

On-line monitoring of a sugar crystallization process

A. Simoglou^a, P. Georgieva^c, E.B. Martin^a, A.J. Morris^{a,*}, S. Feyo de Azevedo^b

^a Center for Process Analytics and Control Technology, Merz Court, University of Newcastle, Newcastle upon Tyne NE1 7RU, UK

^b Department of Chemical Engineering, Faculty of Engineering, University of Porto, R. Dr. Roberto Frias, 4200-465 Porto, Portugal

^c Department of Electronics and Telecommunications, IEETA, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal

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Abstract

The present paper reports a comparative evaluation of four multivariate statistical process control (SPC) techniques for the on-line monitoring of an industrial sugar crystallization process. The process itself is challenging since it is carried out in multiple phases and there exists strong non-linear and dynamic effects between the variables. The methods investigated include classical on-line univariate statistical process control, batch dynamic principal component analysis (BDPCA), moving window principal component analysis (MWPCA), batch observation level analysis (BOL) and time-varying state space modelling (TVSS). The study is focused on issues of on-line detection of changes in crystallization process operation, the early warning of process malfunctions and potential production failures; problems that have not been directly addressed by existing statistical monitoring schemes. The results obtained demonstrate the superior performance of the TVSS approach to successfully detect abnormal events and periods of bad operation early enough to allow bad batches and related losses in amounts of recycled sucrose to be significantly reduced.

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1. Introduction

Sugar crystallization occurs through the mechanisms of nucleation, growth and agglomeration. The impact of operating conditions on these activities is not always well-understood. It can be characterised as a non-linear, non-stationary process. Significant research has been carried out into the development of first principles models (Feyo de Azevedo, Chorão, Gonçalves, & Bento, 1994) to describe the process. More recently hybrid models based on both first principles and neural network models have been proposed (Georgieva, Feyo de Azevedo, Goncalves, & Ho, 2003a; Georgieva, Meireles, & Feyo de Azevedo, 2003b). However, these models have been developed for process state estimation, the prediction of crystal size distribution (CSD) and for various control objectives including tracking, optimisation

and robustness. The issues of the on-line detection of changes in process operation, early warning of process malfunctions and potential production failures have not been directly addressed by the existing models.

In this paper, an empirical statistical approach is adopted for the development of a statistical model based on the available process measurements. Techniques investigated include moving window principal component analysis (MWPCA, Lennox, Montague, Hiden, Kornfeld, & Goulding, 2001); batch observation level (BOL, Wold, Kettaneh, Friden, & Holmberg, 1998), batch dynamic principal component analysis (BDPCA, Chen & Liu, 2002) and time-varying state space modelling (TVSS, Simoglou, Martin, & Morris, 2002a, 2002b). These approaches assume that the available data captures the underlying process operating conditions. Then multivariate statistics such as Hotelling's T^2 and the squared prediction error (SPE) are to be calculated along with their appropriate control limits. These metrics and associated control limits are then used for the on-line monitoring of the process and the classification of a batch as in- or out-of-specification.

* Corresponding author. Tel.: +44 191 222 7342; fax: +44 191 222 5748.

E-mail addresses: petia@det.ua.pt (P. Georgieva), e.b.martin@ncl.ac.uk (E.B. Martin), julian.morris@ncl.ac.uk (A.J. Morris), sfeyo@fe.up.pt (S. Feyo de Azevedo).

2. Process operation

The batch cycle of white sugar production is divided into several sequential phases. During the first phase, the pan is partially filled with a juice containing dissolved sucrose (termed liquor). The liquor is concentrated by evaporation, under vacuum, until supersaturation reaches a predefined value (typically 1.15). At this stage, seed crystals are introduced into the pan to induce the production of crystals. This is the beginning of the second (crystallization) phase. As water is evaporated, the dissolved sugar concentration increases, resulting in crystal growth. As evaporation takes place, further liquor or water is added to the pan to maintain the level of supersaturation and increase the volume. For economical reasons, towards the end of this phase, the liquor is replaced by other juices of lower purity (termed syrup). The third phase consists of tightening which is principally controlled by evaporation capacity. At the end of a batch, the pan is filled with a suspension of sugar crystals in heavy syrup, which is dropped into a storage mixer before centrifugation. Present pan control involves the manipulation of the feed flow rate of sugar liquor/syrup and the vacuum pressure. The process objective is to obtain sugar of high quality, which is measured in terms of the purity, shape and CSD at the batch end. CSD is quantified by the mass averaged crystal size (MA) and the coefficient of variation (CV). The desired values for MA are 0.5–0.6 mm and for CV: 28–32%.

2.1. Available measurements

The industrial unit is equipped with 15 sensors. The on-line recorded physical measurements relating to a batch are summarised in Tables 1 and 2, Measured input and output measurements, respectively, and Table 3 those variables that are constant for each batch. These are all known to be reliable measurements.

Table 1
Measured variable input data

Notation	Process variable
F_f	Liquor/syrup feed flowrate
B_f	Brix of the feed
T_f	Temperature of the feed
F_w	Water feed flowrate
F_s	Steam flowrate
T_s	Steam temperature
P_s	Steam pressure
I_{agit}	Intensity of stirrer current
P_{vac}	Vacuum pressure
T_{vac}	Vacuum temperature

Table 2
Measured variable output data

Notation	Process variable
B_{sol}	Brix of the solution
T_m	Temperature of the solution
L	Level in the pan

Table 3
Constant (for each batch) data

Notation	Process variable
T_w	Temperature of the feed water
Pur_f	Purity of the liquor/syrup
t_{syr}	Initial time for introducing syrup
t_{seed}	Initial time of seeding

The brix of the solution is the concentration of total dissolved solids (sucrose plus impurities) in the solution and is measured by a refractometer. Supersaturation is not a measured variable but can be determined from the available measurements.

3. On-line multivariate statistical process control (SPC) techniques

Batch process modelling and monitoring has been always a challenging problem in chemical engineering due to the presence of non-linear behaviour and serial correlation, correlated and/or collinear data, varying batch lengths and multi-product production. Current state of the art empirical techniques include the bi-linear approaches of multi-way principal component analysis (MPCA) and multi-way partial least squares (MPLS), Nomikos and MacGregor (1994) and the tri-linear methodologies of PARAFAC (Bro, 1997) and PARAFAC II (Wise, Gallagher, & Martin, 2001 and Smilde, 1992). Although the above bi-linear and tri-linear techniques have been successfully applied to batch processes, they experience a number of limitations. For example, they do not incorporate the process dynamics and with the exception of PARAFAC II, the duration of the batches are assumed to be constant. Moreover, for on-line monitoring, it is required that the whole batch trajectory is known or is predictable. This requirement results in certain assumptions being made in order to in-fill the unknown future values of the batch trajectory. Finally, all these techniques are linear and to a greater or lesser extent fail to capture the non-linear nature of a batch process. To overcome the issues of data in-filling and unequal batches, alternative approaches have been proposed.

3.1. Moving window principal component analysis

Moving window principal component analysis was proposed by Lennox et al. (2001). Typically measurements from a batch process are arranged in a three-dimensional matrix \mathbf{X} ($NB \times NV \times NT$) where NB, NV and NT are the number of batches, variables and time instants (Fig. 1a). The three-dimensional matrix \mathbf{X} can be transformed to a bi-dimensional matrix by unfolding over the batch dimension ($NB \times (NV \times NT)$) as shown in Fig. 1b. A scaling is usually applied to the unfolded matrix \mathbf{X} before an ordinary PCA analysis. The mean of each column of \mathbf{X} is subtracted from each data element of this column. This way of mean centring is very important since it results in the removal of the

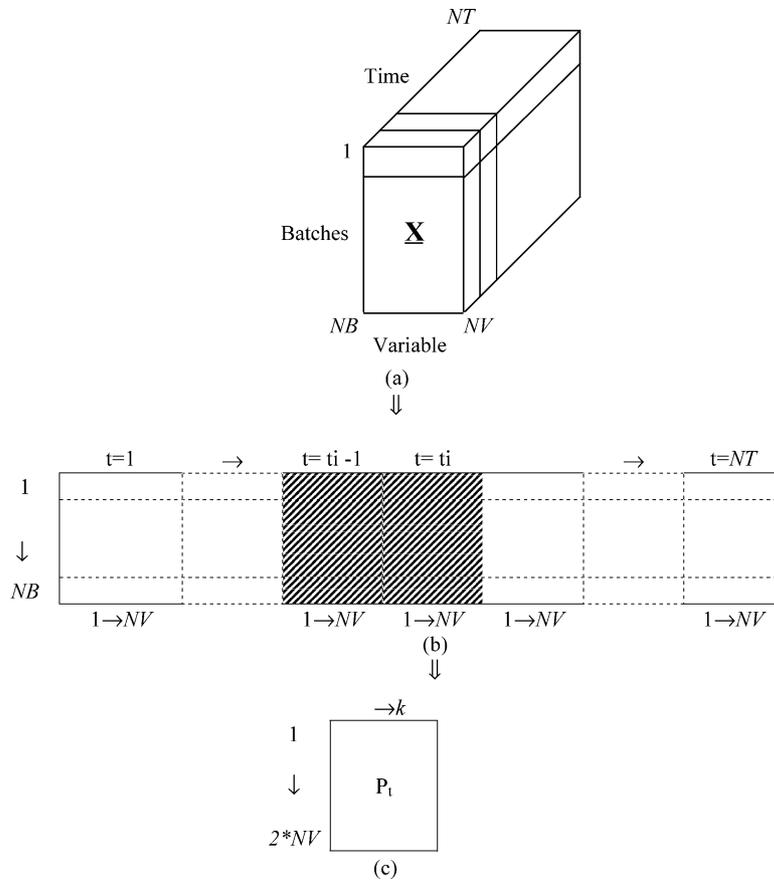


Fig. 1. Moving window principal component analysis (MWPCA).

main non-linear component in the data. Furthermore, by scaling the variables in each column of \mathbf{X} , the differences in the measurement units between variables can be handled to allow equal weight to be given to each variable at each time interval. A PCA model is then developed on a moving window of data. Having selected the length of the moving window (L), MWPCA then develops $NT - L + 1$ PCA models for each time interval by decomposing the $(NB \times NV)$ matrix \mathbf{X} into a systematic and noisy part:

$$\mathbf{X} = \mathbf{T}_k \mathbf{P}_k^T + \mathbf{E} \quad (1)$$

where \mathbf{T}_k and \mathbf{P}_k are the matrices of the k retained principal component scores and loading, respectively, while \mathbf{E} is the matrix of the residuals. The number of the retained principal components, k , is usually determined by the means of cross-validation. For the application considered, the order of the moving window was selected to be $L=2$ which takes into account the desired previous data over two past sample intervals. For each of the $NT - L + 1$ PCA models the loading matrix \mathbf{P}_k , is stored.

Having performed a PCA analysis, a set of on-line monitoring tools can then be developed. Typically these tools are Hotelling's T^2 and squared prediction error control charts. Consider that a new batch \mathbf{x}_{new} is to be monitored. Then,

Hotelling's T^2 is calculated using the k retained PCA scores:

$$\mathbf{t}_k = \mathbf{x}_{\text{new}} \mathbf{P}_k \quad (2)$$

$$T^2 = \mathbf{t}_k \mathbf{S}_t^{-1} \mathbf{t}_k^T \quad (3)$$

where \mathbf{t}_k are the k retained PCA scores and \mathbf{S} is their covariance matrix. The SPE is then calculated as follows:

$$\text{SPE} = \mathbf{e}_t \mathbf{e}_t^T \quad (4)$$

$$\mathbf{e} = \mathbf{x}_{\text{new}} (\mathbf{I} - \mathbf{P}_k \mathbf{P}_k^T) \quad (5)$$

3.2. Batch dynamic principal component analysis

The MWPCA approach does not capture the dynamic behaviour within a batch process. Chen and Liu (2002), proposed batch dynamic principal component analysis, in an attempt to explain the batch process dynamics. They suggested the use of lagged variables to incorporate process dynamics. More specifically in BDPKA, each batch is isolated from the others (Fig. 2a). A matrix \mathbf{X}_{iv} ($NT \times NV$) is formed for each iv batch. Then each of the NV variables is lagged d times resulting in an lagged \mathbf{X}_{iv} [$(NT - d) \times (NV \times (d + 1))$] matrix (Fig. 2b). The covariance matrix of the lagged \mathbf{X}_{iv} matrix, \mathbf{S}_{iv} , is then calculated (Fig. 2c). The procedure is

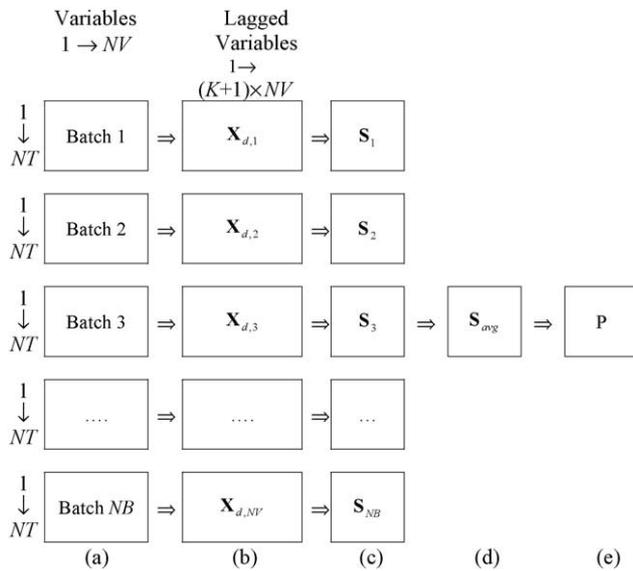


Fig. 2. Batch dynamic principal component analysis (BDPCA).

repeated for all NB batches, resulting in NB S_{iv} covariance matrices. The elements in each of the S_{iv} matrices are a measure of the dynamic relationship between variables in Batch iv . Having calculated these dynamic correlations for all NB batches an average covariance matrix, S_{avg} , is then calculated based on the NB S_{iv} covariance matrices (Fig. 2d):

$$S_{avg} = \frac{(NT - d - 1) \sum_{iv=1}^{NB} S_{iv}}{NV(NT - d)} \quad (6)$$

The average covariance matrix, S_{avg} , expresses the average dynamic relationships between the process measurements. A PCA model is then developed based on S_{avg} (Fig. 2e). The resulting BDPCA model is finally used to calculate the T^2 and SPE statistics for monitoring purposes.

3.3. Batch observation level

To overcome the problem with unequal batch lengths an alternative monitoring approach was proposed by Wold et al. (1998), termed batch observation level. In BOL, the original three-way data are unfolded over the variables dimension (Fig. 3a). A dummy y-variable that can be a time index or a batch maturity index is then specified. Data are scaled and a partial least squares (PLS) analysis is then performed between the unfolded matrix X and the dummy y vector:

$$X = T_k P_k^T + E \quad (7)$$

$$y = T_k c + f \quad (8)$$

where c is the regression vector of y onto the PLS scores T_k (Fig. 3b), and f are the PLS model residuals. The number of PLS latent variables to be retained are selected as those that provide an adequate description of both the X and y spaces.

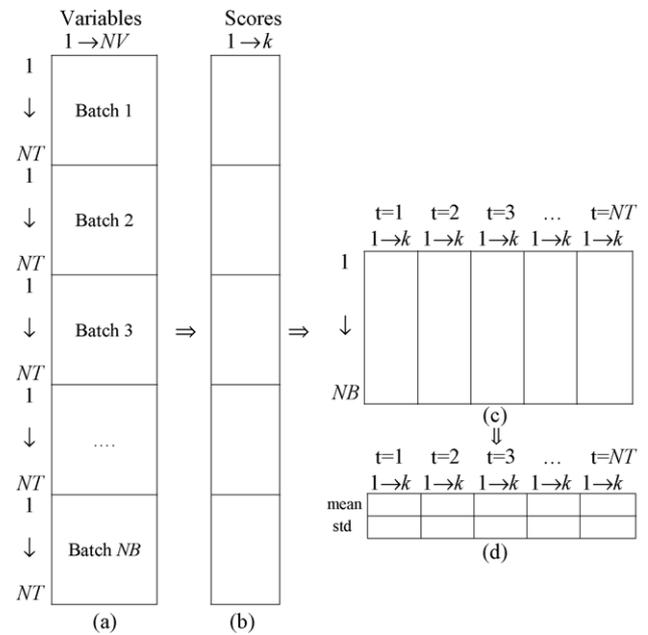


Fig. 3. Batch observation analysis (BO).

For setting up an on-line monitoring scheme, the scores of the retained PLS scores are then rearranged over the batch dimension resulting in a $[NB \times (NT \times k)]$ matrix, Fig. 3c and their mean and standard deviation calculated for each sample point and stored (Fig. 3d.). In an on-line situation, when a new sample is obtained, the scores are initially calculated and then scaled using the mean and the standard deviation of the corresponding sample point. These scaled scores are plotted against their control limits in univariate score plot charts. Similar to the previous approaches, T^2 and SPE charts can also be constructed.

3.4. Time-varying state space modelling

A different approach to batch process modelling and monitoring is currently under investigation, introduced by Simoglou et al. (2002a), namely time-varying state space (TVSS) modelling. The state space model developed takes the form:

$$t_{t+1} = C_t t_t + w_t \quad (9)$$

$$y_t = H_t t_t + e_t \quad (10)$$

where t are the system states, y are the available process measurements, w and e are the state and output residuals with covariance matrices Q and R , respectively. Finally, C and H are the state space model matrices, which are assumed to be time-varying since they aim to describe a non-stationary process. To develop the model ((9) and (10)), the data are initially unfolded and scaled as in MWPCA. The procedure to compute the TVSS matrices C and H then proceeds through the identification of the system states. For a time interval $t = k$, the past and the future of the system is defined as shown in

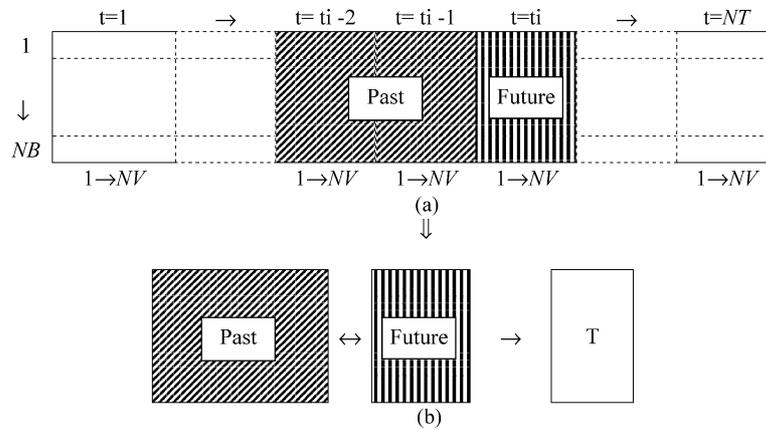


Fig. 4. Time-varying state space model.

Fig. 4a. The past (\mathbf{p}) of the process is associated with the past process measurements of all batches at time k up to a specific lag (in Fig. 4a the time lag, K , was set to a value of two past sample intervals to encapsulate the relevant past data):

$$\mathbf{p}_t = [\mathbf{y}_{t-1} \mathbf{y}_{t-2} \cdots \mathbf{y}_{t-k}]^T \quad (11)$$

The future (\mathbf{f}) of the process are the current and future process measurements of all batches (in Fig. 4a the future horizon, L , is set up to a value of one):

$$\mathbf{f}_t = [\mathbf{y}_t \mathbf{y}_{t+1} \cdots \mathbf{y}_{t+L}]^T \quad (12)$$

Now, by applying any one of either partial least squares, principal component regression (PCR) or canonical variate analysis (CVA) between the past (11) and the future (12) of the process, new latent variables can be calculated which provide a reliable approximation of the true system states. PCR scores capture the variability between process measurements while PLS and CVA latent variables are those linear combinations of the past that include the information required to predict process future. The result of applying either a PCR, PLS or CVA analysis is a weighting matrix \mathbf{J}_t which is used to identify the system states through the past vector \mathbf{p}_t :

$$\mathbf{t}_t = \mathbf{J}_t \mathbf{p}_t \quad (13)$$

Once the system states have been identified the state space matrices can be computed using a least squares solution (see Simoglou et al., 2001, for more details).

In the next section, the four multivariate techniques (BOL, MWPCA, BDPCA and TVSS) are applied and compared with the univariate SPC for the ‘on-line’ performance monitoring of the sugar crystallization process.

4. On-line SPC of sugar crystallization

Data from 14 industrial runs were available from a sampling period of 4 months. Batches were discriminated as being ‘in-specification’ or ‘out-of-specification’ based on the

final CSD properties. Eleven batches were identified as being in-specification whilst three had MA values out with the specification range.

4.1. Data pre-processing

Prior to developing the statistical models it was necessary to make decisions related to the selection of the crystallization phases and the process variables to be included in the monitoring model. The phases to be modelled were selected to be the crystallization phase and the tightening phase. The initial operations before seeding (charging and concentration) were excluded from the analysis because their objectives are to feed a certain initial quantity of juice into the pan and to concentrate it until a predefined level as soon as possible. Therefore, the main effect of these stages on the next operations is the time it takes to reach the same initial conditions (supersaturation set point) for the crystallization period. Moreover, in practice, no specific faults are observed during this phase of process operations.

The variables included in the analysis were vacuum pressure, steam flowrate, steam pressure, steam temperature, brix of the solution, supersaturation and temperature of the solution. To control the supersaturation around the metastable zone, process operators periodically open and close the respective liquor/syrup and water flow valves. Thus, in the available data set, there are periods where both feed flowrates are equal to zero. Building a statistical model based on this data set results in the model being trained on data where the feed flow rates are zero. However, if for a new batch, process conditions force operators to open one of the feed valves for control purposes, then for this particular time point the statistical model will move outside of the limits resulting in a possible false alarm. The feed variables were thus excluded which does not result in a loss of information since their effect directly impacts on the other process variables (Brix of the solution and the supersaturation) included in the data set. A calculated variable (supersaturation) was also included as a critical sugar crystallization parameter.

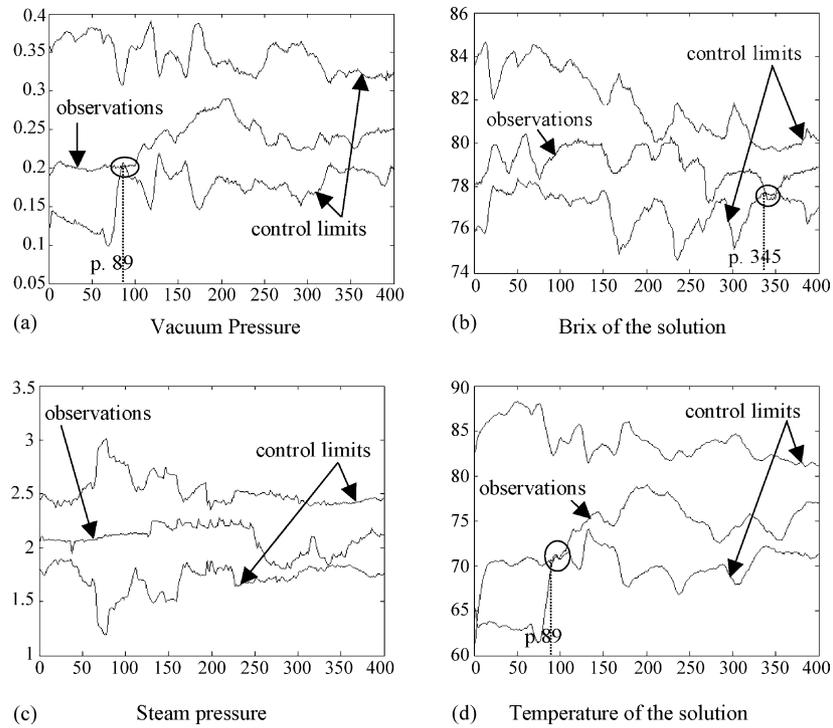


Fig. 5. Time series plots and control limits of out-of-spec Batch 1.

4.2. On-line univariate SPC

Figs. 5–7 show the most significant variables for the three bad batches along with univariate, $\pm 3\sigma$, control limits. For Batches 1 and 3, the variables lie within the univariate control limits for most of the batch run. Those observations that

marginally lie out with the statistical limits, for example, time point 89 in Fig. 5a, are very close to the statistical control limit and it was concluded that they were statistically spurious signals (on average one in hundred observations will lie outside the 99% action limits). It is observed that only Batch 2 has variables that exceed the univariate control limits. It was only

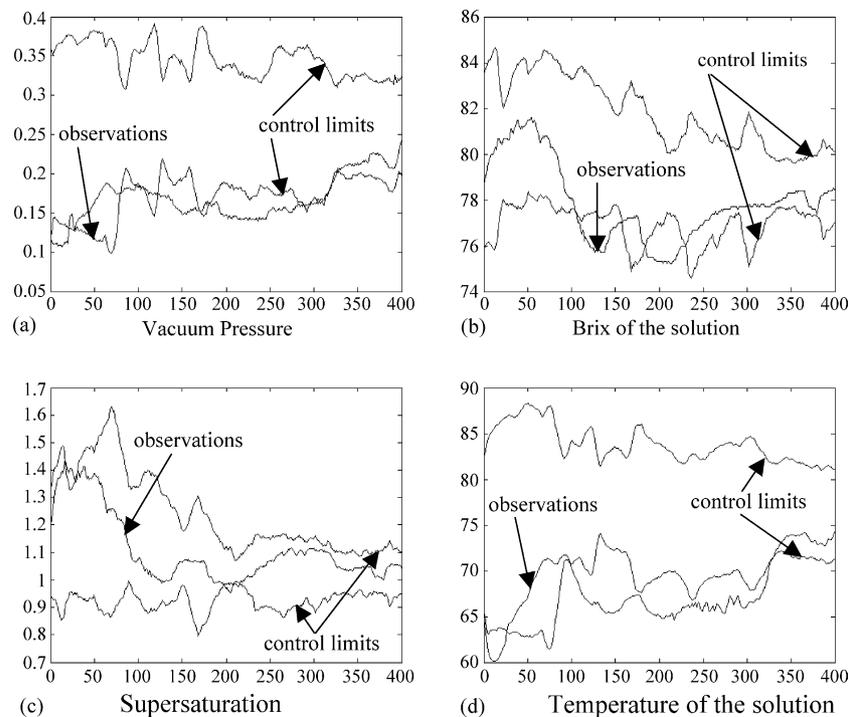


Fig. 6. Time series plots and control limits of out-of-spec Batch 2.

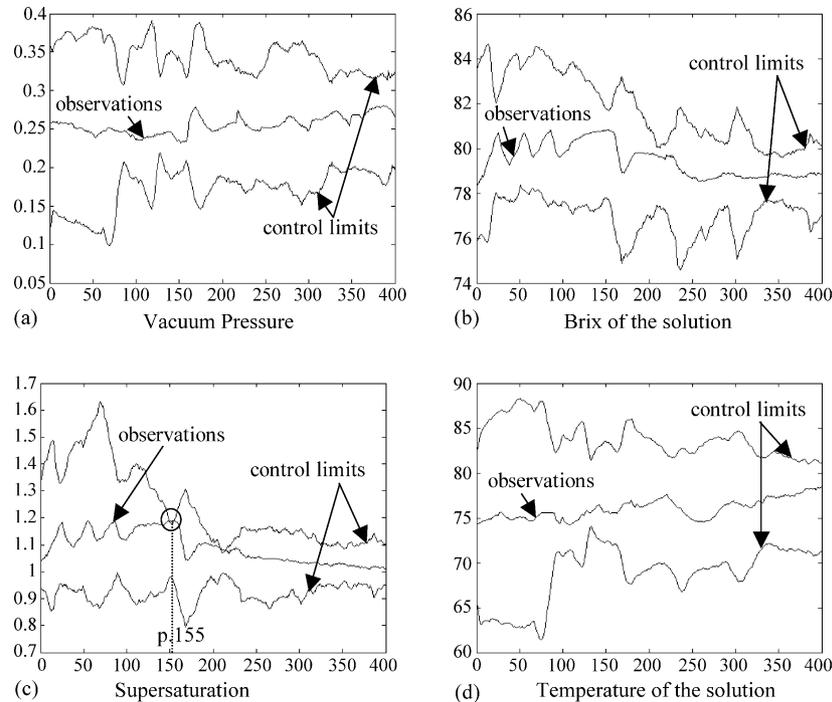


Fig. 7. Time series plots and control limits of out-of-spec Batch 3.

in this particular case, that the application of univariate SPC could detect periods of out-of-specification operation.

4.3. On-line multivariate SPC

The multivariate SPC techniques of MWPCS, BOL, BDPCA and TVSS discussed in Section 3 were then used to ‘monitor’ the real process data. All the approaches compared are linear, can deal with unequal batch lengths and to a greater or lesser extent can describe the underlying batch process dynamics. Having built and validated the four models from in-specification process data, the next step was to evaluate their ability to detect the out-of-specification batches and provide information as to the variable(s) responsible for the out-of-specification signal. The results are summarised in Figs. 8–11. T^2 and SPE control charts are shown alongside their corresponding contribution plots. The contribution plot (Miller, Swanson, & Heckler, 1998) shows the contribution of the original seven process variables to the T^2 or SPE value for the maximum out-of-control value. For example, Fig. 8a shows how the T^2 statistic would evolve in an on-line manner with MWPCA for out-of-specification Batch 1. T^2 takes its maximum value at time point 89, and Fig. 8b shows the T^2 contribution plot for this particular point. In all the control charts, the values shown were scaled so that the run-time control limits were equal to unity for the whole batch run. This way of presenting the control charts is more user-friendly for process operators. It also allows the four statistical methods to be compared on a common basis as the degree to which the T^2 and SPE statistic exceed the limits can be quantified.

In general, it can be seen that the four methods identify periods of out-of-specification operation during the run in all three batches for both SPE and T^2 control charts. It is only for the T^2 metric of BDPCA, Fig. 10e, where there is no out-of-control signal for Batch 3. Thus, by applying multivariate SPC as opposed to univariate SPC periods of out-of-specification operation can be detected. The SPE and T^2 control charts for Batch 2 (not included in this paper but available in the authors graph set) lead to similar conclusions as for the other two batches. Since the univariate control charts clearly detected out-of-specification operation for Batch 2 (Fig. 6), it was decided to illustrate only the batches for which the univariate approach was not efficient.

In Fig. 8a, the MWPCA based T^2 control chart for Batch 1, there is a period of out-of-specification operation around time point 89. The univariate control charts indicated out-of-specification operation for the time period 88–90. More specifically, the univariate control charts of vacuum pressure (Fig. 5a) and solution temperature (Fig. 5d) move outside the limits for these time points. In the multivariate T^2 control chart, out-of-specification operation is detected earlier and takes its maximum value at time point 89. The T^2 contribution plot for time point 89 (Fig. 8b) indicates that variable 1 (vacuum pressure) is responsible for the out-of-control signal. This conclusion is in accordance with the univariate SPC control charts.

T^2 control charts for the other three methods for Batch 1, TVSS (Fig. 9a), BDPCA (Fig. 10a) and BO (Fig. 11a) provided maximum T^2 out-of-control signals for the time period around point 345. Univariate SPC provides an out-of-

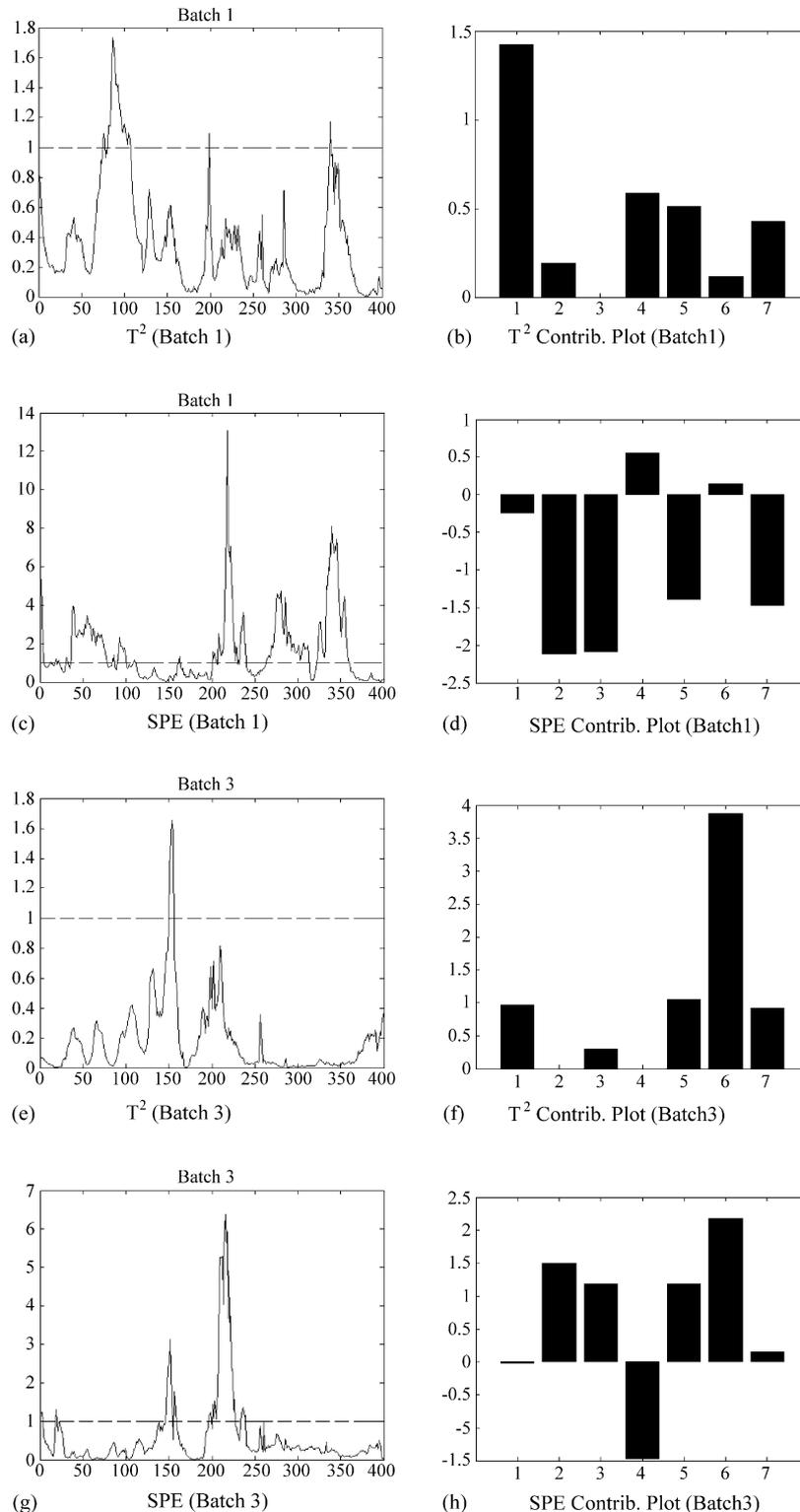


Fig. 8. MWPCA based on-line monitoring for out-of-spec Batches 1 and 3, variables: (1) vacuum pressure, (2) steam flowrate, (3) steam pressure, (4) steam temperature, (5) brix of the solution, (6) supersaturation and (7) temperature of the solution.

control signal for the brix of the solution for this time period Fig. 5b. However, the fault is not detected as early as for the multivariate control charts and the level of excursion outside the limits is smaller for the univariate control charts. The contribution plot for TVSS (Fig. 9b) indicates that the steam

temperature and the brix of the solution are mainly responsible for the out-of-control signal. The respective contribution plots for BDPCA (Fig. 10b) and BOL (Fig. 11b) also indicate that the brix of the solution is mainly responsible for the out-of-control signal.

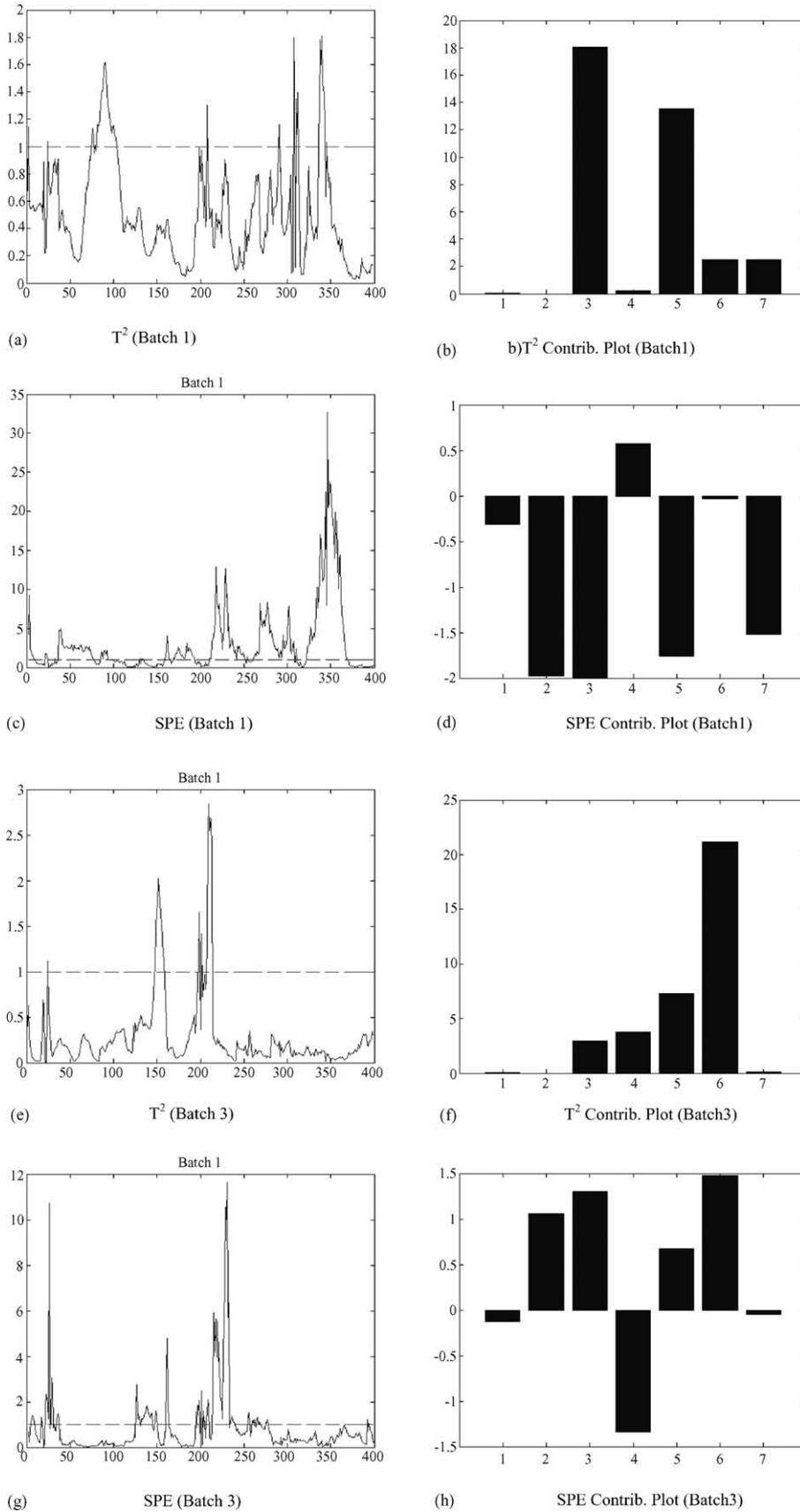


Fig. 9. TVSS based on-line monitoring for out-of-spec Batches 1 and 3, variables: (1) vacuum pressure, (2) steam flowrate, (3) steam pressure, (4) steam temperature, (5) brix of the solution, (6) supersaturation and (7) temperature of the solution.

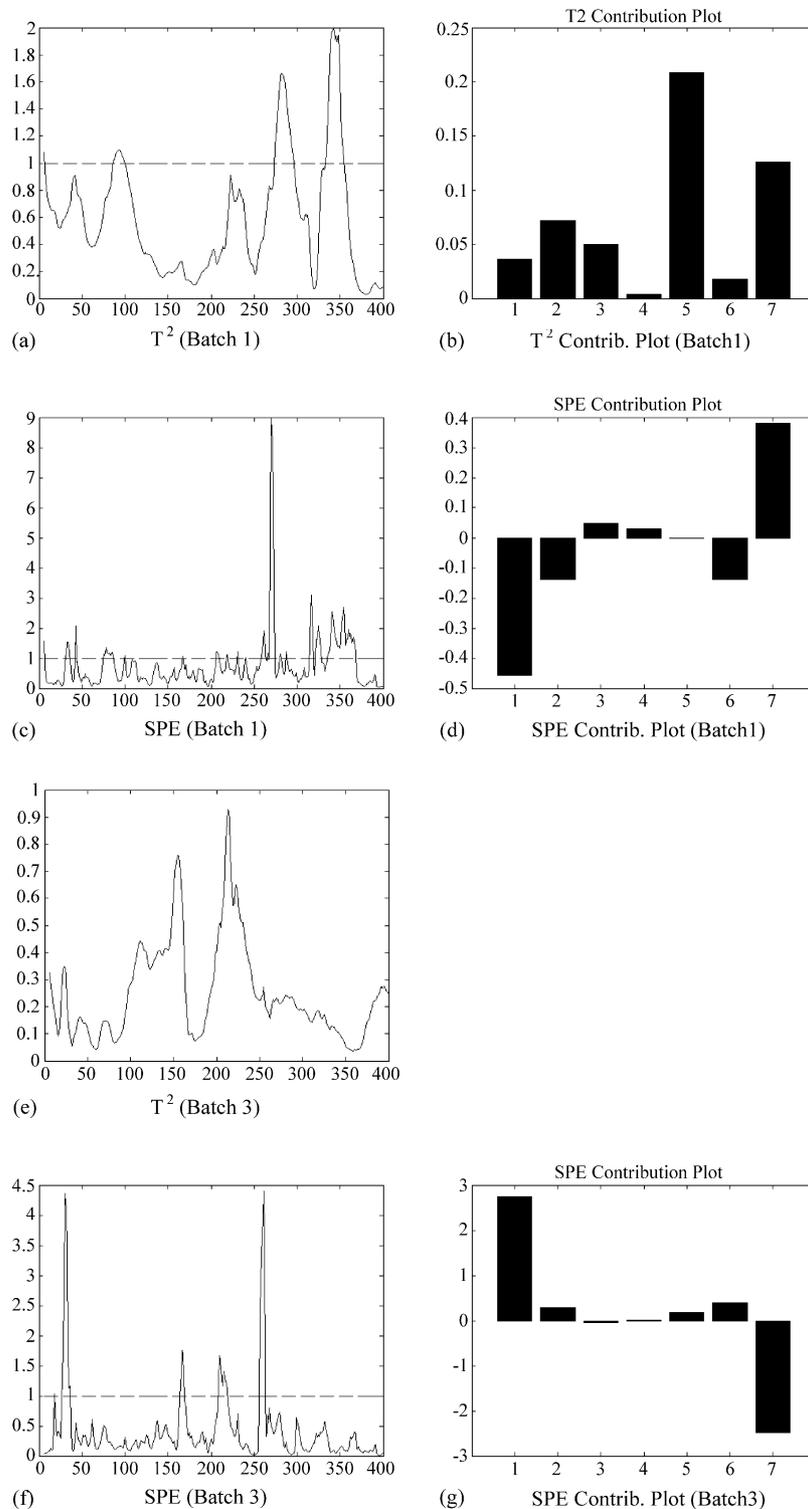


Fig. 10. BDPCA based on-line monitoring for out-of-spec Batches 1 and 3, variables: (1) vacuum pressure, (2) steam flowrate, (3) steam pressure, (4) steam temperature, (5) brix of the solution, (6) supersaturation and (7) temperature of the solution.

Similar conclusions can be drawn for the monitoring of Batch 3. The multivariate SPC techniques provide an earlier warning of the process faults than univariate SPC with the T^2 statistic clearly exceeding the control limits. For example, in Batch 3 there is a time period around point 155 where T^2

exceeds the limit. With the exception of BDPCA, all the MSPC approaches provided an alarm indicating that supersaturation is responsible for the out-of-control signal. This conclusion is in agreement with the respective univariate SPC chart.

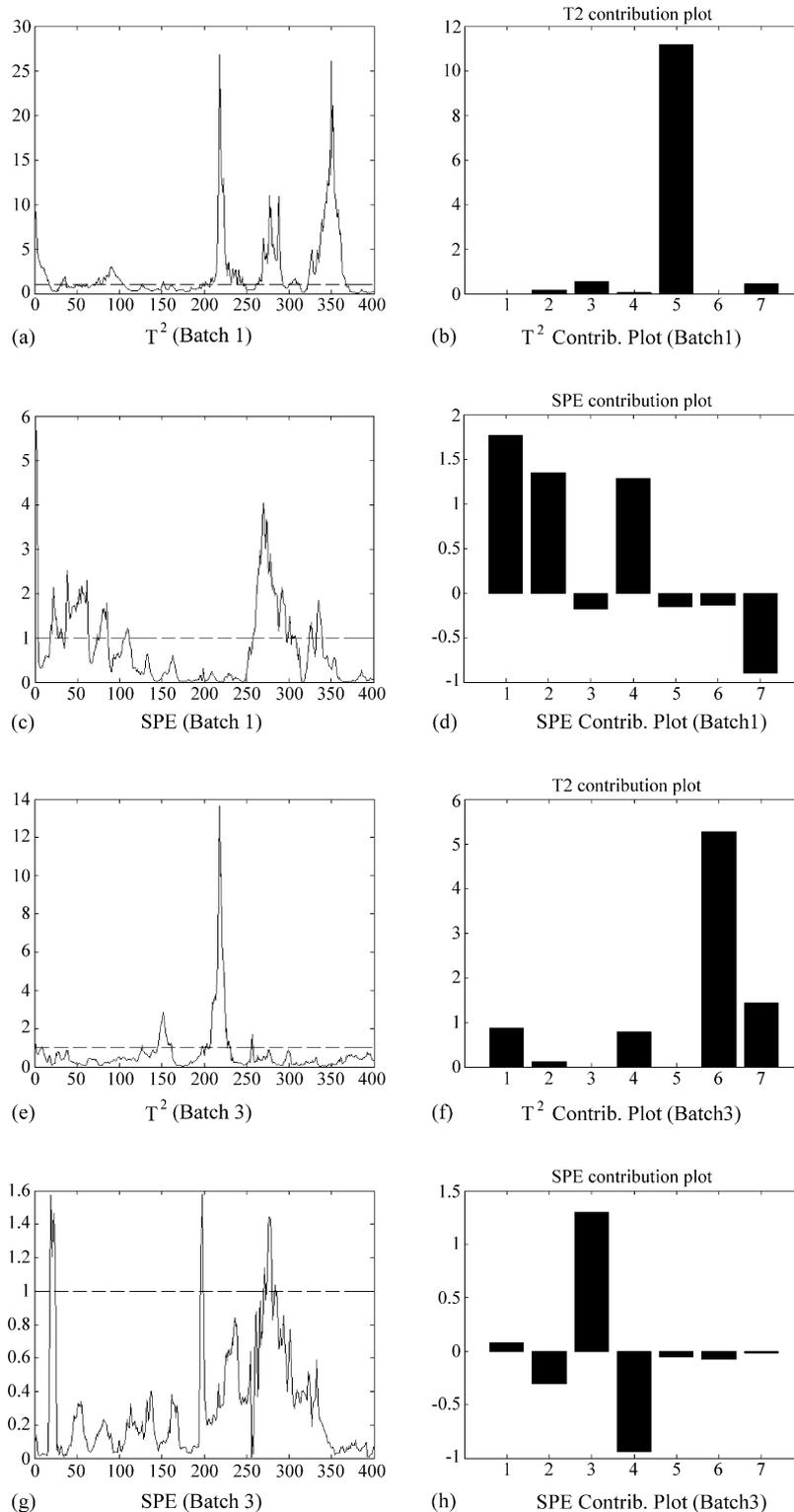


Fig. 11. BO based on-line monitoring for out-of-spec Batches 1 and 3, variables: (1) vacuum pressure, (2) steam flowrate, (3) steam pressure, (4) steam temperature, (5) brix of the solution, (6) supersaturation and (7) temperature of the solution.

The four multivariate monitoring techniques of MWPCS, BOI, BDPCA and TVSS exhibit similar performance and capability in terms of distinguishing between in and out-of-specification behaviour. However, the TVSS approach captures the underlying dynamic relationship between the

process variables more clearly than the other three approaches. For example, according to the control charts in Fig. 9a and c, an abnormal situation arises around time interval 325–375. Examining the time trajectories of the measured variables for Batch 1, it is observed that for the same

period the steam pressure (Fig. 5c) that operationally should be kept at around 1.9–2.2 bar for safety reasons, goes outside of this limit. This causes a rapid decrease in the brix (Fig. 5b) and subsequently supersaturation moves out-of the metastable zone (decreases), which results in the dissolution of the existing crystals. These variations are captured by the contribution plots (Fig. 9b and d) and an alarm signal generated by the monitoring scheme is justified.

For Batch 3, by observing the time series plots, it can be concluded that the main variables that determine the working conditions, namely vacuum pressure, steam pressure, flowrate and temperature are controlled around their nominal values. However, after time point 150, the brix (Fig. 7b) and supersaturation (Fig. 7c) start to decrease for no obvious reason. This experience has shown that this effect is due to unexpected changes in the purity of the feed, which is not an on-line measured variable and thus not included in the data set. Thus, for this reason the BDPCA T^2 statistic did not identify the problem whilst the corresponding SPE control charts only detected very short periods of out-of-specification operation.

5. Conclusions

In this paper, four on-line multivariate process performance monitoring schemes for an industrial sugar crystallization process were applied and compared with univariate SPC techniques. The process itself is challenging since it is carried out in multiple phases and there exists strong non-linear and dynamic effects between the variables. The methods proposed to develop the on-line monitoring scheme were moving window principal component analysis, batch observation level, batch dynamic principal component analysis and time-varying state space modelling. The monitoring schemes were applied in an on-line mode for three batches whose final product was out-of-specification. It was found that all methods could identify clearly periods of bad operation for all three batches and perform better than the traditional univariate SPC. Although the BDPCA approach is attractive in that the quality variables are closely correlated with and are reflected by the process measurements, the TVSS methodology is much more effective in handling varying batch lengths, non-linear data, and presence of serial correlation between measurements.

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