THE ADAPTIVE SENSOR CONCEPT: ON-LINE MODELLING OF THE ACTIVATED SLUDGE PROCESS WITH OPTIMAL IN-SENSOR-EXPERIMENTS

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Abstract

Important features of biological wastewater treatment processes such as their nonlinear and time-varying nature impose considerable strains on control systems required for their optimal performance: time-varying parameters in the process models integrated in the control systems should be updated and the nonlinearity requires that either adaptive linear controllers are applied (with additional adjustment needed to cope with changing operating points) or that nonlinear controllers are devised. Sensors play a key role in such control loops: Monitoring equipment is not only needed to indicate deviations from desired behaviour to the regulator, but they must also provide the necessary data for adjustment of the control laws to the changing process conditions.

The main goal of the work presented in this paper was to develop sensor technology capable of providing this information. Special attention was paid to make sure that this information would be easy to incorporate in the models on which the control system is based. A methodology was sought that would facilitate the on-line modelling of the interaction between wastewater and activated sludge.

Because it is relatively hard to obtain sufficiently rich information from a plant that operates in closed-loop, a new approach is introduced consisting of what has been termed 'In-Sensor-Experiments'. The main characteristic of this approach is that the information on process behaviour is no longer obtained directly from the plant, but from a sidestream sensor in which small-scale experiments are performed which are relevant to the behaviour of the full-scale process. In such sensing device, the excitation signals can be chosen without restriction and, consequently, process behaviour can be characterized under much wider conditions than possible in the treatment plant itself. Hence, if model-based interpretation of the sensor data is applied, rather sophisticated nonlinear models can be identified allowing to devise more elaborate control strategies.

Because the changes in wastewater composition are rather important, not only the parameters but also the structure of the models describing the wastewater/sludge interaction are subject to change. Therefore the model identification encompasses both model structure characterization and parameter estimation.

The hardware of the sensor allows to adjust the In-Sensor-Experiments in such a way that the highest possible information content is obtained under the time-varying conditions the sensor is confronted with. The on-line optimal experimental design (OED) methods that will be presented are the heart of the 'Adaptive Sensor Concept'. It will be shown that optimal experiments can be proposed for structure characterization (OED/SC) and parameter estimation (OED/PE). A very important part of the development work was due to the need to fulfill the real-time requirement imposed by the on-line operation of the adaptive sensor. Real-life experimental results will illustrate the potential of the adaptive sensor concept for the control of activated sludge wastewater treatment plants.

Keywords

Model Identification, Optimal Experimental Design, On-line Monitoring, Wastewater Treatment

1. Introduction

Important features of biological wastewater treatment processes such as their nonlinear and time-varying nature impose considerable strains on the control systems required for their optimal performance. First, the time-varying parameters in the process models integrated in the control systems need continuous update. Second, the nonlinearity requires that either adaptive linear controllers are applied (with additional adjustments needed to cope with changing operating points) or that nonlinear controllers are devised. Sensors play a key role in such control loops (Fig. 1). They are not only needed to indicate deviations from desired behaviour to the regulator, but they must also provide the necessary data for adjustment of the control laws to the changing process conditions.

In case model-based control systems are applied to time-varying processes as the one considered here, it is essential to be able to perform on-line modelling in order to track the bioprocess model and maintain the controller's efficiency. "Modell-

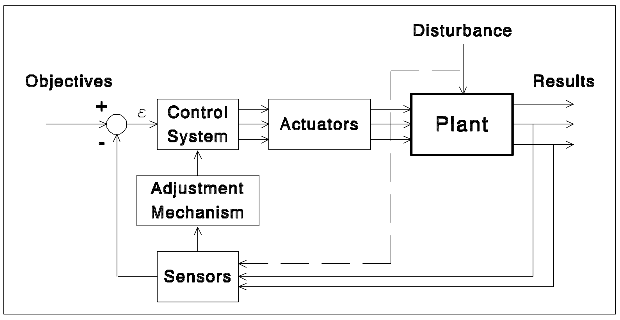

Figure 1. *Building blocks of an adaptive control chain.*

ing" is used here in the broad sense, i.e. both model structure and parameters are to be identified. To achieve this, large amounts of on-line information are required. Two problems have been identified in this respect:

- Although considerable research has focussed on the development of new 'bio'sensing technologies [1], a lack of reliable monitoring equipment is still recognized [2].
- The information content of the data is often insufficient to identify the increasingly complex models required for adequate description of the bioprocess [3].

To tackle these problems, new sensor technology was developed to characterize the main disturbance to the treatment process, i.e. the wastewater composition. In addition, a new approach was sought to obtain highly informative data.

Indeed, except for some process configurations that inherently yield important transients [4-5], it is relatively hard to obtain sufficiently rich information from a plant that operates under closed-loop control. A possible approach is to loosen the control by introduction of some excitation signals superimposed on the control action. This approach induces transients in the state variables and has been proven succesful (e.g. [6]). Still, restrictions must be imposed on the excitation to keep the plant within its operating limits. Hence, a lack of information may remain. In the next section an alternative way to obtain the necessary information is proposed.

In-Sensor-Experiments

The new approach introduced in this work consists of what has been termed 'In-Sensor-Experiments'. The main characteristic of this approach is that the information on process behaviour is no longer obtained directly from the plant, but from a sidestream sensor in which small-scale experiments are performed. Because the behaviour of the process in these experiments is very similar to the one at full-scale, relevant information can be provided by such sensor. Moreover, in such sensing device excitation signals can be chosen without restriction and, consequently, process behaviour can be characterized under much wider conditions than possible in the treatment plant itself. Hence, if model-based interpretation of the sensor data is applied, rather sophisticated nonlinear models can be identified, allowing to devise more elaborate control strategies.

In this paper attention is focussed on a first application of this principle in a new sensing device. The In-Sensor-Experiments performed within the device allow to characterize the interaction between the wastewater and the activated sludge [7]. This characterization is performed by identification of biodegradation models on the basis of the raw data obtained from the In-Sensor-Experiments. Details are developed in the sequel.

The Adaptive Sensor Concept

If the hardware of such sensor allows to adjust the In-Sensor-Experiments performed in it, one may aim to adjust the way the experiments are done. This makes it possible to maintain the quality of the sensor's outputs under the time-varying conditions the sensor is confronted with.
To achieve this, each experiment is designed using optimal experimental design (OED) procedures. These procedures take advantage of previously acquired process knowledge (in the form of process models) to maximize the information content of the next In-Sensor-Experiment.

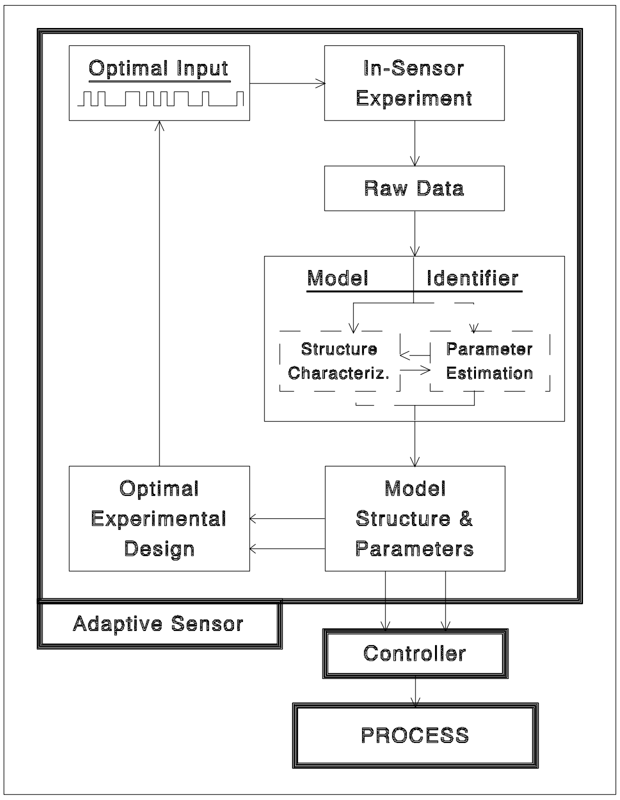

Figure 2. *Flowchart of the operation of an adaptive sensor.*

A sensor that is based on a combination of In-Sensor-Experiments and OED that is performed on-line has been termed an 'Adaptive Sensor' (Fig. 2).

2. A Respirographic Biosensor as Case Study of the Adaptive Sensor Concept

All research on the adaptive sensor concept has been tightly coupled with the development of a sensor that operates on the basis of In-Sensor-Experiments. The experiments in this new device consist of pulse injections of wastewater to activated sludge residing in the bioreactor integrated in the sensor (for more details, see [7]). Biodegradation of the injected waste results in an oxygen uptake rate (OUR) profile (also term-ed respirogram) that represents the impulse response of the biosystem to the injected wastewater. Some typical impulse responses are given in Fig. 3.

The central goal of the study was to identify process models on the basis of these impulse responses. In the work, it was found that most OUR profiles could be adequately described by three candidate models (Fig. 3): a first order, a single Monod and a double Monod model. Each of these models describes the degradation of a wastewater component S by a biocatalyst X according to some degradation kinetics r_s. The OUR is proportional to the degradation rate of the substrate(s). The yield coefficient Y is the fraction of S which is not oxidized but incorporated in the biomass X. The biokinetic parameters μ and K_s describe the dependency of the degradation rate on S.

Modelling these OUR data means finding the best model structure and the associated parameters.

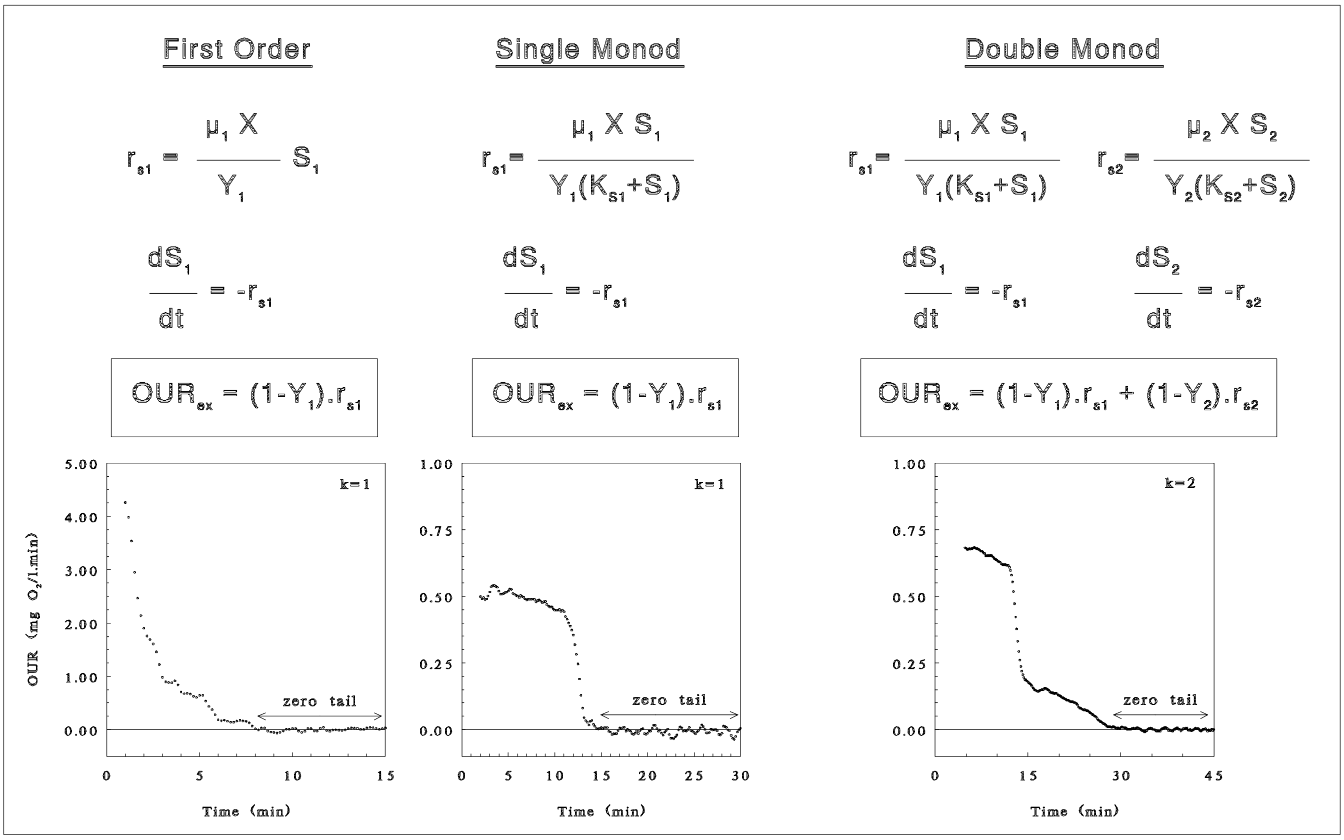

Figure 3. *Model equations of candidate models and typical raw oxygen uptake rate data*

3. Structure Characterization (SC)

Parameter estimation and model structure selection are two closely related stages in any modelling exercise. In fact, the sequence in which these stages are performed is chosen by the model builder. The structure characterization methods are termed *a posteriori SC* if the choice among the candidate models is postponed until all model candidates are fitted to the data, i.e. their parameters are estimated. *A priori SC* methods, on the contrary, can precede the parameter estimation stage since they don't rely on fitting results to select among the different models. An evaluation of different SC methods was reported in [8]. Here, the main conclusions of this study are summarized.

a priori SC

In real-time applications (as the one presented here), a priori SC methods have a distinct advantage over a posteriori methods because the computing-intensive parameter identification stage has to be performed only once, i.e. only with the selected model. To discriminate between candidates, model-specific features must be extracted from the data.

Two approaches were developed for the OUR profiles. One is an ad hoc method based on the number of inflection points in the impulse response (see Fig. 1: the first order model has none, the Single Monod has one and the double Monod model has three inflection points). The other method is intrinsically more general and is based on the pattern recognizing ability of neural networks. Training of the neural net was performed by applying a set of 750 Monte Carlo simulations with the candidate models.

a posteriori SC

Different a posteriori methods were evaluated. Traditional model selection criteria are based on a decision criterion that looks for the optimal trade-off between model complexity and fit. However, due to some unmodelled dynamics in the raw data, these methods proved unsuccesful, except for the GIC-approach in which an explicit quantification of 'undermodelling' is performed. Minimization of the undermodelling allowed to point to the most appropriate model. Methods based on the analysis of the statistical properties of the residuals also provided a good means of a posteriori model selection.

4. Optimal Experimental Design for SC

In view of the noisy data, a good experimental design may be an invaluable tool to increase the discriminative power of the data [9]. Optimal experimental design (OED) procedures are aimed at designing experiments in which the difference among the structure characterization criterions for the different models is maximized.

Vanrolleghem & Van Daele [10] describe procedures for OED/SC in case the a priori SC method based on the number of inflection points is used for model selection. Figure 4 is illustrative of the case in which the experimental design consists of finding the optimal ratio between two substrates in the sample. In Fig. 4a, the OUR profile of the 'worst case' mixture is given, i.e. although biology tells that Double Monod kinetics prevail, the experimental conditions are such that a Single Monod model would be selected because only one inflection point can be detected. The respirogram of Fig. 4b is a good example of data that allows reliable structure characterization.

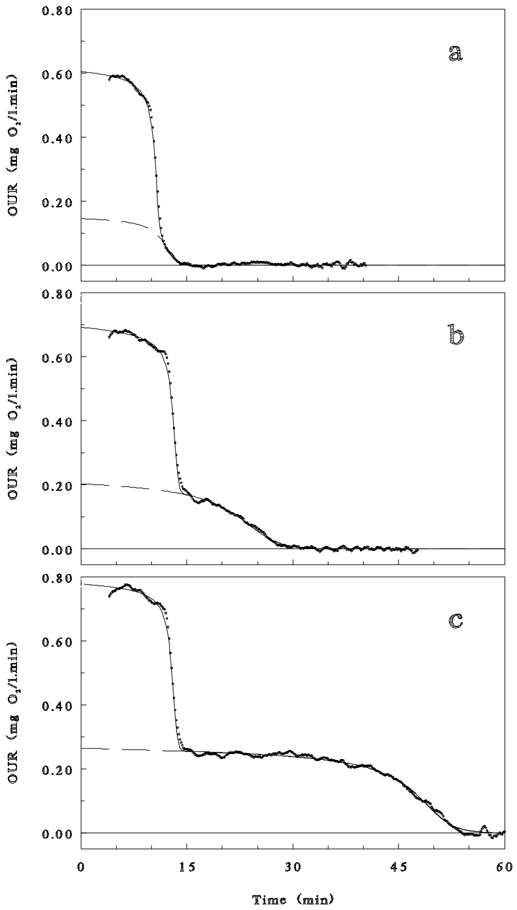

Figure 4. *OUR profiles obtained for different experimental designs of the sample mixture.*

In Fig. 4c reliability is even somewhat higher, but the experiment takes prohibitively long, endangering the real-time constraint of the sensor's operation. This example illustrates that a compromise must be sought between modelling accuracy and real-time operation. The same constraint prohibited the use of a posteriori SC methods as a basis for OED.

5. Parameter Estimation (PE)

Estimating nonlinear parameters of a model poses both theoretical and practical identifiability problems. Vanrolleghem [11] studied the identifiability of the candidate models of Fig. 3, both in case of perfect, i.e. noiseless, OUR data (the theoretical identifiability) and in case of a real-life finite data-set with a particular realization of the noise (the practical identifiability).

Theoretical Identifiability

Although the Monod model has been subject to intense research regarding its theoretical identifiability (e.g. see [12]), these studies were always initiated on the assumption that both biomass X and substrate S were measured. In this application, however, the aim is to estimate biokinetic parameters on the basis of OUR data only.
Hence, a new study was required to evaluate if it is possible at all to find unique estimates of the model parameters on the basis of perfect data, or alternatively, that only some parameter combinations are identifiable. The tools for evaluation of the theoretical identifiability are however rather restricted. There exists no generally applicable methodology that guarantees the solution of a nonlinear identifiability problem [13]. The approach taken for this application is to transform the model into a linear regression form from which the parameter identifiability can be deduced.

Table 1. *Identifiable parameter combinations of different biodegradation models if only OUR measurements are available.*

Exponential	Double Monod
$(1-Y_1)\,S_1(0)$	$(1-Y_1)\,S_1(0)$
$\dfrac{\mu_{max1}X(1-Y_1)}{Y_1}$	$\dfrac{\mu_{max1}X(1-Y_1)}{Y_1}$
Single Monod	$(1-Y_1)\,K_{m1}$
$(1-Y_1)\,S_1(0)$	$(1-Y_2)\,S_2(0)$
$\dfrac{\mu_{max1}X(1-Y_1)}{Y_1}$	$\dfrac{\mu_{max2}X(1-Y_2)}{Y_2}$
$(1-Y_1)\,K_{m1}$	$(1-Y_2)\,K_{m2}$

Table 1 summarizes the results of Vanrolleghem [11]. It is observed that only a number of combinations of parameters can be attributed unique values. Not surprisingly these combinations always include the yield coefficient Y since this parameter quantifies the fraction of substrate which is not oxidized, i.e. no observations can be made on this fraction using oxygen uptake measurements only.

Practical Identifiability

The practical identifiability is concerned with the problem of evaluating whether the (combinations of) parameters can be estimated reliably considering the measurement noise.

Quantification of the estimation accuracy is based on an evaluation of the Fisher Information Matrix, which corresponds to the inverse of the parameter covariance matrix [14]. The output sensitivity equations are central to the calculation of this matrix. These equations quantify the sensitivity of the model predictions on the parameter values. The elements of the information matrix are calculated on the basis of the sensitivities of the measured variable(s) evaluated at the different measuring instants.

When the sensitivity equations are (nearly) linearly dependent, the Fisher matrix becomes ill-conditioned or even singular, indicating practical identifiability problems with the available experimental data. As shown in the sequel, a good experimental design may eliminate such problems.

6. Optimal Experimental Design for PE

On the basis of the Fisher Information Matrix the value of a particular experimental design can be assessed. Consequently, it is possible to initiate an optimization procedure in order to maximize the information content of a forthcoming experiment. different objective criteria have been proposed that can be traced back to Fisher Matrix characteristics [14]. All except one are directly concerned with the parameter variances.

Either the largest variance is minimized (E-criterion), or the arithmetic or geometric mean of the parameter variances (D- and A-criterion respectively). The exception is the modified E criterion which allows to maximize the numerical stability of the parameter estimation problem (by improving the condition number of the Fisher Matrix). To complete the list of criteria, the modified A criterion has to be mentioned. Here the sum of variances is minimized.

Vanrolleghem [11] evaluated the optimal experimental designs for these different criteria in case of the Monod model and an additional pulse of sample during the experiment as a design variable. Figure 5 illustrates the evolution of the substrate concentration in the sensor's reactor and the resulting OUR predictions. The proposed experiments diverge for the different OED/PE criteria. While for the A- and modified A criteria experiments are proposed that prolong the phase in which the maximum degradation rate is observed (so as to minimize the variance of μ_{max1}), the D- and E-criteria focus on the estimation of K_{m1} by allowing the substrate to evolve three times through the concentration range in the neighbourhood of this parameter. The modified E criterion is an intermediate design by which the numerical properties of the identification problem are addressed.

Validation of these experimental design procedures was performed for the modified E-criterion. In Fig. 6 both the reference (top) and optimized (middle) experimental data and the corresponding model fit are summarized. The change in shape of the objective functional is apparent from the contour plots and is indicative of the improved conditioning: the valley has become more cone-like. Table 2 shows that considerable improvements in parameter variance can be obtained (50 %) at the expense of little experimental effort.

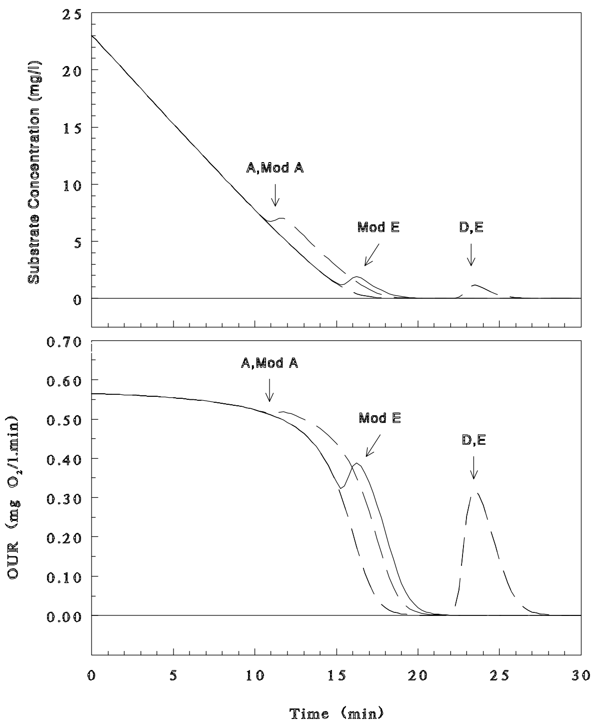

Figure 5. *Substrate (top) and OUR trajectories (bottom) of simulated experiments with additional pulse injections at different times as proposed by different OED/PE criteria.*

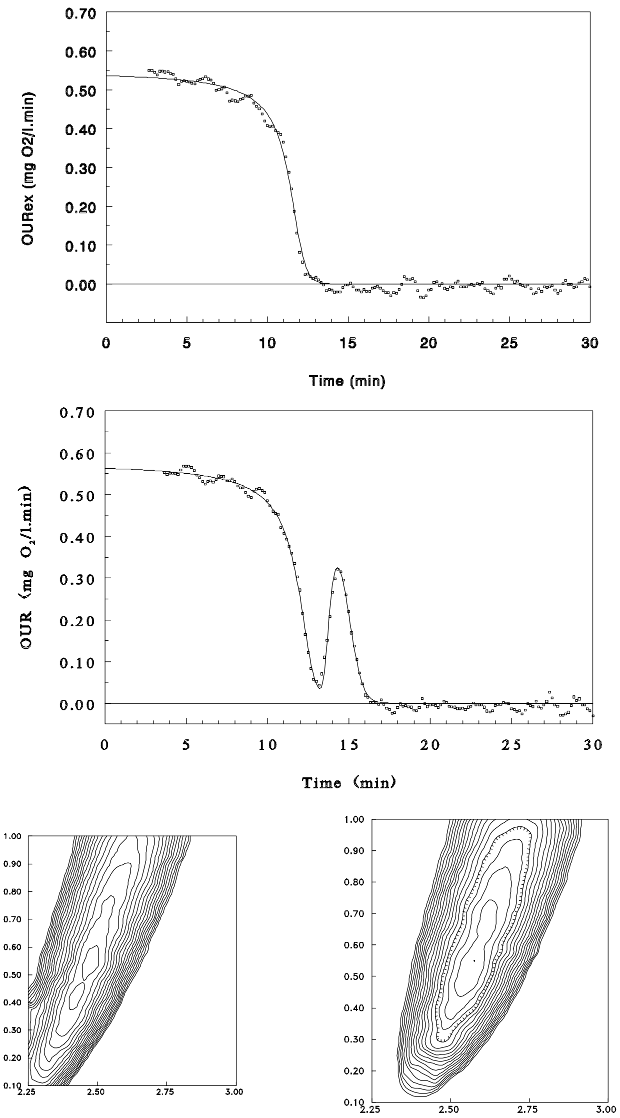

Figure 6. *Reference experiment (top) and optimal experiment with additional pulse addition after 14.1 min (middle). Contour plots of the sum of squared errors as function of the Monod biokinetic parameters for both designs (bottom, left: reference; right: optimal).*

7. Control Applications

The In-Sensor-Experiment application presented in this paper allows a rather detailed characterization of the main disturbance of the process, i.e. the wastewater composition. Hence, feedforward control strategies can be devised that take advantage of this information.

An important feature of feedforward schemes is their reliance on a proper process model for optimum performance. As the considered process is highly time-varying, not only in model parameters but also in model structure, it is essential that on-line modelling of the process is performed. In-Sensor-Experiments as described above may provide an important part of the necessary information. Evidently, as the wastewater treatment process does not only consist of biodegradation of waste components but also involves settling and thickening of the biocatalysts, other sensors are required to complete the on-line modelling of the system.

Table 2. *DependencY of modified E criterion and parameter variances on the time of pulse addition. Results are relative to the reference validation experiment.*

tpuls (min)	Modified E	Var(μ_{max1})	Var(K_{m1})	Covariance
No pulse	1	1	1	1
13.0	0.676	0.411	0.422	0.381
14.1	0.624	0.535	0.465	0.468
14.6	0.619	0.480	0.409	0.417

Van Impe et al. [15] studied a control system as summarized in Fig. 7. It consists of a combination of an adaptive linearizing controller and an Extended Luenberger software sensor. Information to adjust the control law and feed the state and parameter estimator is obtained from the respirographic biosensor presented in this paper and turbi- dimetric measurements of biomass concentration. A simulation study indicated good convergence and tracking properties of the observer and the linearizing controller.

The adaptive sensor concept as proposed in this contribution guarantees that the In-Sensor-Experiments are adjusted to ensure the highest possible quality of the sensor outputs, an important assett for model-based controllers that rely on its data.

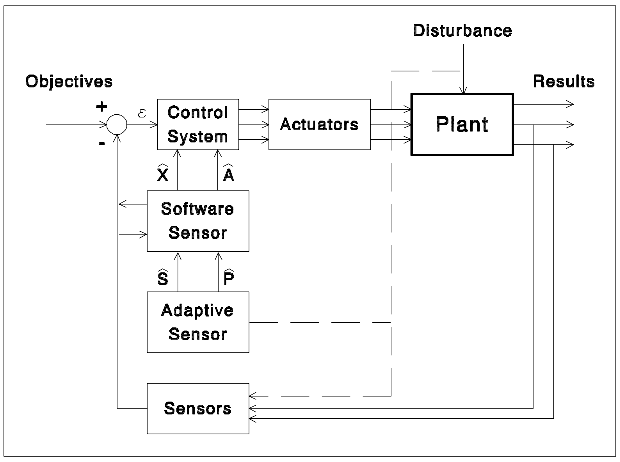

Figure 7. *Structure of an adaptive model-based control system with adaptive and software sensors.*

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