PLS-based supervisory control of the Single Reactor High Activity Ammonia Removal Over Nitrite (SHARON) Process

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Abstract
In the past, applications of statistical modelling, typically put within statistical process control (SPC) have typically been limited to on-line monitoring of processes. Statistical model-based control design is hardly found in literature. A straightforward application method of PLS modelling to control is therefore presented in an attempt to close the gap between statistical monitoring and process control. Based on an extensive simulation study, covering several steady-state situations of the SHARON process, several PLS models were constructed. Based on captured cumulative variance and CUMPRESS (cumulative squared sum of prediction errors) statistics, the number of retained latent variables were determined. The resulting PLS models were tested in closed loop control by means of dynamic influent data of the full scale SHARON process in Rotterdam. The control performance was however unsatisfying, either due to bad prediction or due to insensitivity of the model output to the selected control handles. This observed insensitivity was caused by an improper selection of historical data. In order to fit a linear model, certain steady-states were removed from the modelling data set. By doing so, only steady state situation where the DO setpoint and HRT control handles showed little effect on the output variables were selected for modelling purposes. Faced with the observed pitfall in PLS modelling, some suggestions for future research are given.

Keywords
Partial least-squares, Multivariate statistical process control, model based process control, Nitrogen removal, Supervisory control, Wastewater treatment.

INTRODUCTION

The Single reactor High activity Ammonia Removal Over Nitrite (SHARON) process is designed and applied for the treatment of wastewater with high ammonia concentrations by means of nitritation. The successful combination of this process with the Anammox autotrophic nitrogen removal process, in which equimolar ammounts of ammonia and nitrite are converted to nitrogen gas, can result in a reduction of the stoichiometrically required oxygen down to 40% of the oxygen demand in conventional N-removal, while no carbon source needs to be added and sludge production is negligible (van Dongen et al., 2001). The success of this strategy is however highly dependent on the control of the nitrite:ammonia ratio in the effluent of the SHARON process (van Dongen et al., 2001, Volcke et al., 2005). A suitable control strategy, which aims at an optimal nitrite:ammonia ratio of 1:1 and reduced aeration and acid and base addition at the same time, may be troubled by the nonlinear, time-varying and fast-responding nature of the process.

A project has been set up in which a supervisory control system for wastewater treatment systems, including monitoring, diagnosis and control modules, is developed. The intention is that the control module that is aimed for will, based on the output of the monitoring and diagnosis modules, select between alternative control strategies. The subject of this paper discusses the control strategy in normal operational conditions.
In the past decade, several applications of PLS (partial least-squares) modelling for monitoring of chemical processes have been described (MacGregor and Kourti, 1995, Kourti and MacGregor 1995,

Wise and Gallagher, 1996). Lee *et al.* (2005) discuss hybrid applications of PLS and mechanistic modelling to process monitoring in a full-scale wastewater treatment plant. In the aforementioned cases, PLS models provide a link between process data and qualities of the final product. As such, deviating quality or abnormal products can possibly be detected at an early stage of the process, hereby allowing corrective actions in time without excessive costs. However, these models do not necessarily allow to determine the appropriate action that should be taken. Indeed multivariate statistical monitoring is typically put under the moniker of multivariate statistical process control (MVSPC). Applications of PLS modelling as a basis for control design are however limited. Kaspar and Ray (1992) show how PLS models can be used as compensators for controllers to tackle the uncertainty in the mechanistic models that were used in control design. Piovoso and Kosanovich (1994) applied multivariate statistical methods to process monitoring and controller design, where a feedback controller design based on the principal component analysis (PCA) and principal component regression (PCR) was developed.

In this work, a straightforward application of PLS models in control design is formulated. First, an explanation of the methodology is given. Second, the results of the applied methodology to the SHARON process are shown and finally, conclusions are drawn and future perspectives are indicated.

MATERIALS AND METHODS

Partial least-squares (PLS) regression is a linear multivariate method to relate input data (X-space) to output data (Y-space) (Geladi and Kowalski, 1986). Analysis of collinear, noisy and highly dimensional data sets is possible by application of PLS (Wold *et al.*, 2001). By means of extraction of so called latent variables, which are highly correlated with the data in Y-space and capture a large part of the variance in X-space, PLS maximizes the covariance between the input and output data. In this way, the latent variables provide linear combinations of X-data and linear combinations of Y-data that are highly correlated. A PLS model is typically presented by the following set of equations:

$$X = \sum_{i=1}^{k} t_i p_i^T + E \tag{1}$$

$$Y = \sum_{i=1}^{k} u_i q_i^T + F \tag{2}$$

$$u_i = b_i t_i + h_i \tag{3}$$

k is the number of latent variables that are retained in the model. The PLS model is uniquely defined by means of the loading vectors in X-space, p_i, the loading vectors in Y-space, q_i, and the coefficients of the linear regression equations between the corresponding loading vectors, b_i and h_i. Vectors t_i and u_i represent the transformed data, also called scores, in the X- and Y-space respectively. E and F are the residual errors in X- and Y-space. In case prediction is the purpose of modelling, the number of latent variables is typically chosen on the basis of the prediction residual sum of squares (PRESS) in Y-space, generally obtained by cross-validation.

In this work, the data set for PLS model identification is derived from an extensive simulation study using the detailed nonlinear SHARON-model of Volcke *et al.* (2002). Different combinations of influent conditions and feasible slave controller setpoints are simulated in order to cover different states of the process. The input data (X-space) consist of ammonia load (TNHiTNHi), inorganic carbon load (TICi), ratio of inorganic carbon load to ammonia load (TICi:TNHi), hydraulic residence time (HRT), influent flow rate (Q), dissolved oxygen setpoint (DOsp), dissolved oxygen (DO) and pH. The output data (Y-space) consist of ammonia-nitrogen (TNHo), nitrite-nitrogen (TNO2o) and nitrate-nitrogen (NO3o). It was intended to link the effects of two X-variables, namely DOsp and HRT, to the effluent quality variables TNHo, TNO2o and NO3o by means of PLS modelling.

Selection of the number of retained latent variables was based on cross-validation using contiguous blocks. Each block represented 20% of the total dataset, each corresponding to one simulated value of the ammonia load. Besides this criterion, the cumulative variance captured in X- and Y-space, was used for latent variable selection. The performances of several models, with different numbers of latent variables, were tested in closed loop in a simulation study through dynamic influent data of the full-scale SHARON reactor in Rotterdam. The daily values for influent pH and the concentrations of ammonia and inorganic carbon in this dataset were used. Flow rates to the SHARON reactor were not taken from this data set. Instead the control algorithm was allowed to control the influent flow rate independently, at this stage of the study not being limited by any feasibility or cost restrictions. The supervisory control was allowed to change the setpoints every 6 hours.

RESULTS AND DISCUSSION
Proposed methodology
The methodology proposed here is summarized in Figure 1. Firstly, a PLS model is constructed based on historical process data. Successful PLS modelling enables the prediction of output variables (in this case effluent quality) by means of input variables (in this case influent measurements, operational conditions and control setpoints).

The PLS model, once established, becomes an essential part of the master controller. With a certain time interval, newly derived process data enter the control algorithm as non-controllable input variables (imposed X-variables). Other variables, such as the setpoints of slave controllers can be changed (controllable X-variables). The output variables (Y-variables) are then predicted for each possible combination of imposed X-variables and controllable X-variables. For each of the predictions, a measure of control quality is calculated, expressed as a cost function. In turn, the setpoint combination that yields the lowest cost function are communicated to the slave controllers. The setpoints remain the same until the next evaluation by the master controller. Each time the designed time interval has elapsed, new process data are entered to the master controller and the procedure is repeated.
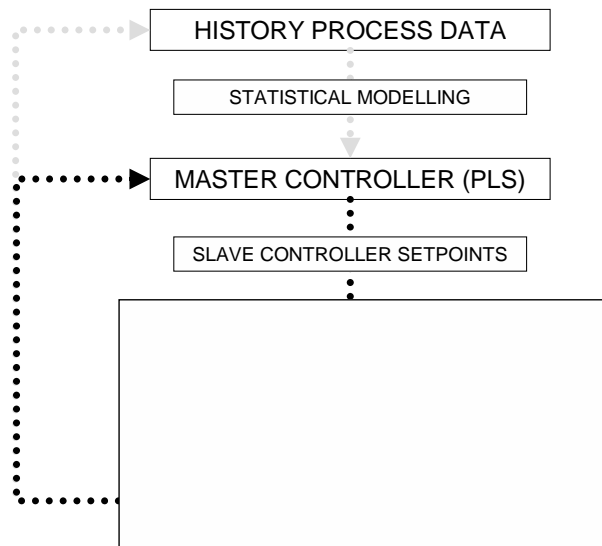
Figure 1. Conceptual Basic flow chart of the proposed methodology. The master control loop setpoints for slave controllers are set on the basis of statistical modelling.

As biological systems are subject to changing environmental conditions such as temperature changes, the history data will possibly be extended with process conditions that were not present before in the historical dataset. Therefore, repeated or adaptive statistical modelling can be used to adapt to changes in the process. This is however not the subject of this study.

Possible benefits of the proposed approach are:
- no mechanistic or precise knowledge of a process is necessary if sufficient historical process data are available
- if necessary, easy adaptation to new situations is possible by repeated automated statistical modelling or model updating

Application to the SHARON process: PLS modelling

The behaviour of the SHARON process was simulated for a range of influent conditions and slave control setpoints. The used slave controllers were PID controllers that controlled DO and HRT at the given setpoint and maintained the pH between 6.75 and 8.00. The values for each of the changed variables, that is the experiment design, are given in Table 1.

Table 1. Simulated steady-state values for influent variables and control setpoints

| variable	simulated values
TNHi [mg/l]	500 – 750 - 1000 – 1250 -1500
TICi:TNHi [-]	0.5 - 0.75 – 1.0 – 1.25 – 1.5
pHin [-]	7.8 – 8.0 – 8.2
DOsp [mg/l]	1 – 1.5 – 2.0 – 3.0
HRT [d]	1 – 1.1 – 1.2 – 1.3

A range of PLS models were identified from the resulting data. Steady state results where biomass washout was observed were omitted from the dataset. The first models (PLS1) were identified with all the described data. However, in the X-space of these models, the ratio of the ammonia load to the inorganic carbon load (TICi:TNHi) and the flow rate (Q) appear to be redundant variables. They can be mathematically written as a function of other variables as follows:

$$TICi:TNHi = \frac{TICi}{TNHi} \qquad (4)$$

$$Q = \frac{V}{HRT} \text{ where V, the reactor volume, is constant} \qquad (5)$$

Such redundancies may induce a risk of overfitting. Therefore, it was investigated whether any of the redundancies could be removed by removing one or more variables. Based on the PRESS results, it was found that either TICi:TNHi or TICi can be removed from the dataset without significant losses of prediction capacity. Removing TNHi, Q or HRT resulted in a large loss of prediction capability. Based on loading plots and biplots of corresponding scores, t_i (reduced X-space) and u_i (reduced Y-space), it was seen that the removal of any of these variables upsets the covariance structure. In the further course of the research, only the model without TICi:TNHi (PLS2) and the model without TICi (PLS3) in the input space were therefore used.

Figure 2 shows the cumulative variance and CUMPRESS inferences for both selected data structures (PLS2 and PLS3). CUMPRESS is the sum of PRESS for all observations. For both model types, retaining 3 LV's seems the best option as the captured variance does not increase much and no significant improvement of the PRESS statistic is seen beyond 3 LV's. Moreover, with 3 LV's about 90% of the variance in the Y-space can be captured.
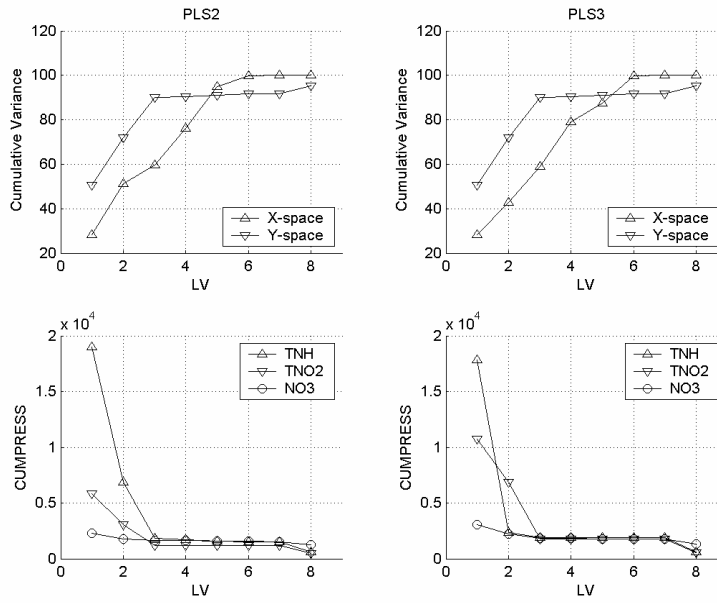
Figure 2. Cumulative captured variance in X- and Y-space and CUMPRESS statistic for the output variables TNH, TNO2 and NO3 as a function of retained variables. Graphs at the left show results for the PLS2 models (TICi:TNHi left out of X-space). Graphs at the right show results for the PLS3 models (TICi left out of X-space).

Application to the SHARON process: PLS-based control

The two resulting models were tested in by simulated closed loop control as follows. Measurements of the reactor pH and the influent variables TNHi and TICi are made.In this case, the output space variables TNHo and TNO2o are then predicted for a range of combinations of HRT, Q, DOsp and DO. DO values were set equal to their setpoints. This is justified as long as the DO control dynamics are much faster than those of the biological process, as in this case. Each set of control setpoints, combined with the measurements, defines a single virtual observation in the X-space. The cost function is then evaluated for all observations and the observation that leads to the smallest cost, is selected. The slave setpoints are communicated to the slave controllers. This procedure is repeated every 6 hours.

The following simple cost function was implemented:

$$COST = (y - y^{sp})^2 = \left(\frac{TNO_2}{TNH + TNO_2} - 0.5 \right)^2 \tag{6}$$

This cost function becomes zero when the ratio of nitrite nitrogen to the sum of ammonia and nitrite nitrogen is 1:2, as aimed for when it is intended to couple the SHARON process with an Anammox unit.

The minimum value, maximum value and interval for the control setpoints that are evaluated are given in Table 2. The interval between evaluated control setpoints was set small in order to reduce possible effects of the discretization of the controller. In any case, computation times were negligible compared to the process dynamics.

Table 2. Evaluated control setpoints

| setpoint variable	minimum value	interval	maximum value
DOsp [mg/l]	1.00	0.01	3.0
HRT [d]	1.00	0.01	1.30
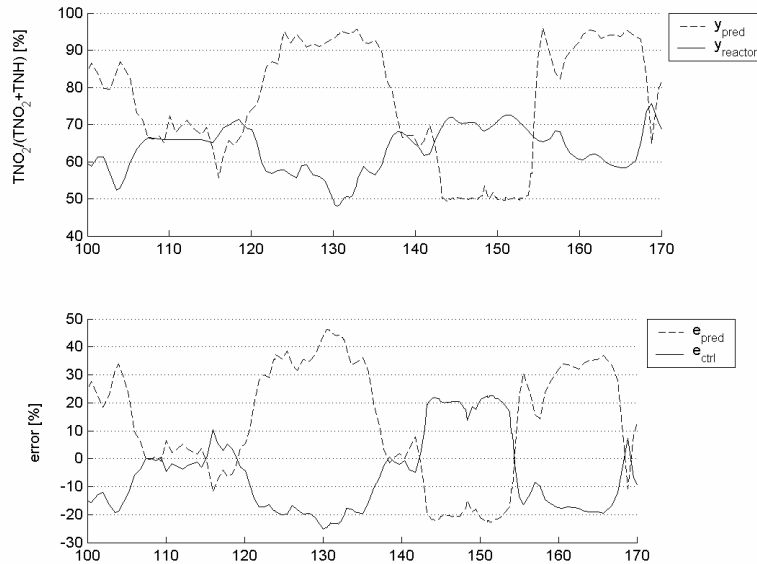
Figure 3. Results of the application of the PLS3 model (3 LV's) in closed loop.

Results of the closed-loop tests are shown in Figure 3 for the PLS3 (3 LV's) model for days 100 to 170. In this period the influent variables remained well between the previously simulated ranges of influent variables, so that extrapolation is avoided. The predicted value for $TNO_2/(TNH+TNO_2)$, the actual value for $TNO_2/(TNH+TNO_2)$, the deviation from the setpoint (e_{ctrl}) and the prediction error (e_{pred}) are shown. The graphs show that the model is not able to predict the conversion of ammonia to nitrite in a satisfying manner. In turn, it is obvious that it is not possible to control the conversion of ammonia to nitrite by means of the PLS-based controller. Similar results were obtained by means of the PLS2 (3 LV's) model.

As the first models (with 3 LV's) led to poor control of the process, the same tests were repeated with the same model structures. Only two LV's were retained now, as it was thought that the seemingly interesting third LV may be largely influenced by the extrapolation of the model to a dynamic situation, which in turn leads to erroneous predictions. Results of these new tests are shown in Figure 4 for the PLS3 (2 LV's) model. Visual inspection (Figure 4) shows that the selection of 2 LV's is indeed better as the prediction value and actual value of the controlled variable $TNO_2/(TNH+TNO_2)$ are much closer to each other and the same trends in the predicted and the actual values of the controlled variable are seen. Even though satisfactory prediction is now obtained, the control is still far from optimal, as the setpoint is never reached. To evaluate this in more detail, the control actions that were taken were investigated. Over the whole period no changes of HRT or the DOsp were communicated to the slave controllers. Moreover, the HRT setpoints remained at the minimum (1 day) and the DO setpoint remained at its maximum (3 mg/l). It is remarkable that, faced with a conversion which is too high, the controller never lowers the setpoint of oxygen. Indeed, process knowledge says that the growth rate of the ammonia oxidizers can be limited by lowering the oxygen concentration.

Faced with this incompatibility between observed control actions and process knowledge, the steady state response of the controlled variable $TNO_2/(TNH+TNO_2)$ to HRT and DOsp was investigated. Figure 5 shows this response for the case where TNHi is 1000 mg/l and TICi:TNHi is 1:1. Clearly, in

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a large part of the shown area a flat response to HRT and DOsp is observed. The output variable, $TNO_2/(TNH+TNO_2)$, shows a different response only when DO is below 1.5 mg/l and HRT is lower than 1.1 days. However, this area is exactly the area where biomass washout is observed, causing these data to be omitted from the modelling dataset. It is fairly logic that PLS regression by means of the resulting dataset will hardly relate the values of $TNO_2/(TNH+TNO_2)$ to the variables DOsp and HRT, resulting in control actions that are not sound with existing process knowledge. Thus, the simulated control setpoint changes do not excite the system sufficiently to identify a model for control of the selected output variable.
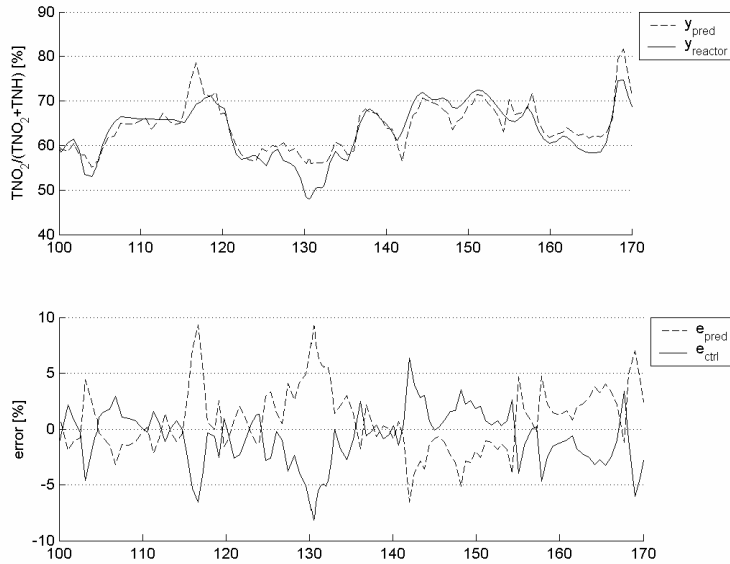
Figure 4. Results of the application of the PLS3 model (2 LV's) in closed loop. Predictions, and in turn the controller performance, are far from satisfying.
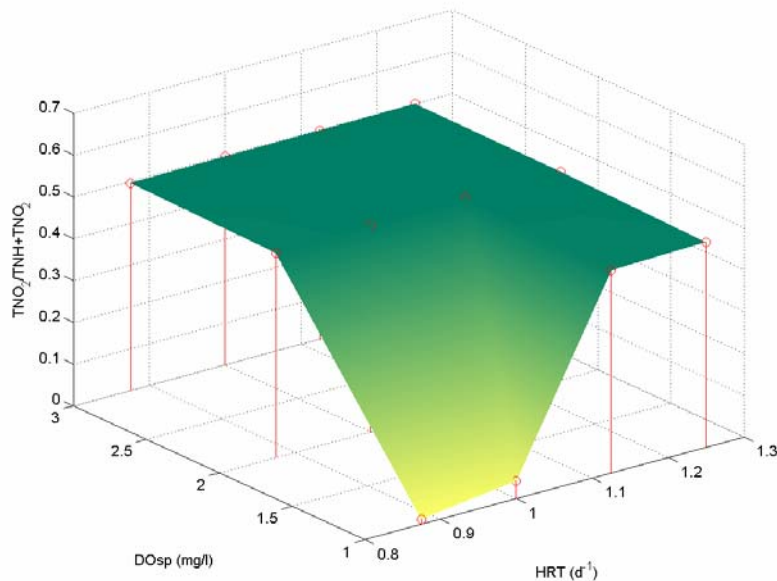
Figure 5. Steady state values of $TNO_2/(TNH+TNO_2)$ as a function of DOsp and HRT, where $TNHi = 1000$ mg/l and TICi:TNHi = 1:1.

It can thus be stated that in order to identify a PLS model that is useful for control of the SHARON process, data should be obtained that shows a responsiveness of the output variable to the control setpoints that are intended to be used. From Figure 5, it can be expected that these data will show non-linear behaviour. In order to tackle this problem, the data space can possibly be divided into several subspaces so that a linear PLS model can be fitted in each discrete subspace.

CONCLUSIONS AND FUTURE PERSPECTIVES
In this paper, the possibility of direct use of PLS modelling as a strategy in process control is introduced. In the past, PLS applications, traditionally put under the moniker of statistical process *control* (SPC), have been limited to statistical *monitoring* of processes and little applications in actual control design has been found. With the proposed methodology, a step towards filling the gap between statistical monitoring and automatic process control in wastewater treatment plants has been attempted.

While applying the proposed methodology, a pitfall in data-driven modelling was encountered. By insecure selection of the data for fitting statistical models, models with poor sensitivity of their outputs to the selected control handles were obtained. In order to obtain efficient and robust statistical model-based controllers in the future, proper data selection method to increase its extrapolation capability should be performed prior to PLS regression. It is observed that the SHARON process shows highly non-linear behaviour in the desired conditions. This behaviour may request a multiple modelling approach, where the data space is divided into several subspaces, in which local linear PLS models can be fitted.

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