

Available online at www.sciencedirect.com



Journal of Biotechnology 116 (2005) 195-210



www.elsevier.com/locate/jbiotec

Adaptive multiscale principal component analysis for on-line monitoring of a sequencing batch reactor

Dae Sung Lee^{a,*}, Jong Moon Park^{a,b}, Peter A. Vanrolleghem^c

 ^a Advanced Environmental Biotechnology Research Center (AEBRC), School of Environmental Science and Engineering, Pohang University of Science and Technology, San 31, Hyoja-dong, Nam-gu, Pohang, Gyeongbuk 790-784, Republic of Korea
 ^b Department of Chemical Engineering, Pohang University of Science and Technology, San 31, Hyoja-dong, Nam-gu, Pohang, Gyeongbuk 790-784, Republic of Korea
 ^c BIOMATH, Department of Applied Mathematics, Biometrics and Process Control, Ghent University,

Coupure Links 653, B-9000 Gent, Belgium

Received 3 April 2004; received in revised form 11 October 2004; accepted 25 October 2004

Abstract

In recent years, multiscale monitoring approaches, which combine principal component analysis (PCA) and multi-resolution analysis (MRA), have received considerable attention. These approaches are potentially very efficient for detecting and analyzing diverse ranges of faults and disturbances in chemical and biochemical processes. In this work, multiscale PCA is proposed for fault detection and diagnosis of batch processes. Using MRA, measurement data are decomposed into approximation and details at different scales. Adaptive multiway PCA (MPCA) models are developed to update the covariance structure at each scale to deal with changing process conditions. Process monitoring by a unifying adaptive multiscale MPCA involves combining only those scales where significant disturbances are detected. This multiscale approach facilitates diagnosis of the detected fault as it hints to the time-scale under which the fault affects the process. The proposed adaptive multiscale method is successfully applied to a pilot-scale sequencing batch reactor for biological wastewater treatment. © 2004 Elsevier B.V. All rights reserved.

Keywords: Principal component analysis; Process monitoring; Multiscale; Batch process

1. Introduction

* Corresponding author. Tel.: + 82 54 279 8650; fax: +82 54 279 8659.

E-mail address: dslee@postech.ac.kr (D.S. Lee).

Batch operations are the prevalent mode, e.g. in chemical and biological processes, when highvalue-added, low-volume products are produced or they have an inherent flexibility. In general, batch processes exhibit some batch-to-batch variations

^{0168-1656/\$ –} see front matter © 2004 Elsevier B.V. All rights reserved. doi:10.1016/j.jbiotec.2004.10.012

due to composition disturbances, equipment defects and deviations of the process variables from their specified trajectories. Abnormalities during batch operations can lead to undesirable products in at least one batch or a whole sequence of batches. Therefore, on-line monitoring of batch processes is very crucial as it allows to detect potential problems and make modifications when necessary.

With the advent of improved on-line sensor technology and automation, batch processes with wellequipped computerized measurement devices produce large amounts of data. It becomes therefore very important and essential to extract the useful information from the measurement data and to infer the state of an ongoing process. However, this task is a really challenging one due to the complexities of chemical and biological processes originating from the large number of measurement variables, strong interactions among those measurements, missing data, considerable effects of control loops, etc.

Multivariate statistical process control (MSPC) has been successfully applied to monitoring, fault detection and diagnosis of batch processes (Nomikos and MacGregor, 1994; Lennox et al., 2001). Multiway principal component analysis (MPCA) is a projection method for analyzing a historical reference distribution of measurement trajectories from past successful batches in a reduced latent-vector space and comparing the behaviors of new batches to this reference distribution. Several extensions of MPCA have been proposed to take into account various factors such as dynamic MPCA (Chen and Liu, 2002), nonlinear MPCA (Dong and McAvoy, 1996), hierarchical MPCA (Ränner et al., 1998), multi-group MPCA (Lane et al., 2001) and multiblock MPCA (Lee and Vanrolleghem, 2003). All these techniques are based on a single-scale presentation of the collected data. However, data from almost all practical processes are inherently multiscale due to events occurring at different locations and with different localization in time and frequency.

In recent years, there has been significant interest in combining the conventional PCA with wavelet transforms (Bakshi, 1998; Kosanovich and Piovoso, 1997; Misra et al., 2002; Rosen and Lennox, 2001). Those PCA-based process monitoring methods employ wavelet analysis to transform time-domain signals into the time-frequency domain. Especially, Bakshi (1998) proposed the multiscale PCA methodology, which determines separate PCA models at each wavelet scale. The scales where significant events occur are recombined to obtain a PCA model for all scales together. Multiscale PCA is useful for modeling data containing contributions that change over time and frequency.

In the application investigated here, a variant of MPCA technique, adaptive multiscale MPCA, is used as a basis to develop a monitoring system for a sequencing batch reactor (SBR) process for biological wastewater treatment. A SBR process has a unique cyclic batch operation for wastewater treatment (Demuynck et al., 1994; Lee and Park, 1999). Most of the advantages of SBR processes may be attributed to their single-tank designs and their flexibility that allows them to meet many different treatment objectives (Wilderer et al., 2001). The SBR process is highly nonlinear, time-varying and subject to significant disturbances like hydraulic changes, composition variations and equipment defects. Disturbances and events in SBR processes occur in different time-scales ranging from minutes (sensor faults), hours (toxic shocks) to months (seasonal effects). Thus, a multiscale MPCA seems to be better suited for extracting information from SBR processes.

Multiscale MPCA decomposes process data into different time-scales using the wavelet transform. Separate MPCA models at each scale can be expected to have a better ability to detect events whose magnitude is most significant at that scale. The SBR process itself evolves over time as the microorganisms adapt to changing operating conditions like surrounding temperature and varying process loads. To overcome the problem of changing process conditions, an adaptive MPCA model can be developed at each scale. The proposed adaptive multiscale MPCA model is used to detect abnormal batch behaviors and to identify the major sources of process disturbances. Real-time detection of abnormalities directly after completion of a batch cycle may even prevent detrimental effects on the following batch run. The proposed methodology is applied to a pilot-scale SBR for biological nutrient removal. When the SBR is free from major upsets the process is likely to be more stable than when it is subject to significant disturbances. The adaptive multiscale MPCA supervision is used as a tool to monitor the stability of the process on the basis of simple on-line data.

2. Materials and methods

2.1. Multiway principal component analysis

In a typical batch run, $j = 1, \dots, J$ variables are measured at each of k = 1, 2, ..., K time intervals throughout the batch. Similar data will exist on a number of batches $i=1, 2, \ldots, I$. All the data can be summarized in the $X(I \times J \times K)$ of a historical database (Fig. 1). It can be decomposed using various three-way techniques, including MPCA. MPCA is equivalent to unfolding the three-dimensional data matrix X into a large twodimensional matrix X, and then performing a regular PCA (Henrion, 1994; Nomikos and MacGregor, 1994). In case of monitoring batch processes, it is important to determine differences between batches and to project new batches on the model. Therefore, X was unfolded in such a way as to put each of its vertical slices (I)side by side to the right, starting with the one corresponding to the first time interval. The resulting twodimensional matrix has size $(I \times JK)$. This unfolding allows for analyzing the variability among the batches in X by summarizing the information in the data with respect to both variables and their time variation.

Then MPCA decomposes the data into a series of principal components consisting of score vectors (t_r)

and loadings (p_r) , plus residuals (E):

$$X = \sum_{r=1}^{K} t_r p_r + E \tag{1}$$

The loading vectors (\mathbf{p}_r) define the reduced dimension space (R) and are the directions of maximum variability. Each element of the score vectors (t_r) corresponds to a single batch and depicts the overall variability of this batch with respect to the other batches in the database throughout the whole batch duration (Nomikos and MacGregor, 1995). Usually, a few principal components can express most of the variability in the data when there is a high degree of correlation among the data $(R \ll \min(I, JK))$. R is chosen such that most of the systematic variability of the process data is described by these principal components and that the residual matrix E is as small as possible in a least-squares sense. The NIPALS (nonlinear iterative partial least-squares) algorithm can be used for sequential computation of the dominant principal components (Geladi and Kowalski, 1986).

Abnormal behavior of new batches is identified by projecting the new batches onto the model. Control charts that are used in monitoring batch processes are generally based on the Q- and T^2 -statistics in which

Variables × Times

Fig. 1. Decomposition of a three-way data matrix \underline{X} by MPCA.

control limits are used to determine whether the process is in control or not. The assumption behind these approximate confidence limits is that the underlying process exhibits a multivariate normal distribution with a population mean zero. This is to be expected since any linear combination of random variables, according to the Central Limit Theorem, should tend toward a normal distribution.

The Q-statistic is a measure of the lack of fit with the established model. For batch number i, Q is calculated as follows:

$$Q_{i} = \boldsymbol{e}_{i} \boldsymbol{e}_{i}^{T} = \sum_{c=1}^{JK} \boldsymbol{e}_{i,c} \ g x_{(h)}^{2}$$
(2)

where e_i is the elements of E. Q_i indicates the distance between the actual values of the batch and the projected values onto the reduced space. The distribution of the calculated Q_i values can be approximated by a chisquared distribution, $g\chi^2_{(h)}$, where g is a constant and h is the effective degrees of freedom of the chi-squared distribution.

Hotelling's T^2 -statistic measures the degree to which the calibration model fists the data:

$$T_i^2 = t_i^T S^{-1} t_i \sim \frac{I(I-R)}{R(I^2-1)} F_{R,I-R}$$
(3)

where *S* is the estimated covariance matrix of the scores. The distribution of the T^2 -statistic for all batches can be approximated by an *F*-distribution, $F_{R,I-R}$, and confidence limits for the T^2 -statistic are calculated from this *F*-distribution.

2.2. Multiscale MFCA

2.2.1. Wavelet transform

Wavelets are a family of basis functions generated from a mother wavelet $\psi(t)$ by translation and dilation:

$$\psi_{a,b} = a^{-1/2}\psi\left(\frac{t-b}{a}\right) \tag{4}$$

where *a* and *b* are the dilation and translation parameters, respectively. Then a family of discrete wavelets is represented as

$$\psi_{m,s} = 2^{-m/2} \psi(2^{-m}t - s) \tag{5}$$

where m and s are integers. For most practical applications, the wavelet coefficients are discretized dyadically (i.e. in integer powers of two) by a factor of 2^m for translation and by a factor of $2^m s$ for dilation. The dilation parameter determines the location in the frequency domain, while the translation parameter determines the location of the wavelet in the time domain. The discrete wavelet transform (DWT) projects a signal on orthonormal basis functions to analvze the signal at different scales by decomposing the signal at each scale into coarse approximation (lowfrequency components) and details (high-frequency components). Multi-resolution analysis (MRA) uses decomposition and reconstruction algorithms to obtain a multilevel representation of the signal by an efficient series of filtering and down-sampling operations (Mallat, 1989). High-pass filters are associated with the wavelet functions, while low-pass filters correspond to the scaling function. The wavelet transform can be used to decompose multivariate signals x into an approximation A_1 (low-frequency components) and details D_1 (high-frequency components). The decomposition process can continue, with successive approximations being decomposed in turn, so that signals are broken down into a desired number of levels L. In this application, the simplest discrete wavelet Haar is used:

$$\psi_H(t) = \begin{cases} 1 & 0 \le t \le 1/2 \\ -1 & 1/2 \le t \le 1 \\ 0 & \text{otherwise} \end{cases}$$
(6)

The mother wavelet $\psi_H(t)$ is localized in time and frequency with an equal area above and below the *t*-axis, as shown in Fig. 2. As an example, pH originating from the measurement data of the SBR was reconstructed after applying MRA (Fig. 3). The approximation coefficient at scale 4 (A_4) represents the underlying trend of the signals while the details coefficients (D_1-D_4) represents the high-frequency details.

2.2.2. Adaptive multiscale MPCA methodology

Multiscale PCA combines the strengths of PCA with the attractive properties of wavelet analysis. PCA has the ability to decorrelate the variables by extracting a linear relationship between variables, and wavelet analysis has the ability to extract features in the measurements and approximately decorrelate the autocorrelation among the measurements. In this work, the basic structure of the multiscale PCA method as introduced by Bakshi (1998) is employed. There are,



Fig. 2. Orthonormal scaling function and wavelet function of Haar wavelet.

however, some differences in the application and in the extension of the multiscale PCA approach. First, the multiscale PCA is adapted to batch processes as a multiscale MPCA method. Second, adaptive MPCA models with recursive updating of the covariance matrices are used at each scale to make the MPCA models follow the evolution of the process. Finally, a multiscale fault identification method is proposed once a fault is detected through the multiscale MPCA. The proposed methodology for adaptive multiscale MPCA is illustrated in Fig. 4 and can be summarized in the following steps:

Modeling procedure

1. Select *N* historical batches which represent normal operation. Then the data matrix $\underline{X}(N \times J \times K)$ is normalized using the mean and standard deviation of each variable at each time in the batch cycle over all batches. Subtracting the average batch trajectory generally eliminates the major nonlinear and non-stationary behavior of the process.



Fig. 3. Multi-resolution plot of pH (decomposition level: 4).



Fig. 4. Adaptive multiscale PCA (AMPCA) methodology.

- Compute the wavelet decomposition for each variable for all the batches by applying a wavelet transform W(K × K) with decomposition level *L*, and generate *L* detail coefficient matrices, X_{D1}(N × J × K/2), X_{D2}(N × J × K/2²), ..., X_{DL}(N × J × K/2^L) and one approximate coefficient matrix X_{AL}(N × J × K/2^L).
- 3. Apply adaptive MPCA to each of the L+1 matrices and determine control limits of the monitored indices, T^2 and Q, at each scale.
- 4. Select wavelet coefficients larger than the appropriate threshold and reconstruct the approximated data matrix \underline{X}_T .

Apply adaptive MPCA to the reconstructed data matrix \underline{X}_T and calculate overall control limits, T_T^2 and Q_T .

On-line process monitoring procedure

- 5. Scale the current batch data with the mean and standard deviation obtained at step 1.
- 6. Compute the new wavelet coefficients, project these coefficients onto their respective scale model and calculate the monitoring indices, T^2 and Q, against the limits at each scale.
- 7. Reconstruct the approximate measurements from the scores at the scales where one of the current monitoring indices violates the limits.
- 8. Project the reconstructed measurements onto the unified adaptive MPCA model and calculate the overall monitoring indices, T_r^2 and Q_T .

2.3. Sequencing batch reactor

The data used in this study were collected from a pilot-scale SBR system shown in Fig. 5. The filland-draw sequencing batch reactor (SBR) system with a 80-1 working volume was operated in a 6 h cycle mode and each cycle consisted of 1 h fill/anaerobic, 2 h 30 min aerobic, 1 h anoxic, 30 min aerobic and 1 h settling/draw phases. The hydraulic retention time (HRT) and solid retention time (SRT) were maintained at 12 h and 10 days, respectively. Loading amounts of COD as synthetic municipal-like sewage, NH_4^+ –N and PO_4^{3-} –P per cycle in standard conditions were 440, 60 and 9.5 mg/l, respectively.

The controls of the duration/sequence of phases and the on/off status of the peristaltic pumps, mixer and air supply were automatically achieved by a LabView data acquisition and control (DAC) system. The DAC system consisted of a computer, interface cards, meters, transmitters and solid-state relays. Electrodes for pH, ORP (oxidation-reduction potential), DO (dissolved oxygen), temperature, weight and conductivity were installed and connected to the individual meters. The status of the reactor was displayed on the computer and the time series of the electrode signals were stored in a data file.

A set of on-line measurements was obtained every 1 min (360 time instants) containing pH, ORP, DO, conductivity, temperature and weight of the SBR reactor. Thus, no advanced or expensive measurement devices had to be installed in order to make the methods work. All measurements are simple standard measurements. These measurements were stored for 280 cycles (=70 days) forming a database of historical information about the process. Only the measurement data from the first 300 sampling time instants of the cycles were used to develop the monitoring models since the biological reactions in the settling and drawing phases (corresponding to those of the last 60 time instants) were assumed to be negligible. Moreover, due to the absence



Fig. 5. Schematic diagram of a sequencing batch reactor system.

of mixing, the sensor signals were unreliable in these two phases. Therefore, the multiscale MPCA algorithm was applied to the three-way data array \underline{X} with dimensions $280 \times 6 \times 300$. Typical batch trajectory profiles of the measurement data are shown in Fig. 6.

3. Results and discussion

3.1. Multiway principal component analysis (MPCA)

A MPCA model for on-line monitoring was built from a historical data set of batches, where five abnormal batches (batch numbers: 8, 51, 60, 85, 86) were excluded from the normal operating condition model. Four principal components, which explained approximately 82% of the total variability, were determined by cross-validation (Krzanowski, 1987). The validation data set consisting of the 180 remaining batches were projected onto the model space. Fig. 7 shows the Q and T^2 monitoring charts of the MPCA model. It can be seen that the T^2 hardly exceeds its limit, while the Q values is far above the 99% limit from batch 110 on. This indicates that the process variation in the validation batches cannot be described by the developed model. It is obvious that the typical MPCA model is not valid since the fixed reference database

is not representative of the SBR process that is time varying. In the SBR operation the influent wastewater is fed into the reactor and mixed with already existing microorganisms. Therefore, the performance of the current batch highly depends on microorganism activity in the previous batches. In addition, the SBR process is subject to significant disturbances like hydraulic changes and composition variations. Small changes in concentrations or flows can have a large effect on the kinetics of biological reactions leading to batchto-batch variability in effluent quality and microorganism growth. When the typical MPCA model is used to monitor the SBR process with time-varying behaviors, false alarms often result, which significantly compromises the reliability and acceptance of the monitoring system.

3.2. Adaptive MPCA

To overcome the problem of changing process conditions as the SBR process itself evolves over time, an adaptive MPCA model with the recursive updating of the covariance matrices can be developed. When a new block of batch data becomes available, the covariance matrix is updated by exponentially discounting the old data (Dayal and MacGregor, 1997):

$$\boldsymbol{X}^{T}\boldsymbol{X}(i) = \boldsymbol{\alpha}\boldsymbol{X}^{T}\boldsymbol{X}(i-1) + \boldsymbol{x}^{T}\boldsymbol{x}(i)$$
(7)



Fig. 6. Typical batch trajectory profiles of the measurement data.

where $X^T X(i)$ is the covariance matrix at batch *i*, x(i) is the unfolded operation vector at batch *i* and α is a forgetting factor. The forgetting factor α is a tuning parameter that varies depending on how fast the process change. In this application it is set to 0.9897, which corresponds to 96 batch operations. Since the number of significant principal components can change over time, it is necessary to determine the number of principal components recursively. However, the cross-validation approach that was used for the MPCA model above is



Fig. 7. MPCA. Q and T^2 monitoring charts with 99% confidence limits.

not suitable because old data are not representative for the current process. Therefore, the number of significant principal components was calculated recursively using the cumulative percent variance (CPV) method (Li et al., 2000). The CPV is a measure of the percent variance captured by the first R principal components:

$$CPV(R) = \frac{\sum_{l=1}^{R} \lambda_l}{\text{trace}(V)} \times 100\%$$
(8)

where the λ_l are the eigenvalues of X and $V = EE^T/(I - 1)$. The number of principal components is chosen when CPV reaches a predetermined limit (80%). A potential adaptation problem is that the model could adapt not only to normal process evolution, but also to disturbances and failures. To prevent this, the model updating was skipped when the Q and T^2 values of new batches were exceeding predetermined limits. The Q and T^2 values in Fig. 8 are mostly well inside



Fig. 8. Adaptive MPCA. Q and T^2 monitoring charts with 99% confidence limits.

the confidence limits; this implies that as the covariance structure adapts to new process conditions, the updating model effectively captures the variability of the process.

3.3. Adaptive multiscale MPCA

For the adaptive multiscale MPCA formulation, each variable in the previous examples is first decomposed into a number of scales using the Haar wavelet. The number of scales is four, i.e. four detail scales $(D_1, D_2, D_3 \text{ and } D_4)$ and one approximation scale (A_4) . Then, adaptive MPCA models with the recursive updating of the covariance matrices are developed at each scale. Each adaptive MPCA uses the same forgetting factor ($\alpha = 0.9897$) and computes its optimal number of principal components adaptivity based on the CPV. The detection limits at each scale are adjusted to account for the overcompleteness of the on-line wavelet decomposition by the following equation (Bakshi, 1998):

$$C_L = 100 - \frac{1}{L+1}(100 - C) \tag{9}$$



Fig. 9. Unifying adaptive multiscale MPCA. Q and T^2 monitoring charts with 99% confidence limits.

where *C* is the desired overall confidence limit and $C_{\rm L}$ is the adjusted confidence limit at each scale. Therefore, if either the *Q* or T^2 value at any scale is above the corresponding 95% limit, the scale is considered to be significant. The data on that scale is then used in the reconstruction of a unifying estimate of the original data. The reconstructed data are then monitored using a unifying adaptive MPCA with the confidence limit 99%. The resulting Q or T^2 charts of the unifying adaptive MPCA are shown in Fig. 9. Both the Q and T^2 charts indicate that the multiscale model is valid during the whole period. Most of the significant features in the unifying adaptive MPCA results are qualitatively similar to those of the adaptive MPCA. However, there are some differences. It can be seen from Fig. 9 that the Q values of batch numbers 162 and 163 violate the 99% confidence limits. The adaptive MPCA



Fig. 10. Q monitoring charts at each scale.



Fig. 11. T^2 monitoring charts at each scale.



Fig. 12. Contribution plot at the approximation scale A₄ (batch 274).

method only detects the fault only at batch number 163. Considering the fact that the batch data in the model are updated at the end of a batch cycle, the adaptive MPCA detects the fault 6 h later. In addition, the Q values in Fig. 9 violate their limits more than five times between batch numbers 220 and 230, compared with those of the adaptive MPCA model (Fig. 8). During this period, the performance of the SBR process

was unstable and gave relatively poor effluent quality. Therefore, the adaptive multiscale MPCA gave proper false alarms in the period whereas the adaptive MPCA failed to detect the significant events. Thus, the adaptive multiscale MPCA method is not only more successful in early detection but also in detection itself of less pronounced process faults than the adaptive MPCA approach.



Fig. 13. Univariate profiles of DO concentrations for normal batches and batch 274.

Scale Q and T^2 charts (Figs. 10 and 11) can help to determine the nature of a disturbance. Fast disturbances are mainly detected in the higher scales whereas slow disturbances are found in the lower scales (Lennox and Rosen, 2002). In addition, the way a disturbance appears across scales can reveal information on the disturbance characteristics. For instance, the disturbance at batch 163 is a rather spiky disturbance since it is strong in the highest scale (D_1) but becomes weaker in the lower scales. On the other hand, the disturbance at batch 197 is a step disturbance as it appears clearly for all scales.

In order to identify the disturbance for batch 274, a multiscale identification scheme was adopted. The multiscale identification approach diagnoses a fault in the most significant scale Q and T^2 charts rather than the O and T^2 charts of the unifying adaptive MPCA. For instance, it is quantitatively identifiable from the adaptive multiscale MPCA that the ratio between the T^2 value and the 99% confidence limit at batch 274 is highest at the approximation scale (A_4) . The contributions to the T^2 value in the approximation scale show that it was mainly the DO concentrations that contributed to the disturbance (Fig. 12). Fig. 13 shows the univariate plots of DO concentrations for normal batches and for batch 274. It can be seen that the DO concentrations of batch 274 are lower than those of normal batches during the aerobic phase.

Compared with the adaptive monitoring results, the multiscale approach provides more information on the disturbance characteristics and can detect a disturbance more rapidly than adaptive MPCA in this application. However, these advantages come at the price of a higher complexity of the monitoring model. For a simple process, where most events occur in single time scale, the simplest model should be used for monitoring. When dynamics with a wide range of time constants are to be modeled, the proposed multiscale MPCA method may be more suitable and effective.

4. Conclusions

Dealing with evolving processes is a key concern in monitoring wastewater treatment processes. To deal with this problem, an adaptive multiscale MPCA methodology is proposed for batch process monitoring and fault detection. In the adaptive multiscale MPCA formulation, the individual variables are decomposed into wavelet coefficients at different scales. The wavelet coefficient at each scale is used to recursively develop adaptive MPCA to extract correlations at each scale. Only significant scales are combined to construct a uniscale batch data set in the time domain, which is then used to develop a unifying adaptive MPCA model for process monitoring and diagnosis. The application of the proposed algorithm to a pilot-scale SBR process demonstrated the feasibility and effectiveness of this adaptive process monitoring approach. With respect to detecting disturbances, the performance of the adaptive multiscale MPCA algorithm is not only more successful in early fault detection but also in detection of less pronounced process faults than typical single time scale MPCA methods. Moreover, the multiscale approach provides information on the time scale under which a fault affects process, which can be used for diagnosis of the fault to find the physical cause.

Acknowledgement

This work was financially supported by the Korea Science and Engineering Foundation through the Advanced Environmental Biotechnology Research Center at Pohang University of Science and Technology. This research was also supported by the Fund for Scientific Research-Flanders (F.W.O.) and the Ghent University Research Fund.

References

- Bakshi, B.R., 1998. Multiscale PCA with application to multivariate statistical process monitoring. AIChE J. 44 (7), 1596–1610.
- Chen, J., Liu, K.-C., 2002. On-line batch process monitoring using dynamic PCA and dynamic PLS models. Chem. Eng. Sci. 57, 63–75.
- Dong, D., McAvoy, T.J., 1996. Nonlinear principal component analysis-based on principal curves and neural network. Comp. Chem. Eng. 20 (1), 65–78.
- Dayal, B.S., MacGregor, J.F., 1997. Recursive exponentially weighted PLS and its applications to adaptive control and prediction. J. Proc. Cont. 7 (3), 169–179.
- Demuynck, C., Vanrolleghem, P.A., Mingneau, C., Liessens, J., Verstraete, W., 1994. NDBEPR process optimization in SBRs: reduction of external carbon source and oxygen supply. Water Sci. Technol. 30, 169–179.

- Geladi, P., Kowalski, B.R., 1986. Partial least squares regression: a tutorial. Anal. Chim. Acta 185, 1–17.
- Henrion, R., 1994. N-way principal component analysis: theory, algorithms and applications. Chemom. Intell. Lab. Syst. 25, 1–23.
- Kosanovich, K.A., Piovoso, M.J., 1997. PCA for wavelet transformed process data for monitoring. Intell. Data Anal. 1, 85–99.
- Krzanowski, W.J., 1987. Cross-validation in principal component analysis. Biometrics 43, 575–584.
- Lane, S., Martin, E.B., Kooijmans, R., Morris, A.J., 2001. Performance monitoring of a multi-product semi-batch process. J. Process. Cont. 11, 1–11.
- Lee, D.S., Park, J.M., 1999. Neural network modeling for on-line estimation of nutrient dynamics in a sequentially operated batch reactor. J. Biotechnol. 75, 229–239.
- Lee, D.S., Vanrolleghem, P.A., 2003. Monitoring of a sequencing batch reactor using adaptive multiblock principal component analysis. Biotechnol. Bioeng. 82, 489–497.
- Lennox, B., Montague, G.A., Hiden, H.G., Kornfeld, G., Goulding, P.R., 2001. Process monitoring of an industrial fed-batch fermentation. Biotechnol. Biogen. 74, 125–135.
- Lennox, J., Rosen, C., 2002. Adaptive multiscale principal components analysis for online monitoring of wastewater treatment. Water. Sci. Technol. 45 (4–5), 227–235.

- Li, W., Yue, H., Valle-Cervants, S., Qin, S.J., 2000. Recursive PCA for adaptive process monitoring. J. Process. Cont. 10, 471– 486.
- Mallat, S.G., 1989. A theory for multiresolution signal decomposition: the wavelet representation. IEEE Trans. Pattern Anal. Mach. Intell. PMAI-11, 674–693.
- Misra, M., Yue, H.H., Qin, S.J., Ling, C., 2002. Multivariate process monitoring and fault diagnosis by multi-scale PCA. Comp. Chem. Eng. 26, 1281–1293.
- Nomikos, P., MacGregor, J.F., 1994. Monitoring batch processes using multiway principal component analysis. AIChE J. 40, 1361–1375.
- Nomikos, P., MacGregor, J.F., 1995. Multivariate SPC charts for monitoring batch processes. Technometrics 37 (1), 41–59.
- Ränner, S., MacGregor, J.F., Wold, S., 1998. Adaptive batch monitoring using hierarchical PCA. Chemom. Intell. Lab. Syst. 41, 73–81.
- Rosen, C., Lennox, J.A., 2001. Multivariate and multiscale monitoring of wastewater treatment operation. Water Res. 35, 3402–3410.
- Wilderer, P., Irvine, R.L., Goronszy, M.C., 2001. Sequencing batch reactor technology. IWA Scientific and Technical Report No. 10, London.