A TIME VARYING STATE SPACE APPROACH FOR SUGAR CRYSTALLIZATION PROCESS MODELLING AND MONITORING

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Abstract: The present paper contributes to the issues of batch process modelling and monitoring by proposing a time-varying state space (TVSS) model for the evaporative sugar crystallization industrial process. 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 TVSS methodology is compared with current state-of-the-art techniques and the results obtained demonstrate the superior performance of the TVSS approach to successfully detect abnormal events and periods of bad operation.

Keywords: Statistical process control, dynamic principal component analysis, batch sugar crystallization

1. INTRODUCTION

Sucrose crystallisation, carried out in evaporative crystallisers, operating under vacuum in a semi-batch regime, constitutes a relevant industrial crystallization process. It can be characterised as a strong non-linear and non-stationary process. Significant scientific work has been carried out into the development of mechanistic dynamical models to describe the process, Feyo de Azevedo et al., 1996. More recently a knowledge-based hybrid model (KBHM) based on a combination of a partial mechanistic and artificial neural network (ANN) model was proposed by Georgieva et al., 2003. However, these models were focused on various estimation, optimization and feedback control problems. 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 the present paper, a new methodology for crystallization modelling and monitoring is proposed. It is a fully data driven approach based on a time varying state space (TVSS) model. A TVSS model is developed for each time interval of the batch duration. The approach is multivariate and dynamic while by building successive local models over the batch duration faces more efficiently than current techniques the issue of non-linear behaviour. It can deal with unequal batch lengths while for on-line monitoring it does not require any assumptions for filling missing future data of the batch.
The paper is organized as follows. Section 2 provides a short description of the process operation. In

section 3 current state of the art statistical process control (SPC) methodologies are reviewed. In section 4 the TVSS model is proposed. In section 5 the proposed modelling scheme is validated against a comprehensive crystallization simulation and compared with the reviewed in section 3 approaches. The paper ends up with conclusions and references.

2. PROCESS OPERATION

Sugar crystallization operation takes place in six phases: *i)* initial filling and concentration; *ii)* seeding; *iii)* setting the grain; *iv)* crystallization; *v)* tightening and *vi)* discharging to a storage mixer before centrifugation. Typically seeding is performed at a supersaturation of 1.15. Often at the start of this period some form of thinning with water is required in order to prevent formation of conglomerates. Crystallization takes the longest period and has to be controlled primarily by the feed flow driven by supersaturation, consistency and crystal production requirements. Tightening is principally controlled by the capacity for evaporation.

The unit contains 15 sensors for the following properties and operating variables: *i) inside the pan* - massecuite temperatures at three locations; brix of solution; level; massecuite consistency; stirrer current; vacuum pressure and temperature. *ii) feed conditions* - temperature, brix and flow rate of feed liquor and feed syrups. *iii) steam conditions* - temperature, pressure and flow rate of steam.

Brix is the concentration of total dissolved solids (sucrose plus impurities) in the solution. Supersaturation is not a measured variable but can be determined from the available measurements. The feed flow rate of sugar liquor/syrup and the vacuum pressure are considered as process inputs. The crystal contents and the crystal size distribution (CSD) characterise the productivity and the product quality.

3. CURRENT ON-LINE STATISTICAL PROCESS CONTROL 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 empirical techniques include the bi-linear approaches of multi-way Principal Component Analysis (PCA) and multi-way Partial Least Squares (PLS), and the tri-linear methodologies of PARAFAC. Although the above techniques have been successfully applied to batch processes they experience a number of limitations. For example they do not incorporate the process dynamics and most of them assume the duration of the batches 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. 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 (MWPCA) was proposed by Lennox et al. 2001. Typically measurements from a batch process are arranged in a three-dimensional matrix X ($NB \times NV \times NT$) where NB, NV and NT are the number of batches, variables and time instants. The three-dimensional matrix $\mathbf{X}$ can be transformed to a bidimensional matrix by unfolding over the batch dimension ($NB \times (NV \cdot NT)$). 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 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 X. into a systematic and noisy part:

$$\mathbf{X} = \mathbf{T}_k \mathbf{P}_k^T + \mathbf{E} \tag{1}$$

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 process considered the order of the moving window was selected to be L=2. For each of the $NT-L+1$ PCA models the loading matrix 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 (SPE) 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

$$\mathbf{t}_k = \mathbf{x}_{new} \mathbf{P}_k \tag{2}$$

$$T^2 = \mathbf{t}_t \mathbf{S}_t^{-1} \mathbf{t}_t^T \tag{3}$$

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

$$SPE = \mathbf{e}_t \mathbf{e}_t^T \tag{4}$$

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

3.2 Batch dynamic principal component analysis

The MWPCA approach does not capture the dynamic behaviour within a batch process. Chen and Liu, 2000, proposed Batch Dynamic Principal Component Analysis (BDPCA), in an attempt to explain the batch process dynamics. They suggested the use of lagged variables to incorporate process dynamics. More specifically in BDPCA, each batch is isolated from the others. A matrix $\mathbf{X}$ ($NT \times NV$) is formed for each batch. Then each of the NV variables is lagged d times resulting in an lagged $\mathbf{X}[(NT\text{-}d)\times(NV\cdot(d+1))]$ matrix. The covariance matrix of the lagged $\mathbf{X}$ matrix, $\mathbf{S}_{iv}$, is then calculated. The procedure is repeated for all NB batches, resulting in NB $\mathbf{S}_{iv}$ covariance matrices. The elements in each of the $\mathbf{S}_{iv}$ 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, is then calculated based on the NB $\mathbf{S}_{iv}$ covariance matrices :

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

The average covariance matrix, $\mathbf{S}_{avg}$, expresses the average dynamic relationships between the process measurements. A PCA model is then developed based on $\mathbf{S}_{avg}$. 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 (BOL). In BOL the original three-way data is unfolded over the variables dimension. A dummy y-variable that can be a time index or a batch maturity index is then specified. Data is scaled and a Partial Least Squares (PLS) analysis is then performed between the unfolded matrix $\mathbf{X}$ and the dummy $\mathbf{y}$ vector:

$$\mathbf{X} = \mathbf{T}_k \mathbf{P}_k^T + \mathbf{E} \quad (7)$$

$$\mathbf{y} = \mathbf{T}_k \mathbf{c} + \mathbf{f} \quad (8)$$

where $\mathbf{c}$ is the regression vector of $\mathbf{y}$ onto the PLS scores $\mathbf{T}_k$,, and $\mathbf{f}$ 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. 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 $[NB\times(NT\cdot k)]$ matrix, and their mean and standard deviation calculated for each sample point and stored. 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. Similarly to the previous approaches, T^2 and SPE charts can also be constructed.

4. TIME VARYING STATE SPACE MODELL

The underlying idea of this paper is that a batch process can be described by a time-varying state space (TVSS) model. This new approach was recently introduced by Simoglou et al., 2002a. The state space model developed takes the form:

$$\mathbf{t}_{t+1} = \mathbf{C}_t \mathbf{t}_t + \mathbf{w}_t \quad (9)$$

$$\mathbf{y}_t = \mathbf{H}_t \mathbf{t}_t + \mathbf{e}_t \quad (10)$$

where $\mathbf{t}$ are the system states, $\mathbf{y}$ are the available process measurements, $\mathbf{w}$ and $\mathbf{e}$ are the state and output residuals with covariance matrices $\mathbf{Q}$ and $\mathbf{R}$ respectively. Finally $\mathbf{C}$ and $\mathbf{H}$ 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 (9-10) the data are initially unfolded and scaled as in MWPCA. The procedure to compute the TVSS matrices $\mathbf{C}$ and $\mathbf{H}$ then proceeds through the identification of the system states. For a sample time $t = k$, past and future of the system are considered. The past ($\boldsymbol{p}$) is associated with the past process measurements of all batches at time k up to a specific lag K :

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

The choice of K as the length of the past vector window is in terms of capturing the relevant dynamics of the system being studied. In the case considered K=2. The future ($\boldsymbol{f}$) of the process are the current and future process measurements of all batches (in practical cases the future horizon, L, can be set as one or two):

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

The choice of the length of the moving window L is also based on the dynamics of the process being studied; too large and the sensitivity of the process malfunction is reduced, whilst too small a window would be impacted by process noise. Now, by applying any one of either PLS, 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 $\mathbf{p}_t$:

$$\mathbf{t}_t = \mathbf{J}_t \mathbf{p}_t \tag{13}$$

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 TVSS methodology is validated and compared with the univariate SPC and the multivariate techniques reviewed in section 3 (MWPCA, BDPCA, BOL) using a comprehensive simulation of an industrial white sugar crystallizer.

5. ON-LINE SPC OF SUGAR CRYSTALLISATION

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 CSD values out of the specification range.

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 'crystallisation' phase and the 'tightening' phase. The initial operations before seeding (charging and concentration) were excluded from the analysis because their main 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 flow valve. Thus in the available data set there are periods where the feed flowrate is equal to zero. Building a statistical model based on this data set results in the model being trained on data where the feed flow rate is zero. However if for a new batch, process conditions force operators to open the feed valve 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 (the brix in the solution and the supersaturation) included in the data set. A calculated variable (supersaturation) was also included as a critical sugar crystallisation parameter.

On-line Univariate SPC

On-line univariate SPC was applied to the tree batches identified as out of specification. Only Batch 2 (not depicted in the figure) was clearly detected as out-of-spec. Fig.1 shows the most significative variables for out-of-spec Batch 1 along with univariate, $\pm 3\sigma$, control limits. Note that the variables lie within the univariate control limits for most of the batch run. Those observations that lie out with the limits, for example time point 89 in Fig. 1a, are still close to the limits and thus it is concluded that they are spurious signals, i.e. on average one in hundred observations will lie outside the 99% action limits. As a result, the Batch 1 would be classified by this method as good. Thus, the univariate SPC cannot detect reliably periods of out-of-spec operation.

On-line multivariate SPC

The TVSS approach presented in section 4 and the multivariate SPC techniques of MWPCS, BOL, and BDPCA discussed in section 3 were then used to 'monitor' the real process data. 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 for out-of-spec Batch 1 are summarised in Fig.2 to Fig.5. T^2 statistics are shown alongside their corresponding contribution plots. The contribution plots shows the contribution of the original seven process variables to the maximum out of control value. 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 exceeds the limits can be quantified.

In general it was observed that the four methods identify periods of out-of-specification operation during the run in all three batches (not depicted in the figures) for the T^2 control charts. Thus by applying multivariate SPC as opposed to univariate SPC,

periods of out-of-specification operation can be detected.

In Fig. 2a, 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. 1a) and the temperature of the solution (Fig. 1c) move outside the limits for these time points. In the multivariate T^2 control chart, out-of-spec operation is detected earlier and takes its maximum value at time point 89. The T^2 contribution plot for time point 89 (Fig.2b) 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 of Batch 1, applying BDPCA (Fig. 3a), BOL (Fig.4a) and TVSS (Fig. 5a), provided maximum T^2 out-of-control signals for the time period around point 345. Univariate SPC provides an out-of-control signal for the brix of the solution for this time period (Fig.1b). 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. 5b) 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. 3b) and BOL (Fig. 4b) also indicate that the brix of the solution is mainly responsible for the out-of-control signal.

The four multivariate monitoring techniques of MWPCS, BOL, 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.1d, 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.1b) 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 plot (Fig. 5b) and an alarm signal generated by the monitoring scheme is justified.

5. CONCLUSIONS

A novel modelling approach was proposed to model an industrial sugar crystallization fed-batch process using a time varying state space (TVSS) model. 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 TVSS methodology was compared with current state-of-the-art monitoring schemes as Moving Window Principal Component Analysis (MWPCA), Batch Dynamic Principal Component Analysis (BDPCA) and Batch Observation Level (BOL). 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. However, the results obtained demonstrate the superior performance of the TVSS approach to successfully detect abnormal events and periods of out-of-spec operation. 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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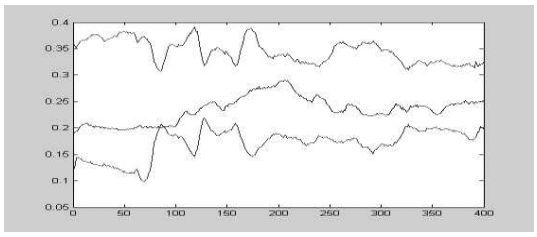
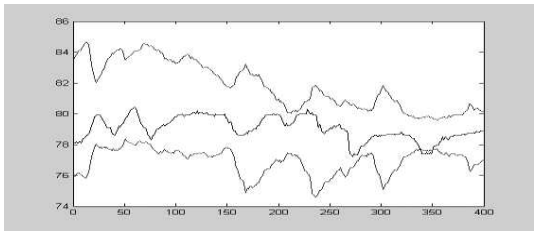
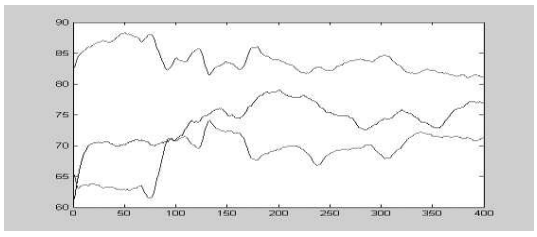
Wold, S., N. Kettaneh, H. Friden & A. Holmberg (1998). Modelling and Diagnostics of Batch Processes and Analogous Kinetic Experiments. *Chemometrics and Intel Lab Systems* **44**, 331.



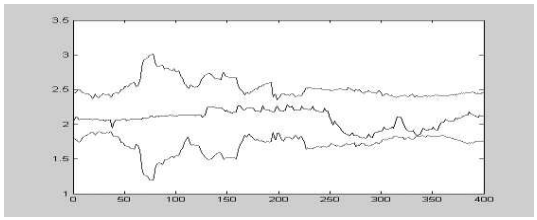
a) Vacuum Pressure



b) Brix of the solution

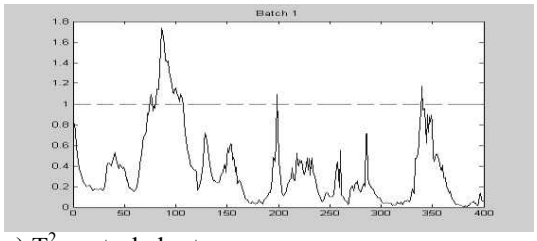


c) Temperature of the solution

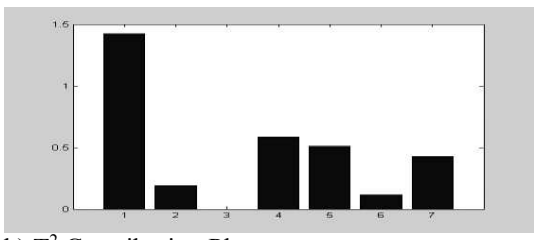


d) Steam pressure

Fig.1 Time series plots (bold line) and control limits of bad Batch1

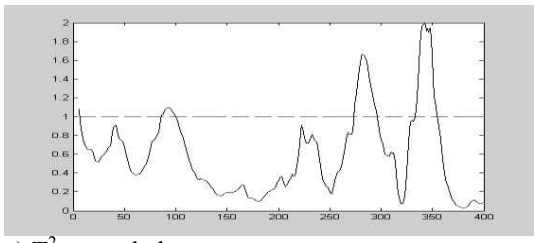


a) T^2 control chart

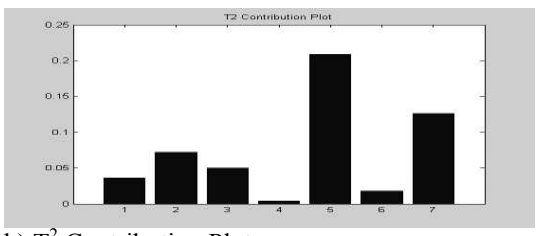


b) T^2 Contribution Plot

Fig.2 MWPCA on-line monitor. for out-of-spec Batch1

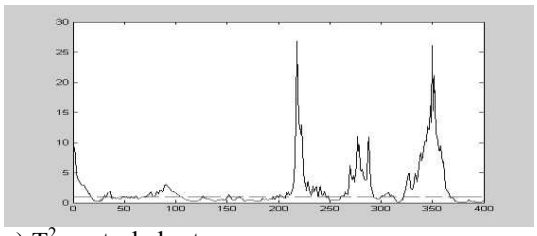


a) T^2 control chart

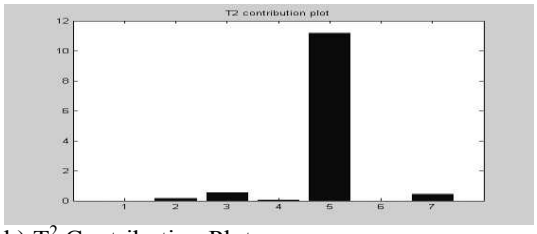


b) T^2 Contribution Plot

Fig.3 BDPA on-line monitor. for out-of-spec Batch1

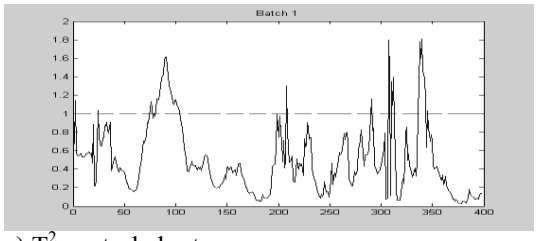


a) T^2 control chart

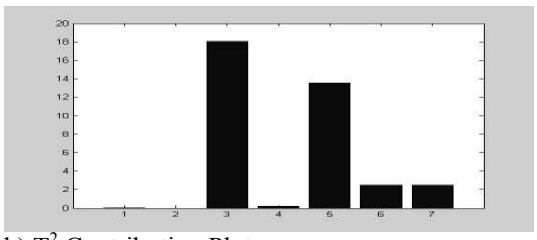


b) T^2 Contribution Plot

Fig.4 BOL on-line monitoring for out-of-spec Batch1



a) T^2 control chart



b) T^2 Contribution Plot

Fig.5 TVSS on-line monitoring for out-of-spec Batch1