Journal of Process Control 21 (2011) 830–839

Contents lists available at ScienceDirect

Journal of Process Control

journal homepage: www.elsevier.com/locate/jprocont

A virtual metrology model based on recursive canonical variate analysis with applications to sputtering process

Tian-Hong Pan[a], Bi-Qi Sheng[a], David Shan-Hill Wong[b,*], Shi-Shang Jang[b,**]

[a] School of Electrical & Information Engineering, Jiangsu University, Zhenjiang, Jiangsu 212013, China
[b] Department of Chemical Engineering, National Tsing-Hua University, Hsin-Chu 30013, Taiwan

ARTICLE INFO

Article history:
Received 10 August 2010
Received in revised form 23 January 2011
Accepted 12 April 2011
Available online 26 May 2011

Keywords:
Canonical variate analysis
Partial least squares
Virtual metrology
Sputtering process
R^2 statistics

ABSTRACT

In data driven process monitoring, soft-sensor, or virtual metrology (VM) model is often employed to predict product's quality variables using sensor variables of the manufacturing process. Partial least squares (PLS) are commonly used to achieve this purpose. However, PLS seeks the direction of maximum co-variation between process variables and quality variables. Hence, a PLS model may include the directions representing variations in the process sensor variables that are irrelevant to predicting quality variables. In this case, when direction of sensor variables' variations most influential to quality variables is nearly orthogonal to direction of largest process variations, a PLS model will lack generalization capability. In contrast to PLS, canonical variate analysis (CVA) identifies a set of basis vector pairs which would maximize the correlation between input and output. Thus, it may uncover complex relationships that reflect the structure between quality variables and process sensor variables. In this work, an adaptive VM based on recursive CVA (RCVA) is proposed. Case study on a numerical example demonstrates the capability of CVA-based VM model compared to PLS-based VM model. Superiority of the proposed model is also presented when it applied to an industrial sputtering process.

1. Introduction

Modern industrial processes, continuous or batch, are usually equipped with a large number of sensors that provide process variables data, such as pressure, temperature, spectroscopic signals and heat or power supply. Such process variables data can be used for process monitoring and fault diagnosis using multivariate statistical analysis methods, such as principle component regression (PCR), partial least squares (PLS) and canonical variate analysis (CVA) [1–4]. However, such process variables data are not a direct indicator of final product quality. Examples of quality variables in continuous chemical process include molecular weight and distribution of polymers, purity of distillates, etc. In multi-step batch-based processes, such as semiconductor or thin-film-transistor liquid-crystal-display (TFT-LCD) manufacturing, intermediate product qualities include product state variables, such as film thickness and critical dimension, and final quality indicators include electrical characteristics such as sheet resistance and threshold voltage [5]. Since product quality measurements may be time-consuming and expensive, they can only be sampled and provided in a less frequent, time-delayed manner. For both monitoring and controlled purposes, it is therefore desirable that such quality data can be predicted using process variables data. Such an approach is well known as soft-senor or virtual metrology (VM). Examples of VM applications can be found in both continuous chemical processing industry [6–8] as well as multi-step batch-wise assembly line processes [9–12].

One approach to development of VM models is to use non-parametric models such as neural networks [13–15]. Neural network models are capable of representing complex non-linear functions, but they usually lack generalization ability unless special attentions are paid to variable selection, architecture determination and data screening and compression [16]. Alternatively, linear model, such as PLS is also commonly used to construct VM models [17]. Such models are capable of overcoming the problem of high dimensionality and collinearity in the process variables data. However, due to the linear nature of the model, adaptive or local model network implementation is usually required for on-line tracking of quality changes [8].

It is well known (e.g. see Borga et al. [18]) that principle component analysis (PCA) finds the direction of maximum variations for a set of data, PLS seeks the direction of maximum co-variation of two sets of data, and CVA identifies the direction of maximum correlation between a set of response data and a set of regressor data. Although PCA can deal with high dimensionality and collinearity in the input data by projecting the original process variables onto

* Corresponding author.
** Corresponding author. Tel.: +886 3 571 3697; fax: +886 3 571 5408.
E-mail addresses: dshwong@che.nthu.edu.tw (D.S.-H. Wong), ssjang@mx.nthu.edu.tw (S.-S. Jang).

0959-1524/$ – see front matter © 2011 Elsevier Ltd. All rights reserved.
doi:10.1016/j.jprocont.2011.04.004