Chemical Engineering Science 63 (2008) 2252–2266

Chemical Engineering Science

www.elsevier.com/locate/ces

Nonlinear multiscale modelling for fault detection and identification

Sang Wook Choi[a], Julian Morris[b,*], In-Beum Lee[c]

[a]Memory Division, Semiconductor Business, Samsung Electronics Co. Ltd., San #16, Banwol-Dong, Hwasung 445-701, South Korea
[b]Centre for Process Analytics and Control Technology, School of Chemical Engineering and Advanced Materials, Newcastle University, Newcastle NE1 7RU, UK
[c]Department of Chemical Engineering, Pohang University of Science and Technology, San 31 Hyoja Dong, Pohang 790-784, South Korea

Received 10 July 2007; received in revised form 3 January 2008; accepted 12 January 2008
Available online 31 January 2008

Abstract

In order to detect abnormal events at different scales, a number of multiscale multivariate statistical process control (MSPC) approaches which combine a multivariate linear projection model with multiresolution analysis have been suggested. In this paper, a new nonlinear multiscale-MSPC method is proposed to address multivariate process performance monitoring and in particular fault diagnostics in nonlinear processes. A kernel principal component analysis (KPCA) model, which not only captures nonlinear relationships between variables but also reduces the dimensionality of the data, is built with the reconstructed data obtained by performing wavelet transform and inverse wavelet transform sequentially on measured data. A guideline is given for both off-line and on-line implementations of the approach. Two monitoring statistics used in multiscale KPCA-based process monitoring are used for fault detection. Furthermore, variable contributions to monitoring statistics are also derived by calculating the derivative of the monitoring statistics with respect to the variables. An intensive simulation study on a continuous stirred tank reactor process and a comparison of the proposed approach with several existing methods in terms of false alarm rate, missed alarm rate and detection delay, demonstrate that the proposed method for detecting and identifying faults outperforms current approaches.

Keywords: Multiresolution analysis; Kernel principal component analysis; Fault detection and diagnosis; Multivariate statistical process control; Multiscale kernel principal component analysis

1. Introduction

In the field of process performance monitoring and fault diagnosis in chemical processes, multivariate statistical process control (MSPC), or process performance monitoring, has been extensively researched over the last decade as an alternative to knowledge-based approaches. The successful application of MSPC to a chemical process is significantly dependent on the quality of process data and the capability of the information extracting methodologies and techniques such as principal component analysis (PCA) and its extensions. Conventional PCA-based MSPC is only valid for the non-autocorrelated data with linear relationships between measured variables. Often, inefficient and unreliable process performance monitoring schemes can materialize as a consequence of the underlying assumptions of PCA-based MSPC being violated. To cope with these restrictions several extended approaches have been proposed, which include the MSPC methods based on nonlinear PCA (e.g. Dong and McAvoy, 1996; Jia et al., 1998; Choi et al., 2005a), dynamic PCA (e.g. Ku et al., 1995), dynamic model-based MSPC (McPherson et al., 2002), and canonical variate analysis (e.g. Negiz and Cinar, 1997; Russell et al., 2000; Simoglou et al., 2002).

Apart from the above modifications and extensions of the original MSPC concepts for dealing with process data with nonlinear and dynamic characteristics, multiscale approaches to MSPC have been proposed to monitor and analyze processes containing various events occurring at multiple scales, which are common in most industrial processes (e.g. Bakshi, 1998). Most existing methods operate on data collected at a fixed scale, whereas the multiscale scheme represents data at several different scales with the help of wavelet analysis (e.g. Mallet, 1989; Strang and Nguyen, 1996). The wavelet transform provides the means of analyzing an input signal into a number of different resolution levels in a hierarchical fashion, known as

* Corresponding author. Tel.: +44 191 222 7342; fax: +44 191 222 5748.
E-mail address: julian.morris@ncl.ac.uk (J. Morris).

0009-2509/$ - see front matter
doi:10.1016/j.ces.2008.01.022

multiresolution analysis. Thus, measured time-series signals containing different physical patterns or disturbances, e.g. sudden changes at the finer resolution levels and slowly time-varying activities at the coarser resolution levels, can be best represented as a combination of several signals at different resolution levels.

There have been a number of approaches where MSPC is combined with multiresolution analysis aimed at enhancing process performance monitoring capabilities. Kosanovich and Piovoso (1997) proposed an approach where the process data are filtered by the univariate finite median hybrid filter and a set of coefficients is obtained from wavelet transform. With these wavelet coefficients, a PCA model is developed for the purpose of process monitoring. Bakshi (1998), in his seminal paper, suggested a multiscale-PCA (MSPCA) for extracting relationships not only between variables by PCA but also measurements by wavelet analysis. A detailed discussion of the benefits of MSPCA in terms of process monitoring was presented in a comparison with conventional PCA. Aradhye et al. (2003) analyzed univariate and multivariate multiscale SPC theoretically and compared their properties with existing SPC methods based on the average run length. They concluded that even though multiscale SPC did not perform better than any conventional SPC designed to detect specific types of changes, it was a general approach that showed better average performance in detecting a range of changes in different types of measurements. Several variants of MSPCA-based monitoring have also been suggested. Teppola and Minkkinen (2000) proposed wavelet-partial least square (wavelet-PLS) models for both data analysis and process monitoring. In their approach, a PLS model is constructed based on the filtered measurements which are obtained by removing the low-frequency scales representing low-frequency components such as seasonal fluctuations and long-term variations. Misra et al. (2002) added an MSPCA scheme to the contribution analysis for fault diagnosis. Yoon and MacGregor (2004) presented a comprehensive study of MSPCA within a fault isolation scheme based on contribution plots extended to multiscale approaches.

In this paper, the concept of kernel PCA (KPCA) is combined with multiresolution analysis for nonlinear multiscale process performance monitoring (multiscale-MSPC). Very often chemical processes can exhibit severe nonlinearities, which makes conventional MSPC inefficient and even unreliable. To cope with multivariate data with nonlinear characteristic several nonlinear MSPC methods such as KPCA-based monitoring (e.g. Choi and Lee, 2004; Choi et al., 2005a) have been suggested. The KPCA approach conceptually consists of two steps; the extended nonlinear mapping of measurements in the original space into the extended feature space and the construction of PCA in the feature space. These two steps are implicitly carried out by using kernel functions without knowledge of the nonlinear functions and without the need to solve any optimization procedure.

With the reconstructed signals in the time domain being separately transformed from all the scales in wavelet domain, KPCA is performed to give a nonlinear multiscale model. The implementation of off-line and on-line multiscale KPCA (MSKPCA) is described. Furthermore, a new algorithm of variable contributions to monitoring statistics is also given for fault identification in nonlinear multiscale processes. A rigorous analysis based on Monte Carlo simulations is performed to demonstrate the potential of the proposed method compared with several existing approaches, including PCA, KPCA, and the MSPCA approach of Yoon and MacGregor.

The paper is structured as follows. Section 2 introduces a brief overview of multiresolution analysis with wavelet that underpins the multiscale approach using KPCA which is reviewed in Section 3. A detail description of the proposed MSKPCA-based process performance monitoring scheme is then given in Section 4. An algorithm for building a suitable model, calculating two monitoring statistics for fault detection and deriving variable contributions to the monitoring statistics for fault identification is then discussed. Finally, in Section 5, the results of the proposed methodology are assessed through rigorously simulated examples where a number of different types of faults are considered including a process disturbance, a process degradation, and sensor faults in a continuous stirred tank reactor (CSTR) process previously used as a demonstration process for MSPC and multiscale-MSPC studies.

2. Multiresolution analysis

Let $\mathbf{x}$ be an input sequence of length N. A two-band discrete wavelet transform (DWT) of $\mathbf{x}$ decomposed with a high pass filter and a low pass filter is defined using the following recursive forms:

$$a_j(k) = \sum_m h_0(m-2k)a_{j-1}(m),$$
$$d_j(k) = \sum_m h_1(m-2k)a_{j-1}(m), \tag{1}$$

where $j = 1, 2, \ldots, J$ denotes the scale (or dilation index) and k represents the translation index. The two coefficients a_j and d_j are the scaling and the wavelet coefficients at scale j, respectively. And, h_0 and h_1 are the scaling and the wavelet function coefficients, respectively. The DWT procedure is depicted in the left side box in Fig. 1(a). This decomposition is carried out to a desired number of scale (or level of the decomposition) J by recursively applying the high and low pass filters to the scaling coefficients at the previous level. The operation at the output of the two filters is known as subsampling by 2, which is represented by the small circle in this figure. Due to subsampling, the total number of coefficients in the wavelet domain is the same as that of the input sequence, i.e. N. On the other hand, the right box in Fig. 1(a) shows a structure that combines all the coefficients through the filters g_0 and g_1 to reconstruct $\mathbf{x}$ in time domain, which is called the inverse DWT (IDWT). The circle symbol in front of the filter denotes the upsampling by 2. Using these two synthesis filters g_0 and g_1 together with upsampling, a reconstruction of $\mathbf{x}$, denoted as $\hat{\mathbf{x}}$, will be achieved in the time domain. In particular, the biorthogonality condition $\langle h_i(m-2k), g_j(2l-m)\rangle = \delta_{ij}\delta_{kl}$ for $i, j = 0, 1$ and $k, l \in \mathrm{Z}$ is satisfied, the perfect reconstruction will be obtained,