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SUBSPACE IDENTIFICATION METHODS APPLIED TO ACTIVATED SLUDGE PROCESSES: A PERFORMANCE COMPARISON STUDY☆

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Abstract: The identification of multivariable systems is of extreme importance in practice. This paper deals with the use of subspace identification methods, to obtain a multivariable linear dynamic model in state-space form of an activated sludge process, around an operating point (a LTI model with lumped parameters). Different subspace algorithms (such as CVA, N4SID, MOESP, DSR) are used and compared, based on performance quality criteria. The selected model is cross-validated. It is a very low-order model and describes well the complex dynamics of the process. This model is asymptotically stable and it can be used specifically for control and also for monitoring purposes.

Keywords: Subspace methods, Multivariable identification, State-space models, Water pollution, Environment engineering.

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1. INTRODUCTION

Advanced engineering applications require suitable mathematical models. System identification deals with the problem of obtaining (approximate) models of dynamic systems from measured input-output data. This issue is of interest in a variety of applications, ranging from chemical process simulation and control to identification of vibrational modes in flexible structures. The most traditional system identification techniques are the prediction error method (PEM) and the instrumental variable method (IVM). These methods are primarily used with the so-called black-box model structures (Viberg, 1995).

The field of linear system identification is by now quite advanced and it has been studied for more than 25 years in the mathematical engineering literature. While at first sight, the linear identification techniques seems to be rather restricted, it turns out that the input-output behavior of many real-world problems, for most practical purposes (such as simulation, prediction, optimization, monitoring or control system design), can be approximated very well by a linear-time invariant (LTI) model. However, several important problems remain to be solved. The PEM has excellent statistical properties provided the "true" PEM estimate can be found. Nevertheless, computing the PEM model can sometimes be overwhelmingly difficult. In general, a multi-dimensional non-linear optimization problem must be solved. On the other hand, the IVM attempts to deliver parameter estimates by only solving linear systems of equations. However, the use of these models is quite cumbersome in the general multivariable case, and the numerical reliability may be unacceptably high for complex cases involving large system orders and many outputs (Viberg, 2000). The preferred model structure for complex problems is therefore a state-space model.

Subspace identification method is a branch that has been recently developed in system identification (around 10 years old by now), which has attracted much attention, owing to its computational simplicity and effectiveness in identifying dynamic state-space linear multivariable systems. These algorithms are numerically robust and do not involve nonlinear optimization techniques, i.e., they are fast (non-iterative) and accurate (since no problems with local minima occur). The computational

complexity is modest compared to PEM, particularly when the number of inputs and outputs is large. Because applications of large dimensions are commonly found in the process industry, subspace identification methods are very promising in this field. As a result, a large number of successful applications of subspace identification methods for simulated and real processes have been reported in the literature.

In this paper, a low-order LTI state-space multivariable model that describes the nitrate concentrations in the anoxic and aerobic zones of an activated sludge process is estimated around an operating point. Several subspace identification methods are applied and their performances are compared in order to select the best obtained model. It can be used to control the process, e.g., as in Lindberg (1997), where a multivariable control algorithm based on a subspace model is used to regulate an activated sludge process. Previous performance comparisons of several subspace methods, applied to other processes, can be found in Abdelghani *et al.* (1998), Katayama *et al.* (1998), Favoreel *et al.* (1999) and Juricek *et al.* (2000).

In this work, the ASWWTP-USP (Activated Sludge Wastewater Treatment Plant – University of São Paulo) benchmark (Sotomayor *et al.*, 2001a) is used as a data generator. This benchmark simulates the biological, chemical and physical interactions that occur in a complex activated sludge plant.

2. SUBSPACE IDENTIFICATION METHODS

The subspace identification methods refer to a class of algorithms whose main characteristic is the approximation of subspaces generated by the row spaces of block-Hankel matrices of the input/output data, to calculate a reliable discrete-time state-space model of the following form:

$$\begin{aligned} x_{k+1} &= Ax_k + Bu_k + w_k \\ y_k &= Cx_k + Du_k + v_k \end{aligned} \tag{1}$$

where w_k is called the process noise and v_k is called the measurement noise. They are assumed to be unmeasurable gaussian-distributed zero-mean white noise vector sequences. In this formula, x represents the model state vector, u is the manipulated input vector and y is the process output vector. A is the system (state transition) matrix, B is the input matrix, C is the output matrix and D is the direct input to output matrix. The time index k denotes a discrete (sampled) system.

The following assumptions have been considered related to equation (1):

- the system is asymptotically stable;
- the pair (A, C) is observable; and
- the pair (A, B) is controllable.

It is common practice to distinguish among the three possible situations regarding the inputs acting on the system:

- the purely deterministic case $(w_k = v_k = 0)$;
- the purely stochastic case $(u_k = 0)$; and
- the combined deterministic/stochastic case.

Subspace-based methods for state-space modeling have their origin in state-space realization, as developed by Ho and Kalman (1966). These techniques determine a state-space model from a given impulse response, which received a tremendous attention in the signal processing area in the late seventies. In system identification area, one usually has available input-output data rather than measured impulse response. In this context, subspace methods were developed in the late eighties.

The term "subspace identification method" was first introduced by Verhaegen and Deprettere (1991). There are now many different versions of subspace algorithms. These include an early version of subspace algorithm presented in the paper by Moonen *et al.* (1989), Canonical Variate Analysis

(CVA) by Larimore (1990), Multivariable Output-Error State-sPace model identification (MOESP) by Verhaegen and Dewilde (1992), Instrumental Variable Subspace-based State-Space System IDentification (IV-4SID) by Viberg *et al.* (1993), Numerical algorithm for Subspace State Space System IDentification (N4SID) by Van Overschee and De Moor (1993) and Deterministic and Stochastic subspace system identification and Realization (DSR) by Di Ruscio (1997).

All subspace identification methods consists of three main step: estimating the predictable subspace for multiple future steps, then extracting state variables from this subspace and finally fitting the estimated states to a state-space model (see Appendix). Nevertheless, each subspace identification method looks quite different from other in concept, computation tools and interpretation. The major differences among these subspace identification methods lie in the regression or projection methods used in the fist step to remove the effect of the future inputs on the future outputs and thereby estimate the predictable subspace, and in the latent variable methods used in the second step to extract estimates of the states. A general overview of the state-of-the-art in subspace identification methods is presented in De Moor *et al.* (1999), Favoreel (1999) and Favoreel *et al.* (2000).

The major advantages of these algorithms are that they only need input-output data and very little prior knowledge about the system. In addition, these algorithms are based on system theory, geometry and numerically stable non-iterative linear algebra operations, such as QR (or LQ)–factorization, SVD (singular value decomposition) and its generalizations, for which good numerical tools are well-known (Golub and VanLoan, 1996). A drawback against subspace identification approach is that the physical insight of the process, in the obtained model, is lost, which is a characteristic of black-box models. For example, the states are "artificial" and it is not possible to understand how a process variable, which is not directly included in the model, affects the process. Furthermore, a large amount of data is required to obtain accurate models. Actually, generating and collecting data of some processes can be too expensive. Important issues involved in developing a model through subspace identification methods can be found in Amirthalingam and Lee (1999).

Subspace identification methods have recently reached a certain level of maturity. The subspace identification algorithms considered in this paper are:

CVA: Canonical Correlation Analysis (CCA) technique - uCCA (unconstrained version) and cCCA (constrained version), both in Peternell *et al.* (1996).

MOESP: Past Output (PO) variant of the MOESP algorithm in the SMI Toolbox by Haverkamp and Verhaegen (1997).

N4SID: N4SID function (n4sid.m) in MATLAB System Identification Toolbox v.4.0.4 (Ljung, 1997), that implements the "standard" N4SID algorithm from Van Overschee and De Moor (1994) and the "robust" N4SID algorithm from Van Overschee and De Moor (1996).

DSR: DSR algorithm in the D-SR Toolbox by Di Ruscio (1997).

As previously mentioned, the purpose of the present paper is to compare the performance of these methods and not to analyze their implementational differences. As for the detailed algorithms, the difference between these subspace identification methods seems so large that it is hard to find the similarities between them. Nevertheless, Van Overschee and De Moor (1995a) showed that the subspace algorithms CVA, MOESP and N4SID are actually related to each other and that they differ only in the choice of weighting functions in a minimization problem. Di Ruscio (2000) reports the main differences and similarities among the algorithms CVA, MOESP, N4SID and DSR.

3. DESCRIPTION OF THE PROCESS

The ASWWTP-USP benchmark is a dynamic model, developed to simulate the processes that occur in a biological wastewater treatment plant (WWTP). The benchmark represents a continuous-flow pre-denitrifying activated sludge process (ASP), a frequently applied system for removal of organic matter

and nitrogen from municipal effluents, predominantly domestic, operating at a constant temperature of 15°C and neutral pH. The layout of the process is shown in figure 1.

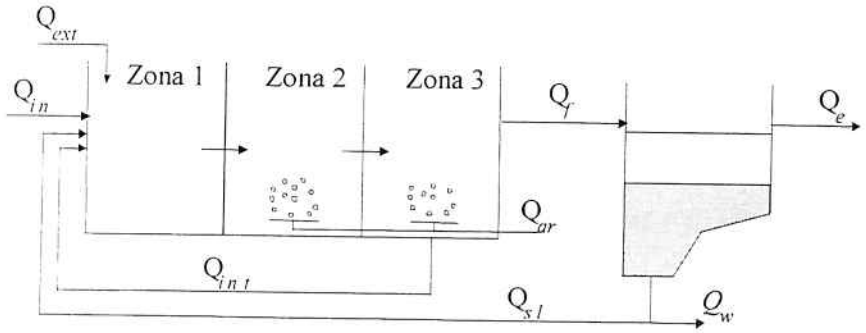


Fig. 1. Layout of the ASWWTP-USP benchmark

The process configuration is formed by a bioreactor composed of an anoxic zone (zone 1 with 13 m^3), two aerobic zones (zone 2 and zone 3 with 18 m^3 and 20 m^3, respectively) and a secondary settler (20 m^3). In nominal steady-state conditions, the influent rate of raw wastewater is $Q_{in} = 4.17$ m^3/h, with an average proportion of 224 mg COD/l of biodegradable organic matter and 44.88 mg N/l of total Kjeldahl nitrogen (TKN) and a hydraulic retention time of 17.0 hours (based on total volume, i.e. bioreactor + secondary settler). The internal recycle flow rate is $Q_{int} = 1.3Q_{in}$, the external sludge recycle flow rate is $Q_{sl} = 0.5Q_{in}$, the wastage flow rate is $Q_w = 25.8$ l/h and the external carbon flow rate is $Q_{ext} = 0.0$ l/h. In this case, an external carbon source is available, constituted by pure methanol, in a 33%-solution with a concentration of 80,000 mg COD/l. In the aerobic zones, the dissolved oxygen (DO) concentration is controlled in 2.0 mg O_2/l by simple PI controllers and in the anoxic zone it is assumed zero DO concentration.

For a reliable simulation of an ASP, the ASWWTP-USP benchmark is based on models widely accepted by the international community. Each bioreactor zone is modeled by IAWQ Activated Sludge Model ASM1 (Henze *et al.*, 1987) and the secondary settler is modeled by the double-exponential settling velocity model of Takács *et al.* (1991). The complete plant model includes 52 large, complex, coupled non-linear differential equations, which were implemented in Matlab/Simulink v.5.3. The values of the process parameters are here omitted, but they can be found in Sotomayor *et al.* (2001a).

For more realistic simulations, a white noise, with zero-mean and standard deviation 0.05, was added to the outputs produced by the benchmark.

4. IDENTIFICATION OF A SUBSPACE MODEL FOR THE ASP

4.1 *Generation and pre-treatment of data set*

It is not very easy to select either the input or the output variables of the process. In this work, the nitrate concentrations in the anoxic zone Sno_1 (mg N/l) and in the last aerobic zone Sno_3 (mg N/l) are selected as outputs. The internal recirculation rate Q_{int} (m^3/h) and the external carbon dosage Q_{ext} (l/h) are considered as inputs. However, to improve the model influent flow rate Q_{in} (m^3/h), influent readily biodegradable substrate Ss_{in} (mg COD/l) and influent ammonium concentration Snh_{in} (mg N/l) are assumed as measurable disturbances, while influent nitrate concentration Sno_{in} (mg N/l) is assumed as an unmeasurable disturbance. The signals used in the identification procedure are summarized in figure 2. Note that all disturbances are considered as inputs.

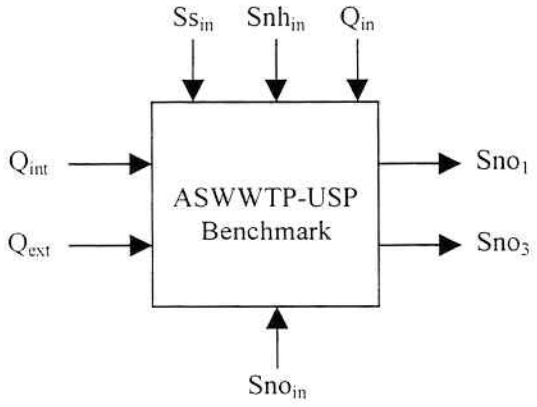


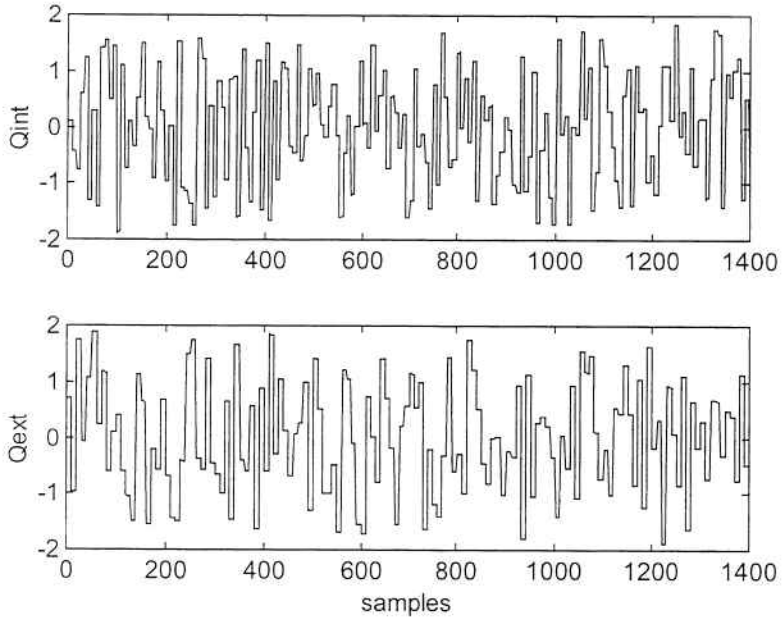
Fig. 2- Signals for subspace identification

Pseudo-random binary sequences (PRBS) are widely used in the identification of linear systems. The advantages of the PRBS input include ease implementation and an autocorrelation function similar to white noise. However, since the PRBS consists of only two levels, the resulting data may not provide

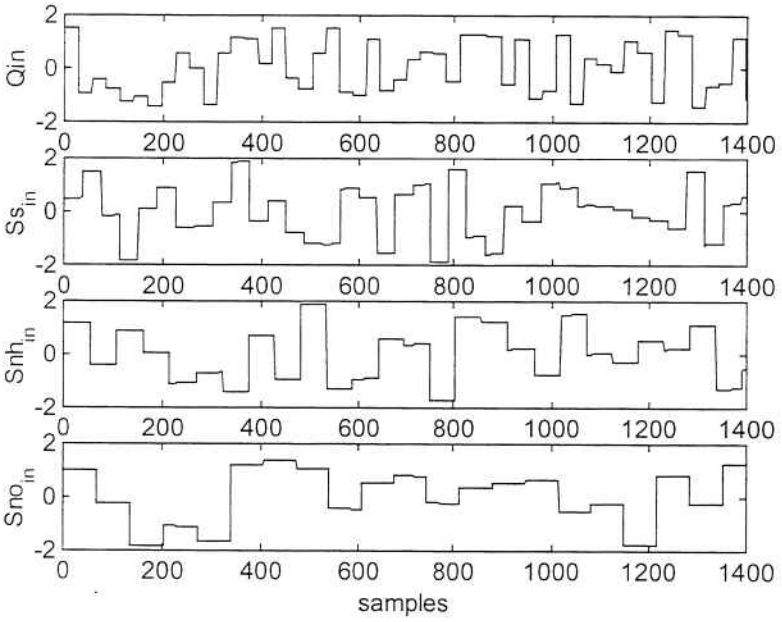
sufficient information to excite nonlinear dynamics. Additionally, a PRBS signal of a too large magnitude may bias the estimation of the linear kernel. Multi-level (m-level) sequences, in contrast, allow the user to highlight nonlinear system behavior while manipulating the harmonic content of the signal, reducing the effect of nonlinearities in the resulting linear model (Godfrey, 1993). On the other hand, the ill-conditioning of probing inputs may lead to a substantial deterioration of performance of the subspace algorithms. This possible cause of ill-conditioning has to do with wide variations in the amplitude of the input spectrum and with frequency bands where the spectrum is nearly zero causing "insufficient excitation" (Chiuso and Picci, 2000).

In the present paper, the data signals correspond to m-level uniformly distributed random sequences. Their amplitudes and frequencies were chosen so as to adequately excite the system, without deviating too much from the normal operating point and, therefore, enabling the identification of a suitable linear model. All data signals are stored at a sampling rate of 0.16 hours to obtain 1400 samples.

For a better identification result, the raw data set is pre-processed. As the data set is generated from a simulation model, no data pre-filtering is necessary. However, since the system is running at an operating point different from zero and hence introducing some D.C. offsets, subtraction of the sample mean from data set is done in order to remove these offsets. This operation is common in system identification (Söderström and Stoica, 1989). As pointed out by Chui (1997), it is important to make sure that the scales of the input-output data are of comparable sizes. Therefore, all data signals are normalized aiming to be equally weighted. Finally, the data set is detrended in order to remove linear trends from input-output data. This step is usual in signal processing. Asymptotic properties of subspace procedures, when the data set is pre-processed by removing trends and periodic components, are presented in (Bauer, 2000a). The pre-processed signals are shown in figures 3 and 4.



(a)



(b)

Fig. 3. Data sequences of the process: (a) inputs and (b) disturbances

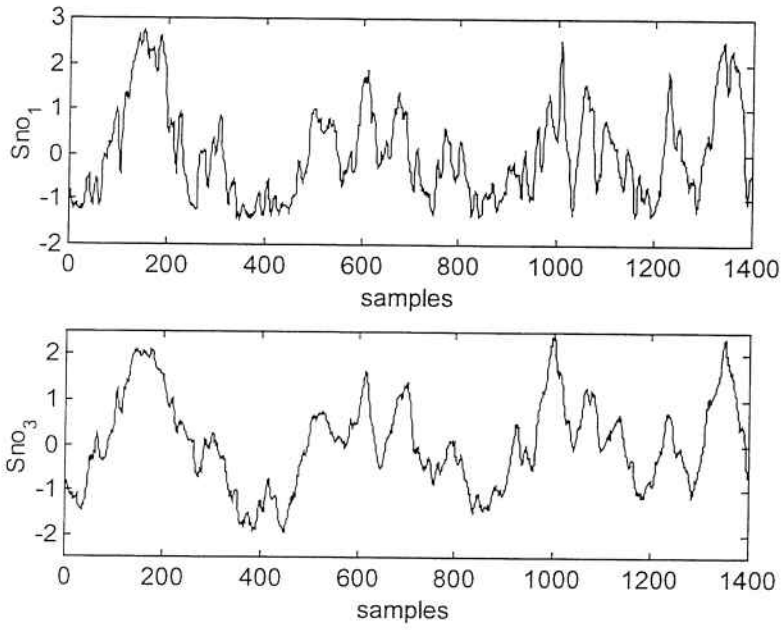


Fig. 4. Output signals of the process

The identification process was carried out off-line in batch form by using the first 1000 points of the data set, whereas the remaining 400 points were applied for model validation. In the identification procedure is done in open loop and the purely deterministic case is considered.

4.2 *Order estimation*

There is an extensive literature for order estimation algorithms for linear, dynamical, state-space systems. Nevertheless, there exist only few references dealing with the estimation of the order in the context of subspace identification methods (Bauer, 2001).

The determination of the system order n is very subtle. Normally, this information is obtained by detecting a gap in the spectrum of the singular values of the orthogonal (or oblique) projections of the row spaces of data block-Hankel matrices. In the present case, the gap is not easy to determine, as it is seen in figure 5, and hence the application of this strategy becomes subjective and the decision regarding the order of the model is an arbitrary one.

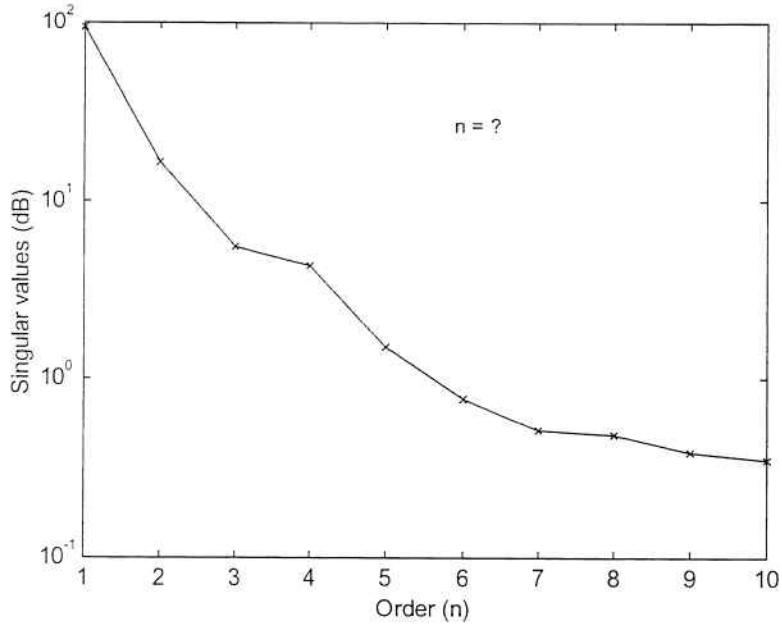


Fig. 5. Singular value spectrum

According to Bastogne *et al.* (1998), a more practical procedure is to choose the value n that minimizes the estimation errors. For instance, subspace identification methods do not involve error minimization schemes. These techniques are exclusive of the "classical" PEMs and they require a larger computational effort. The determination of the theoretical order, in the sense of minimization of the estimation error, is shown in figure 6, which was generated using the "robust" N4SID algorithm. Comparing the relative estimation error indexes, it can be noticed that the 3rd, 6th and 7th-order model have practically the same mean error index, but for $n = 6$ it is slightly lower. Nevertheless, the choice of 6th or 7th-order does not bring enough improvement in comparison with a reduced order given by the 3rd-order model, which is the selected order estimation. For $n = 3$ the relative square error was 34.60% for the case of Sno_1 and 35.07% for the case of Sno_3, with a mean error of 34.84%. This order of the model corresponds to the number of states or poles of the model.

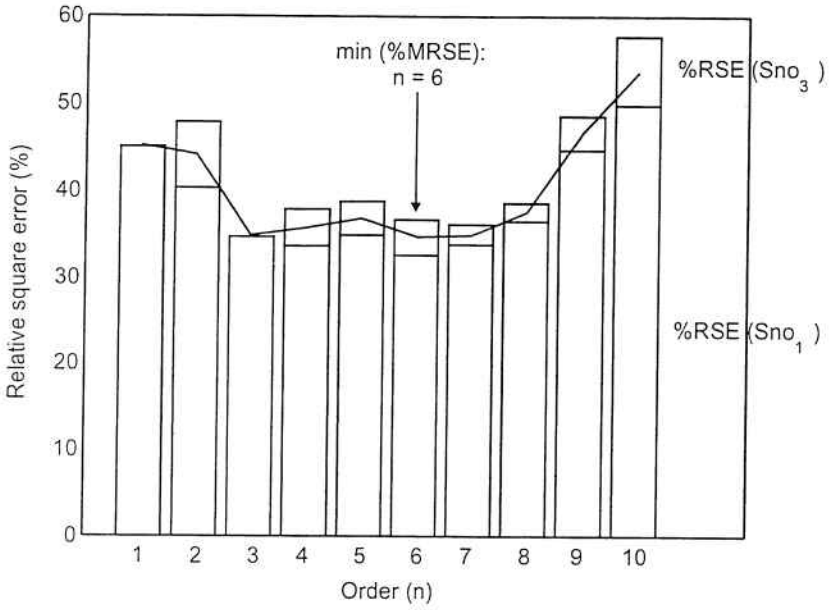


Fig. 6. Estimation error spectrum

4.3 *Performance quality criteria*

In Favoreel *et al.* (1999), three subspace algorithms (CVA, MOESP and "robust" N4SID) were applied to 15 different data sets from real-life systems. They evaluated the algorithms according to computational complexity and prediction/simulation error and concluded that their performance is very similar.

In the present paper, two performance indicators are proposed to measure identification/validation error, in order to obtain the best 3rd-order state-space model. The performance indicators are:

Mean relative square error (MRSE):

$$\%MRSE = \frac{1}{l} \cdot \sum_{i=1}^{l} \sqrt{\frac{\sum_{j=1}^{N} \left(y_i(j) - \hat{y}_i(j)\right)^2}{\sum_{j=1}^{N} \left(y_i(j)\right)^2}} \times 100 \qquad (2)$$

Mean variance-accounted-for (MVAF):

$$\%MVAF = \frac{1}{l} \cdot \sum_{i=1}^{l} \left(1 - \frac{\text{variance}(y_i - \hat{y}_i)}{\text{variance}(y_i)} \right) \times 100 \qquad (3)$$

being N the number of identification data points, l the number of outputs, y_i the *i-th* real output and $\hat{y}_i$ the *i-th* simulated output produced by the model. The MRSE index is widely used in the literature, while the MVAF index is specifically used by the SMI Toolbox. Both performance indexes are used to evaluate the adequacy of the model produced by each algorithm.

Table 1. Numerical results of the performance of the subspace-based algorithms

Algorithm	%MRSE		%MVAF	
	Identification	Validation	Identification	Validation
uCCA	40.4417	69.9404	83.5750	73.5628
cCCA	40.1652	69.2404	83.7998	73.9129
MOESP	**31.8091**	57.5806	**89.9037**	79.3096
N4SID	44.4914	72.9242	80.0546	74.2431
"robust" N4SID	34.8394	57.7508	87.8739	81.2475
DSR	34.2450	**50.9904**	88.2237	**84.4274**

Analyzing the values in table 1, the MOESP model seems to produce a better model in terms of identification, while the DSR model seems to produce a better model in terms of validation. Hence, in this work, the 3rd-order DSR model was chosen to describe the process.

4.4 *Identification results*

The selected deterministic model (proper model) is described by the following matrices:

$$A = \begin{bmatrix} 0.9763 & 0.0194 & 0.3268 \\ 0.0061 & 0.8815 & 0.0893 \\ -0.0023 & 0.0071 & 0.9763 \end{bmatrix}$$

$$B = \begin{bmatrix} 0.0238 & -0.0459 & -0.1488 & -0.0403 & 0.0002 \\ -0.1295 & 0.0299 & 0.0230 & 0.0185 & -0.0052 \\ 0.0097 & -0.0082 & -0.0082 & 0.0004 & 0.0036 \end{bmatrix} \quad (4)$$

$$C = \begin{bmatrix} 0.2253 & -0.4032 & -0.1823 \\ 0.2668 & 0.2880 & -0.4626 \end{bmatrix}$$

$$D = \begin{bmatrix} 0.1292 & -0.0193 & -0.0651 & -0.0312 & 0.0053 \\ -0.0387 & 0.0086 & 0.0126 & 0.0105 & -0.0026 \end{bmatrix}$$

A strictly proper model (i.e, with $D = 0$) is also identified, and it is described by:

$$A = \begin{bmatrix} 0.9763 & 0.0199 & 0.3263 \\ 0.0062 & 0.8818 & 0.0907 \\ -0.0024 & 0.0072 & 0.9758 \end{bmatrix}$$

$$B = \begin{bmatrix} 0.0368 & -0.0434 & -0.1537 & -0.0431 & -0.0045 \\ -0.1505 & 0.0234 & 0.0357 & 0.0283 & -0.0044 \\ 0.0167 & -0.0100 & -0.0091 & 0.0003 & 0.0039 \end{bmatrix} \quad (5)$$

$$C = \begin{bmatrix} 0.2259 & -0.4026 & -0.1810 \\ 0.2664 & 0.2876 & -0.4633 \end{bmatrix}$$

The poles (eigenvalues of A) of the proper model (denoted by the +) and the poles of the strictly proper model (denoted by Δ) are shown in figure 7. The poles closer to the unit circle are related to the slower system dynamics. The poles close to 1, show that the data set seems to contain a phenomenon known as "co-integration" in econometrics. Based on this observation, it is possible to obtain models which produce a one-step-ahead prediction error much smaller (Bauer, 2000b).

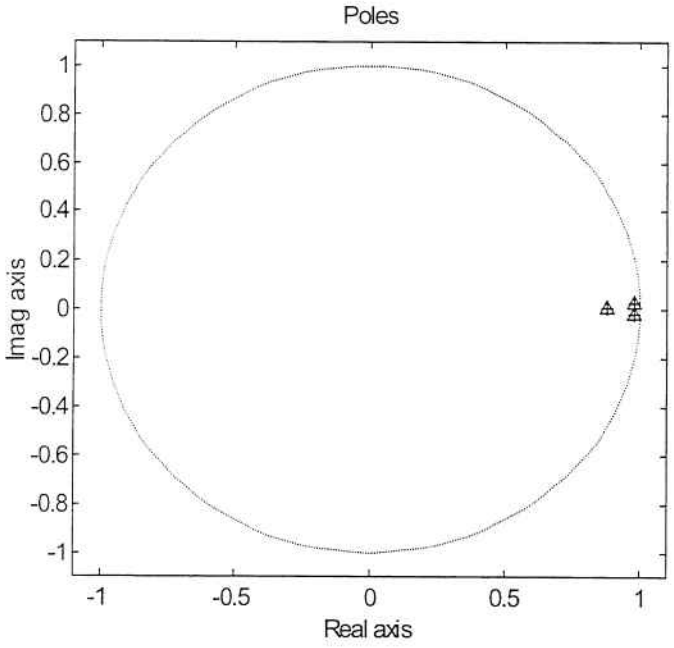


Fig. 7. Location of the poles of the DSR-model.

Figures 8 and 9 show the outputs generated by the identified strictly proper model (dotted line). As it can be observed, the identified model for a given operating points correctly reproduces the main dynamic characteristics of the activated sludge process. In these graphics, either the identification or the validation data were introduced in the obtained model. In both cases the simulation started at zero initial conditions.

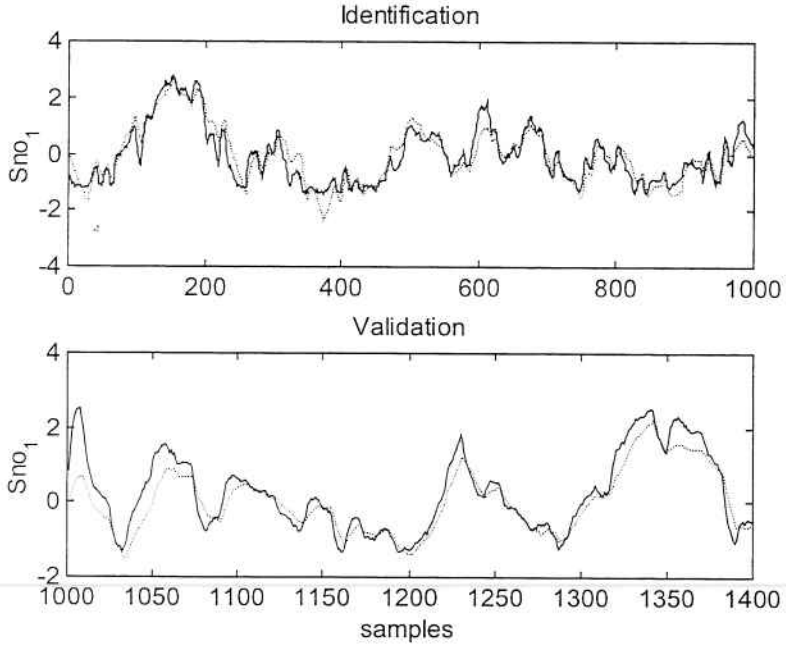


Fig. 8. Response comparison for Sno_1

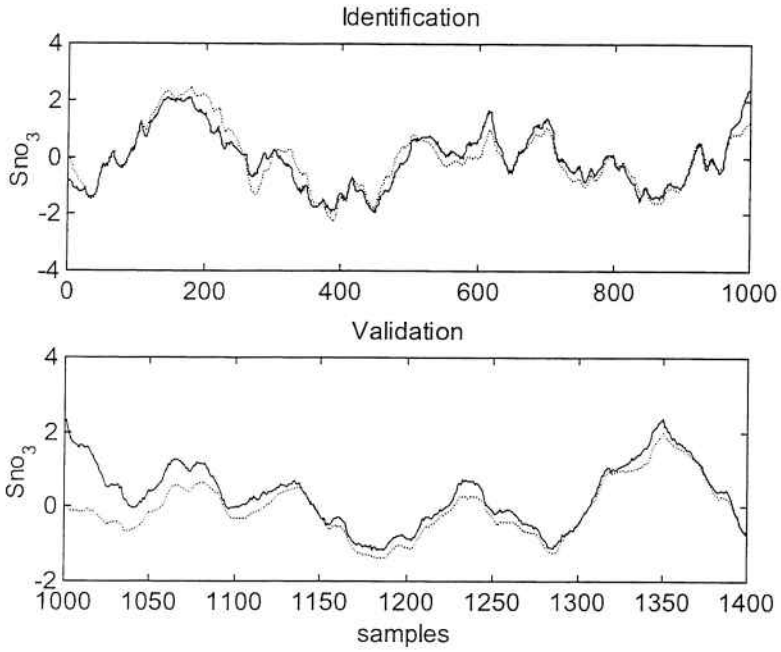


Fig. 9. Response comparison for Sno_3

Given that low-order state-space models sufficiently representative of the nominal system behavior are a prerequisite to the systematic design of control systems, the strictly proper model (5) derived above has been successfully used in the implementation of an infinite-horizon optimal controller. For more details see Sotomayor *et al.* (2001b).

5. CONCLUSIONS

The use of subspace identification methods has proved to be a valuable tool in the estimation of LTI state-space models for the activated sludge process. The performance of different identification algorithms (CVA, MOESP, N4SID and DSR) was compared. Although the used simulation benchmark consists of 52 complex differential equations (3 IAWQ and the settler models), the 3rd-order obtained one (a very reduced order model) manages to describe sufficiently well the process. It is well suited for model-based control (not just for Model Predictive Control) and also for monitoring applications.

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APPENDIX

In this section, we introduce the state-space identification problem and review the main issues related to subspace identification methods and one particular technique (the "standard" N4SID). The text to follow is taken (with some modifications) from Delgado *et al.* (2001).

A.1 *The problem*

The objective is to estimate, from measured input/output data sequences ($\{u_k\}$ and $\{y_k\}$, respectively), the system described by:

$$\begin{cases} x_{k+1} = A\ x_k + B\ u_k + w_k \\ y_k = C\ x_k + D\ u_k + v_k \end{cases} \tag{A.1}$$

$$E\left[\begin{pmatrix} w_p \\ v_p \end{pmatrix}\begin{pmatrix} w_q^T & v_q^T \end{pmatrix}\right] = \begin{bmatrix} Q^s & S^s \\ S^{sT} & R^s \end{bmatrix}.\delta_{pq} \geq 0 \tag{A.2}$$

where:

- $A \in R^{n\times n}$, $B \in R^{n\times m}$, $C \in R^{l\times n}$, $D \in R^{l\times m}$, $Q^s \in R^{n\times n}$, $S^s \in R^{n\times l}$, $R^s \in R^{l\times l}$ and $x_k \in R^n$
- $w_k \in R^n$ and $v_k \in R^l$ denote white noise sequences (process and measurement noise) and
- the input data sequence is assumed to be a persistently exciting quasi-stationary deterministic sequence (Ljung, 1997), with correlation:

$$Ruu(\tau) = E_N\left[u(t+\tau)\,u^T(t)\right] = \lim_{N\to\infty}\frac{1}{N}\sum_{t=1}^{N} E\left[u(t+\tau)\,u^T(t)\right] \qquad (A.3)$$

(where N is the number of measurements)

A.2 *Notations and definitions*

The input and output data will be organized into block Hankel matrices with ($2i$) row-blocks and (j=N-$2i$+1) column-blocks:

- the input block Hankel matrix, $U_{1/2i+j-1(i,j)}$, or just U:

$$U = \begin{bmatrix} u_1 & \cdots & u_j \\ \cdots & \cdots & \cdots \\ u_i & \cdots & u_{i+j-1} \\ u_{i+1} & \cdots & u_{i+j} \\ \cdots & \cdots & \cdots \\ u_{2i} & \cdots & u_{2i+j-1} \end{bmatrix} = \begin{bmatrix} U_{1/i+j-1(i,j)} \\ U_{i+1/2i+j-1(i,j)} \end{bmatrix} = \begin{bmatrix} Up \\ Uf \end{bmatrix} \in R^{2mi\times j}$$

where the subscripts p and f denote *past* and *future*, respectively. In the same way, $U_{0/1} = U_p^{+}$ and $U_{i+1/2i-1} = U_f^{-}$.

- Y (or $Y_{1/2i+j-1(i,j)}$) is the output block-Hankel matrix with $2i$ row-blocks and j column-blocks and $H = \begin{bmatrix} U \\ Y \end{bmatrix}$

- $\hat{X}_f$ is the state sequence generated by a bank of Kalman filters, working in parallel on each of the columns of the block Hankel matrix of past inputs and outputs, illustrated in the next figure:

$\hat{X}_f = [\hat{x}_{i+1/1}\ \hat{x}_{i+2/2}\ \cdots\ \hat{x}_{N-i+1/N-2i+1}] \in R^{n\times j}$ and

$\hat{X}_{f+1} = [\hat{x}_{i+2/2}\ \cdots\ \hat{x}_{N-i+2/N-2i+2}] \in R^{n\times j}$.

$$P_1 \cdot \overline{X}_1 = \left[\overline{x}_1 \ \ldots \ \overline{x}_{q+1} \ \ldots \ \overline{x}_j\right]$$

$$H_p = \begin{pmatrix} U_p \\ Y_p \end{pmatrix} \begin{bmatrix} u_1 & \downarrow & u_{q+1} & \downarrow & u_j & \downarrow \\ \vdots & \downarrow & \vdots & \downarrow & \vdots & \downarrow \\ u_i & \downarrow & u_{q+i} & \downarrow & u_{j+i-1} & \downarrow \\ y_1 & \downarrow & y_{q+1} & \downarrow & y_j & \downarrow \\ \vdots & \downarrow & \vdots & \downarrow & \vdots & \downarrow \\ y_i & \downarrow & y_{q+i} & \downarrow & y_{j+i-1} & \downarrow \end{bmatrix} \begin{matrix} \textit{Kalman} \\ \textit{Filter} \\ \downarrow \\ \downarrow \\ \downarrow \\ \downarrow \end{matrix}$$

$$\hat{X}_f = \left[\hat{x}_{i+1/1} \ \ldots \ \hat{x}_{q+i+1/q+1} \ \ldots \hat{x}_{j+i/j}\right]$$

Fig. A.1 – Interpretation of the sequence $\hat{X}_f$ as a sequence of Kalman filter state estimates based on i measurements of u_k and y_k.

Γ_i is the *extended* observability matrix (since $i>n$) where the subscript i denotes the number of row-blocks (in fact, the estimated order has (li) as an upper bound):

$$\Gamma_i = \begin{bmatrix} C \\ CA \\ \ldots \\ CA^{i-1} \end{bmatrix} \in R^{li \times n} \tag{A.4}$$

H_i^d is a block Toeplitz matrix, built with Markov parameters:

$$H_i^d = \begin{bmatrix} D & \cdots & 0 \\ CB & \cdots & 0 \\ \cdots & \cdots & \cdots \\ CA^{i-2}B & \cdots & D \end{bmatrix} = \begin{bmatrix} H_0 & \cdots & 0 \\ H_1 & \cdots & 0 \\ \cdots & \cdots & \cdots \\ H_{i-1} & \cdots & H_0 \end{bmatrix} \in R^{li \times mi} \tag{A.5}$$

A.3 *One subspace identification technique*

The main principle behind subspace theory is the estimation of the system matrices as the least squares problem:

$$\begin{bmatrix} \hat{X}_{f+1} \\ Y_{i/i} \end{bmatrix} = \begin{bmatrix} \hat{A} & \hat{B} \\ \hat{C} & \hat{D} \end{bmatrix} \cdot \begin{bmatrix} \hat{X}_f \\ U_{i/i} \end{bmatrix} \tag{A.6}$$

where $\hat{X}_{f+1}$ and $\hat{X}_f$ are Kalman filter state estimates, obtained directly from the input-output data. In fact, Van Overschee and De Moor (1994, 1995b) establish a relation between the estimated Kalman filter state sequence and the input and output data – through orthogonal or oblique projections:

- the orthogonal projection of the row space of Y_f (future outputs) into the row space of the past inputs, past outputs and future inputs row space U_f $\left(Z_i = Y_f / \begin{bmatrix} W_p \\ U_f \end{bmatrix} \right)$ is related to $\hat{X}_f$ by the expression $Z_i = \Gamma_i \hat{X}_f + H_i^d U_f$.
- the oblique projection of the row space of Y_f (future outputs), along the future inputs row space U_f, into the row space of the past inputs and outputs W_p, is related to the estimated Kalman filter state sequence $\tilde{X}_i$ by the expression $O_i = \Gamma_i \tilde{X}_f \; : \; O_i = Y_f / U_f W_p = \Gamma_i \tilde{X}_f$.

There is a slight difference between Z_i and O_i. In fact, O_i can be computed from Z_i by just ignoring the information given by U_f. The consequences are clear: part of the information required to estimate $\hat{X}_0$ is no longer available so, the estimated state sequence $(\tilde{X}_f)$ is different from $\hat{X}_f$. Although $\tilde{X}_i$ and $\hat{X}_f$ are not the same bank of Kalman filters, they are still very similar and, actually, under some special conditions ($i \to \infty$ or $\{u_k\}$ is white noise or the system is purely deterministic) they are the same.

This approximation of the state sequences is used to obtain a more elegant and simple algorithm presented in the next section. Unlike the algorithm that considers the "exact" Kalman state estimates

by implementing some orthogonal projections (unbiased for $j \to \infty$), this approximate algorithm is biased for finite i, except under certain special cases (Van Overschee and De Moor, 1994).

A.3 *Algorithm based on the result:* $O_i = \Gamma_i \, \tilde{X}_f$

1. Projections: Compute the oblique projections (LQ-decomposition):

$$O_i = Y_f / U_f \, H_p \quad \text{and} \quad O_{i+1} = Y_f^- / U_f^- \, H_p^+ .$$

2. SVD: Compute the Singular Value Decomposition of the oblique projection O_i:

$$O_i = U \cdot S \cdot V^T = [U_1 \, U_2] \begin{bmatrix} S_1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} V_1^T \\ V_2^T \end{bmatrix} = U_1 \cdot S_1 \cdot V_1^T$$

where $O_i \in R^{li \times j}$, $S \in R^{li \times j}$ (diagonal matrix with the singular values of O_i), $U \in R^{li \times li}$, $V^T \in R^{j \times j}$ (U and V are orthogonal matrices), $U_1 \in R^{li \times r}$, $S_1 \in R^{r \times r}$, $V_1^T \in R^{r \times j}$, $r = \text{rank}(O_i) = n$.

2.1. Order n of the system: can be determined (Van Overschee and De Moor, 1994, 1995a, 1995b) by the number of the nonzero singular values of O_i (dim (S_1)). However, in many practical situations, when the measurements are noise corrupted, it may be not straightforward to distinguish the "nonzero" from the "zero" singular values – we must take a decision by comparing the values or by assuming different orders and then comparing simulation errors.

2.2. Observability matrices: as the column spaces of Γ_i and $U_1 \cdot S_1^{1/2}$ are the same, compute $\Gamma_i = U_1 \cdot S_1^{1/2}$. To compute Γ_{i-1}, remove the last l rows of Γ_i.

2.3. State sequence: since $O_i = \Gamma_i \, \tilde{X}_f$ and $O_i = \Gamma_i - 1 \, \tilde{X}_f + 1$, compute $\tilde{X}_f = pinv(\Gamma_i) \, O_i$ and $\tilde{X}_{f+1} = pinv(\Gamma_{i-1}) \, O_{i+1}$, where *pinv(.)* denotes the Moore-Penrose pseudo-inverse. In order to achieve a more robust algorithm, we can estimate A and

C from $\Gamma_i : C$ from the first l lines of Γ_i and A such that $\Gamma_{i-1} A = \overline{\Gamma}_i$ where

$$\overline{\Gamma}_i = \begin{bmatrix} CA \\ \cdots \\ CA^{i-1} \end{bmatrix}.$$

3. System matrices: the model can now be expressed as a simple least squares problem $\begin{bmatrix} \widetilde{X}_{f+1} \\ Y_{i/i} \end{bmatrix} = \begin{bmatrix} A & B \\ C & D \end{bmatrix} \cdot \begin{bmatrix} \widetilde{X}_f \\ U_{i/i} \end{bmatrix}$ where $Y_{i/i} = \lfloor y_i \ldots y_{i+j-1} \rfloor$ and $U_{i/i} = \lfloor u_i \cdots u_{i+j-1} \rfloor$. Compute the covariance of the residuals, in order to determine the matrices Q^s, R^s and S^s.

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