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Dynamic model-based batch process monitoring

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Abstract

An integrated framework consisting of a multivariate autoregressive (AR) model and multi-way principal component analysis (MPCA) is described for the monitoring of the performance of a batch process. After pre-processing the data, i.e., batch data unfolding, mean-centring and scaling, the data are then filtered using an AR model to remove the auto- and cross-correlation inherent within the pre-processed batch data. Model order is determined using Akaike information criterion and the model parameters are estimated through the application of partial least squares to attain a stable solution. MPCA is then applied to the residuals from the AR model. Three monitoring statistics are considered for the detection of the onset of process abnormalities in the batch process. The main advantage of the proposed approach is that it can monitor batch dynamics along the mean trajectory without the requirement to estimate future observed values. The proposed AR model-based approach is illustrated through its application to two polymerization processes. The case studies indicate that it gives better monitoring results in terms of sensitivity and time to fault detection than the approaches proposed by Nomikos and MacGregor [1994. Monitoring batch processes using multi-way principal components. A.I.Ch.E. Journal 40(8), 1361–1375] and Wold et al. [1998. Modelling and diagnostics of batch processes and analogous kinetic experiments. Chemometrics and Intelligent Laboratory Systems 44, 331–340].

Keywords: Batch process monitoring; Multivariate autoregressive model; Partial least squares; Principal component analysis

1. Introduction

Batch and semi-batch processes have been widely used in the manufacture of high-quality products in many industrial sectors including the chemical, biochemical and pharmaceutical industries. They can be characterized as systems that generate a desired product in a batch reactor through the execution of a planned schedule over a finite duration of time. More recently an integral aspect of batch production has been that of on-line monitoring to ensure that the consistency and quality of the final product is aligned with the requirements of the customer and to detect changes in the operating conditions that may impact on overall quality, as early as possible in the process. Additional advantages of on-line monitoring include the financial savings that can be achieved as a consequence of reducing both the amount of wastage and rework, and hence energy usage. However, in most batch processes, final product quality is measured infrequently, and in some cases is only recorded at the end of the batch, consequently the direct on-line tracking of product quality is not standard in most industrial applications. As a surrogate to these quality measures, more standard measurements such as temperature, concentration, pressure, and flow rate are routinely recorded throughout the duration of the batch. The information from these on-line measurements can be used to analyse process behaviour, and hence improve process operating conditions thereby achieving consistent product quality (Westerhuis et al., 1999).

A number of statistical process monitoring approaches have been developed during the last two decades that utilize on-line process measurements as opposed to direct quality variables. For example Nomikos and MacGregor (1994, 1995a, b) and Wold et al. (1998) proposed on-line batch process monitoring schemes whose basis were the multivariate statistical projection-based techniques of principal component analysis (PCA) and partial least squares (PLS). These methods are

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applicable to two-dimensional data sets and since batch data are inherently three dimensional (batch × variable × time), the first step is to reduce the dimensionality of the problem from three to two dimensions by rearranging the batch data. The two most common structures are (batch × (variable × time)) and ((batch × time) × variable). Alternative approaches that remove the need to reduce data dimensionality and that have been implemented for the monitoring of batch processes are the tri-linear approaches of parallel factor analysis (PARAFAC), PARAFAC2 and Tucker3 (Louwerse and Smilde, 1999; Wise et al., 2001; Meng et al., 2003). A number of comparative studies of the aforementioned monitoring methods have identified the advantages and limitations of the techniques in terms of process modelling and monitoring (Westerhuis et al., 1999; Louwerse and Smilde, 1999; Van Sprang et al., 2002). The batch process monitoring approaches mentioned above deal with within-batch variation and thus they monitor each batch independently during the batch run, or through-batch monitoring, which implies on-line monitoring. Lee and Dorsey (2004) and Flores-Cerrillo and MacGregor (2004) have also suggested monitoring schemes for detecting changes in batch-to-batch variations, which relates to decisions made at the end of the batch, i.e., off-line analysis.

Batch and semi-batch processes typically exhibit significant dynamic behaviour with transient states, consequently measurements collected from these processes are usually auto- and cross-correlated. Thus the direct application of conventional PCA-based monitoring schemes is not possible as the raw batch data violates the underlying assumption that the process is asymptotically stationary. One approach proposed in the literature by Nomikos and MacGregor (1994) to address this issue in batch process monitoring is to subtract the average time-series trajectory from the raw data and use the deviations from the mean trajectory as the inputs into the multi-way principal component analysis (MPCA). By adopting this approach, the loading vectors contain information on the auto- and cross-correlation for all the variables for the duration of the batch. To implement this approach on-line, a key requirement is the need for the complete trajectory of the entire batch run since the score for an individual time point is a weighted sum of all the measurements collected throughout the batch run. Two different approaches to in-filling the unknown future measurements have been proposed: (1) zero deviation, or (2) current deviation. Even though these approaches have worked well in practice, both methods face two limitations. First, unknown future values from the current time to the end of the batch require to be estimated to attain the current score and residual (Nomikos and MacGregor, 1994; García-Munoz et al., 2004). Secondly, the use of all the measurements throughout the duration of the batch assumes that the current condition of a process is affected by future operating conditions, which in practice is not necessarily valid. An alternative approach has been proposed whereby the score for an individual time point can be directly obtained by projecting only the available data onto the plane of a PCA model. Even though this method does not necessitate the estimation of future measurements, it has been shown to give poor monitoring performance especially in the early stage of a batch run (Van Sprang et al., 2002).

Wold et al. (1998) proposed an alternative approach that considered a different unfolding method to the three-dimensional batch data by preserving variable direction, i.e., (batch × time) × variables, and does not require the estimation of future measurements. This method of data matrix unfolding explains the correlations between the variables centred by subtracting their mean over the entire batch; it does not explain their auto- and cross-correlation. As pointed out by Kourti (2003), the variation described by PCA in this method is not the type of variation of interest in on-line monitoring, i.e., dynamic behaviour of the deviations from the optimally desired time trajectory.

To address the limitations identified with the previous approaches, a new dynamic batch on-line process monitoring methodology is proposed. The modelling procedure is performed in three steps as follows: (i) the pre-processing approach of Nomikos and MacGregor (1994) where the batch data unfolding, in the form of 'batch × (time × variables)', centring and scaling, is applied and the subsequent analysis is performed on the deviations from the mean trajectories; (ii) the dynamic structure remaining in the pre-processed data, defined with respect to the auto- and cross-correlation, is estimated through the fitting of a multivariate autoregressive (AR) model; and finally (iii) the AR model residuals are rearranged into a two-dimensional data set preserving the variable direction and PCA is applied. It is conjectured that by filtering the pre-processed data by the dynamic model, the variable dynamics within the residuals will be acceptable for process monitoring. Hence, the assumption of independence between samples, required in the PCA modelling and control limit setting of monitoring statistics, can be realized. Based on the proposed model structure, three monitoring statistics calculated from the current and past measurements underpin the basis of the on-line monitoring strategy. A consequence of this approach is that there is no requirement to estimate future measurements.

The paper is structured as follows. Section 2 presents the background to the proposed method with a short review of MPCA. The methodological development procedure is described in Section 3 along with the concept and algorithm of the proposed batch monitoring scheme. In Section 4, the approach is applied to the polymerization of a methyl methacrylate (MMA) polymerization process and a styrene–butadiene rubber (SBR) polymerization process and the results are compared with the methods of Nomikos and MacGregor (1994) and Wold et al. (1998). Conclusions are drawn in Section 5.

2. Multi-way principal component analysis

A historical data set obtained from a batch process can be arranged into a three-way block $\underline{\mathbf{X}} \in \Re(I \times J \times K)$, where I, J, and K are the number of batches, measured variables, and time points, respectively. Frequently within a batch process, the total duration of the batch and/or the duration of the individual phases within a batch run are not the same and alignment of the variable trajectories should be performed prior to process modelling. A number of methods based on indicator