominant role due to the complexity of the description of the

-> River quality

All in all, it must be evident from the above that the use of models in advanced WWTP control is not limited to model-based predictive control applications.

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