SEMI-BATCH TRAJECTORY CONTROL IN REDUCED DIMENSIONAL SPACES

Jesus Flores-Cerrillo and John F. MacGregor

Department of Chemical Engineering, McMaster University,
Hamilton, Ontario, Canada, L8S4L7

Abstract: A novel inferential strategy for controlling end-product quality properties using complete trajectories of manipulated variables is presented. Control through complete trajectory manipulation using empirical models only is possible by controlling the process in the reduce space (scores) of a latent variable model rather than in the real space of the manipulated variables. Model inversion and trajectory reconstruction is achieved by exploiting the correlation structure in the manipulated variable trajectories captured by a Partial Least Squares (PLS) model. The approach is illustrated with a condensation polymerisation example for the production of nylon. The data requirements for building the model are shown to be modest.

Keywords: Batch control, Partial Least Squares, Statistical process control, Condensation polymerisation, Reduced space control, Trajectory control.

1. INTRODUCTION

Batch/semi batch processes are commonly used because their flexibility to manage many different grades and types of products. In these processes, it is necessary to achieve tight final quality specifications. However, this is not easily achieved because batch operations suffer from constant changes in raw material properties, variations in start-up initialisation, and in operating conditions, all of which introduce disturbances in the final product quality. Moreover, compensating for these disturbances is difficult due to the non-linear behaviour of the chemical reactors and to the fact that robust on-line sensors for quality variable monitoring are rarely available.

Several approaches based on complex theoretical models and computationally intensive control strategies have been presented to control quality properties in batch processes (Kozub, 1989.) However, these strategies are difficult to implement because they require almost perfect model knowledge. Empirical modelling, on the other hand, has the advantage of using information routinely collected and of ease in model building. Yabuki and MacGregor, (1997) used empirical models for the control of product quality-properties. However, control action was restricted to only a few movements in the manipulated variables (injection of reactants) due to effective control action can only be applied at certain reaction stages.

In batch operation is not uncommon to find processes in which the quality properties must be controlled by adjusting several manipulated variables trajectories (MVT) through most of the duration of the process (for example, reactor temperature or pressure). In this case, the conventional approach is to coarsely segment the MVT into a few intervals or decision points (usually 5-10) and characterize them by slope and level (stair-case parameterisation, Russell et al., 1998). Therefore, in controlling a new batch, only the level and/or the slope of such intervals need to be adjusted because it is assumed that the MVT remains constant (same level/slope) until the next decision point. In this form, the number of parameters to be estimated from identification experiments remains relatively small. Studies involving this type of parameterisation can be found in Russell et al., (1998), and Lee, et al., (2001) among others. However, if fine trajectory segmentation is required or if smoother MVTs need to be implemented, a much more comprehensive experimental design need to be performed to allow for an adequate identification of the effect of MV's on the controlled variables over the entire batch trajectory. Moreover, model inversion would be usually difficult because a large number of highly correlated control actions need to be determined at every decision point. A solution to this dilemma is to project such highly correlated process trajectories (MVT and measurements) into lower-dimensional spaces and to perform the control computation in the reduced dimension space. By projecting the original correlated trajectories into a lower dimension we are obtaining a few orthogonal variables that summarizes the original information. In this form, the model parameter estimation is more efficient and the control computation easier. In spite of the inherent advantages in controlling the MVT's of batch processes in the latent variable space, no literature has yet addressed this issue.

Statistical controllers for continuous processes based on Principal component analysis (PCA) have been proposed (Cheng and McAvoy, 1996; Chen et al., 1998), which also express the control objective in the score space of the PCA model. However, the approach taken here is different.

The purpose of this study is to introduce a novel inferential control strategy that allows a much finer characterization and smoother reconstruction (model inversion) of manipulated variable trajectories than those obtained using staircase parameterisation, without increasing the complexity and number of identification experiments needed for model building. These objectives are made possible by formulating the control strategy in the reduced dimensional space of a latent variable model, and then using the model to invert the solution for the MVT's. The contents of this work are as follow: in section 2 the methodology is introduced; in section 3, the control approach is illustrated with a condensation polymerisation case study for the production of nylon 6,6. In section 4, conclusions are drawn.

2. CONTROL METHODOLOGY

2.1 Model building

The proposed methodology uses historical-data bases and a few complementary identification experiments for model building. The empirical model is obtained using Partial Least Squares (PLS). However, other projection methods such as principal component regression may also be applied.

The database from which the PLS model is identified consists of a regressor matrix ($\mathbf{X}$) composed of k row vectors ($\mathbf{x}^T$) of on-line process variable trajectories ($\mathbf{x_{on}}$) and possibly off-line measurements ($\mathbf{x_{off}}$), collected occasionally through the batch, $\mathbf{x_m^T} = [\mathbf{x_{on}^T} \quad \mathbf{x_{off}^T}]$, full manipulated variable trajectories (MVT) $\mathbf{u_c}$, and the matrix ($\mathbf{Y}$) of quality properties measured at the end of the batch. Full MVT's are obtained through trajectory segmentation as illustrated in Figure 1. In this Figure is shown that the MVT's are finely segmented and that decision points (θ_i, i=1,2,…), where control action is taken, are chosen. Notice that the segment size is not necessarily uniform and that decisions points may be chosen arbitrarily. (However, the decision points will usually be selected using prior process knowledge.) In the limit, control action can be taken at every segment (i.e. every segment would represent a decision point).

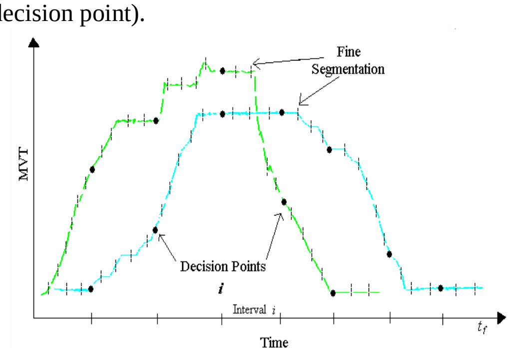

Fig. 1. Fine segmentation of MVT and decision points.

Linear PLS regression is performed by projecting the mean centered and scaled variables onto lower dimensional subspaces:

$$\begin{aligned}\mathbf{X} &= \mathbf{TP^T} + \mathbf{E} \\ \mathbf{Y} &= \mathbf{TQ^T} + \mathbf{F}\end{aligned} \qquad (1)$$

where $\mathbf{T}$ are new latent variables $\mathbf{T{=}XW^*}$ that capture most of the data variability, $\mathbf{P^T}$ is the loading matrix, and $\mathbf{E}$ and $\mathbf{F}$ are residual matrices. Non-linear PLS regression can also be used (Flores-Cerrillo, 2003). However, for simplicity, through this presentation linear models will be assumed.

The control methodology used in this work consists of two stages: 1) at predetermined decision times (θ_i, i=1,2,…) an inferential end-quality prediction using on-line and possible off-line process measurements ($\mathbf{x_m}$) and the MVT's ($\mathbf{u_c}$) up to the current time is performed to determine whether or not the controlled end-qualities ($\mathbf{y}$) fall outside a non-control region, and if needed, 2) model inversion to obtain tne modified MVT for the remainder of the batch that will yield the desired final qualities. This two-stage procedure is repeated at every decision point (θ_i) using all available measurement and MVT's information up to that time. The novelty of the proposed approach is that the model inversion stage is performed in the reduced dimensional space (latent variable or score space) of a PLS model rather than in the real space of the MVT's. Due to the high correlation of measurements and control actions, the true dimensionality of the process, determined in the score variable space (t_a, a=1,2,…,A) of the PLS model, is generally much smaller than the number of manipulated variables points obtained from the MVT segmentation ($\mathbf{u_c}$). Therefore, the control computation performed in the reduced latent variable space ($\mathbf{t}$) is much simpler than that performed in the real space. In the following the control methodology is described for one control decision point during the batch. This is repeated at each future decision point.

2.2 Prediction

For on-line end-quality estimation ($\hat{\mathbf{y}}$), when a new batch k is being processed, at every decision point (θ_i, i=1,2,…) $0 \le \theta_i \le \theta_f$, there exists a regressor row vector $\mathbf{x}^T$ composed of, at least, the following variables

$$\mathbf{x}^T = [\mathbf{x}_{\text{m}}^T \quad \mathbf{u}_{\text{c}}^T] = \qquad (2)$$

$$[\mathbf{x}^T_{\text{m,measured}}, q_i \quad \mathbf{x}^T_{\text{m,missing}} \quad \mathbf{u}^T_{\text{c,implemented}}, q_i \quad \mathbf{u}^T_{\text{c,future}}]$$

The regressor vector $\mathbf{x}$ consists of 1) all measured variables ($\mathbf{x}_{\text{m,measured}}$) available up to time θ_i ($0 \le \theta \le \theta_i$), 2), unmeasured variables ($\mathbf{x}_{\text{m,missing}}$) not available at θ_i, but that will be available in the future ($\theta_{i+1} \le \theta \le \theta_f$), implemented control actions $\mathbf{u}_{\text{c,implemented}}$ ($0 \le \theta \le \theta_{i-1}$), and future control actions $\mathbf{u}_{\text{c,future}}$, ($\theta_i \le \theta \le \theta_f$) which will be determined through model inversion. Note that at the model building stage, the $\mathbf{x}_{\text{m,missing}}$ and $\mathbf{u}_{\text{c,future}}$ vectors are available for each batch.

To estimate whether or not the quality properties, for a new batch, will lie within an acceptable region, the prediction is performed considering $\mathbf{u}_{\text{c,future}} = \mathbf{u}_{\text{c,nominal}}$ (i.e. assuming that the remaining trajectory will be kept at their nominal conditions) using the PLS model:

$$\hat{\mathbf{t}}^T_{\text{present}} = [\mathbf{x}_{\text{m}}^T \quad \mathbf{u}_{\text{c}}^T]\mathbf{W}^* = \qquad (3)$$

$$[\mathbf{x}^T_{\text{m,measured}}, q_i \quad \mathbf{x}^T_{\text{m,missing}} \quad \mathbf{u}^T_{\text{c,implemented}}, q_i \quad \mathbf{u}^T_{\text{c,n}}]\mathbf{W}^*$$

$$\hat{\mathbf{y}}^T = \hat{\mathbf{t}}^T_{\text{present}} \mathbf{Q}^{\mathbf{T}} \qquad (4)$$

W* and $\mathbf{Q}^{\mathbf{T}}$ are projection matrices obtained from the PLS model building stage (Geladi et al., 1986). $\hat{\mathbf{t}}_{\text{present}}$ is the projection of the $\mathbf{x}$ vector onto the reduced dimension space of the latent variable model (scores) at time θ_i, and $\hat{\mathbf{y}}$ is the vector of predicted end-quality properties. From the above equations, it can be noticed that changes in batch operation detected by process measurements ($\mathbf{x}_{\text{m}}$) or produced by changes in the MVT's ($\mathbf{u}_{\text{c}}$) would produce changes in the scores ($\hat{\mathbf{t}}_{\text{present}}$) and therefore in the end-quality properties (i.e. changes in the end-qualities can be detected through changes in the scores).

From equation (3), it can be noticed that in order to compute $\hat{\mathbf{t}}_{\text{present}}$ and $\hat{\mathbf{y}}$, it is necessary to have an estimate of the unknown future measurements ($\mathbf{x}_{\text{m,missing}}$) from ($\theta_{i+1} \le \theta \le \theta_f$). These can be obtained using efficient missing data algorithms available in the literature (Nelson et al., 1996). Alternatively, a multi-model approach in which a model is identified at every decision point can be used as discussed in Russell et al., (1998). The decision of one alternative over other depends on the number of decision points and/or performance of the missing data algorithm. In the example shown in this paper a single PLS model is used for control and the estimation of unknown future measurements is done by a missing data algorithm.

The non-control region can be determined in several ways, such as the one that takes into account the uncertainty of the model for prediction (Yabuki and MacGregor, 1997), from product specifications or from quality data under normal ("in-control") operating conditions. In this work a simple control region based on product quality specifications will be used (section 3).

If the quality prediction is outside the non-control region, then model inversion to obtain the MVT is needed. Obtaining of the full MVT consist of two stages: 1) Computation of the deviation of the scores from the quality targets and 2) Model inversion to obtain the real MVT using the correlation structure of the PLS model. These two stages are explained in as follows.

2.3 Control Computation

At every decision point (θ_i), the distance that the scores need to be changed ($\Delta\mathbf{t}$) to track the end-qualities closer to their set-points ($\mathbf{y}_{\text{sp}}$) can be obtained by solving the linear quadratic regulator (5):

$$\min_{\Delta\mathbf{t}(q_i)} (\hat{\mathbf{y}} - \mathbf{y}_{\text{sp}})^{\mathbf{T}}\mathbf{Q}_1(\hat{\mathbf{y}} - \mathbf{y}_{\text{sp}}) + \Delta\mathbf{t}^{\mathbf{T}}\mathbf{Q}_2\Delta\mathbf{t} + l T^2$$

$$st \quad \hat{\mathbf{y}}^T = (\Delta\mathbf{t} + \hat{\mathbf{t}}_{\text{present}})^T \mathbf{Q}^{\mathbf{T}}$$

$$T^2 = \sum_{a=1}^{A} \frac{(\Delta t + \hat{t}_{present})_a^2}{s_a^2} \qquad (5)$$

$$\Delta\mathbf{t}_{\text{min}} \le \Delta\mathbf{t} \le \Delta\mathbf{t}_{max}$$

where $\Delta\mathbf{t}^T = \mathbf{t}^T - \hat{\mathbf{t}}^T_{\text{present}}$, $\mathbf{Q}_1$ is a diagonal weighting matrix, $\mathbf{Q}_2$ is a movement suppression matrix, T^2 is the Hotelling's statistic, s_a^2 is the variance of the score t_a, and λ is a weighting factor. Hard constrains in the adjustment to the scores ($\Delta\mathbf{t}_{\text{min}} \le \Delta\mathbf{t} \le \Delta\mathbf{t}_{\text{max}}$) are problem dependent and may or may not need to be included.

Equation (5) is a quadratic programming problem that can be restated as:

$$\min_{\Delta\mathbf{t}(q_i)} \frac{1}{2}\Delta\mathbf{t}^{\mathbf{T}}\mathbf{H}\Delta\mathbf{t} + \mathbf{f}^{\mathbf{T}}\Delta\mathbf{t} \qquad (6)$$

where

$$\mathbf{H} = \mathbf{Q}^{\mathbf{T}}\mathbf{Q}_1\mathbf{Q} + \mathbf{Q}_2 + \mathbf{Q}_3$$

$$\mathbf{f}^{\mathbf{T}} = (\mathbf{Q}\hat{\mathbf{t}}_{\text{present}})^{\mathbf{T}}\mathbf{Q}_1\mathbf{Q} + \hat{\mathbf{t}}^T_{\text{present}}\mathbf{Q}_3 \qquad (7)$$

$$\mathbf{Q}_3 = \text{diag}\left[l / s_a^2 \right]$$

and whose interpretation is given in Figure 2 for a two dimensional space. As can be seen in this Figure, the aim of equations (6-7) is to reduce the distance of $\hat{\mathbf{t}}_{\text{present}}$, by an amount D**t**, to get closer to the score value corresponding to the quality set-points

($\mathbf{t_{sp}} = (\mathbf{Q^T Q})^{-1}\mathbf{Q^T y_{sp}}$). Due to the movement suppression matrix ($\mathbf{Q_2}$) and/or λ, the achieved **t** may not achieve $\mathbf{t_{sp}}$, but will be closer to it. If we desire to obtain the D**t** that would force the calculated $\mathbf{t}^T = \mathbf{t}_{\mathbf{sp}}^T$, we could use a minimum-variance like controller. Under this situation equation (5), with $\mathbf{Q_2}$=**I** and λ=0, can be restated as:

$$\min_{\Delta \mathbf{t}(q_i)} \Delta \mathbf{t^T} \Delta \mathbf{t} \qquad (8)$$
$$st \quad \mathbf{y_{sp}}^T = (\Delta \mathbf{t} + \hat{\mathbf{t}}_{\mathbf{present}})^T \mathbf{Q^T}$$

and whose solution can be easily obtained as:

$$\Delta \mathbf{t}^T = (\mathbf{y_{sp}}^T - \hat{\mathbf{t}}^T_{\mathbf{present}} \mathbf{Q^T})(\mathbf{QQ^T})^{-1}\mathbf{Q} = \mathbf{t}^{\mathbf{T}}_{\mathbf{sp}} - \hat{\mathbf{t}}^{\mathbf{T}}_{\mathbf{present}} \mathbf{Q^T}(\mathbf{QQ^T})\mathbf{Q} \qquad (9)$$

If we consider **y** to be deviations from $\mathbf{y_{sp}}$, then $\mathbf{t_{sp}}$=**0** and the last equation is reduced to:

$$\Delta \mathbf{t}^T = -(\hat{\mathbf{t}}^T_{\mathbf{present}} \mathbf{Q^T})(\mathbf{QQ^T})^{-1}\mathbf{Q} \qquad (10)$$

A detuning factor (d) may be included for this minimum-variance like controller to achieve some robustness against model error:

$$\Delta \mathbf{t}^T = -\boldsymbol{\delta}(\hat{\mathbf{t}}^T_{\mathbf{present}} \mathbf{Q^T})(\mathbf{QQ^T})^{-1}\mathbf{Q} \qquad (11)$$

where **0**≤d≤**1**. Δ**t** is computed at every decision point (θ_i).

Notice that the matrix $\mathbf{QQ^T}$ has dimension $m \times m$ (*m* being the number of quality properties). Therefore, in order to do not have an ill-conditioned matrix inversion, the quality properties should not be highly correlated. This poses no problem since one can always perform a PCA on the **Y** quality matrix to obtain a set of orthogonal variables (t) that can be used as new controlled variables, or perform selective PCA (Jackle and MacGregor, 1998) on the **Y** matrix to determine the best independent subset of quality variables to be controlled. Removal of a high correlated *y* variable should not be detrimental to its control since, by controlling the other quality variables, that quality variable will also be controlled.

2.4 *Inversion of PLS model to obtain the MVT's*

Once the low dimensional (*1*×*A*) vector D**t** is computed via one of the control algorithms in the last section, it remains to reconstruct from it, the high dimensional trajectories for the future process variables ($\mathbf{x_{m,missing}}$) and for the future manipulated variables ($\mathbf{u_{c,future}}$) over the remainder of the batch. These future trajectories can be computed from the PLS model (1) in such a way that their covariance structure is consistent with past operation. If there were no additional restrictions on the trajectories, such as might exits for a control action at θ=0, then the model for the X-space can be used directly to compute the **x** vector trajectory for the entire batch (Jaeckle and MacGregor, (1998)) as:

$$\Delta \mathbf{x}^T = [\Delta \mathbf{t}^T]\mathbf{P^T} \qquad (12)$$

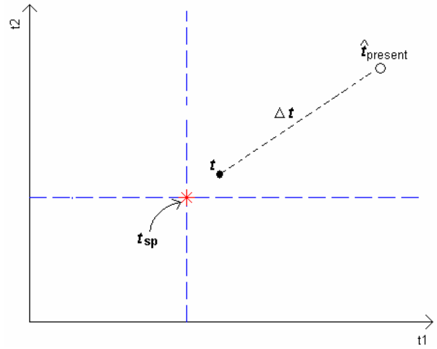

Fig. 2. Control in the reduce space (score control).

However for control intervals at times θ_i >0, there already exits observed trajectories for the interval 0 ≤ θ <θ_i, for the measured process variables ($\mathbf{x_{m,measured}}$) and for the already implemented manipulated variables ($\mathbf{u_{m,implemented}}$) that must be respected when computing their trajectories for the remainder of the batch (θ_i ≤ θ ≤θ_f). From equation (3) it can be seen that the changes in the score vector, D**t**, is related to the changes in the nominal trajectories according to:

$$\Delta \mathbf{t}^T = [\Delta \mathbf{x}^T]\mathbf{W}^* = [\Delta \mathbf{x}^T_{\mathbf{m,measured}} \quad \Delta \mathbf{u}^T_{\mathbf{c,implemented}} \quad \Delta \mathbf{x}^T_{\mathbf{m,missing}} \quad \Delta \mathbf{u}^T_{\mathbf{c,future}}]\mathbf{W}^* \qquad (13)$$

If one is currently at decision time θ_i, then clearly $\Delta \mathbf{x_{m,measured}} = \mathbf{0}$ and $\Delta \mathbf{u_{m,implemented}} = \mathbf{0}$, and the remaining trajectories to be computed for $\theta_i \le \theta \le \theta_f$ (i.e. $\Delta \mathbf{x_{m,missing}}$ and $\Delta \mathbf{u_{c,future}}$) should satisfy the following relation:

$$\Delta \mathbf{t}^T = [\mathbf{0}^T \quad \mathbf{0}^T \quad \Delta \mathbf{x}^T_{\mathbf{m,missing}} \quad \Delta \mathbf{u}^T_{\mathbf{c,future}}]\mathbf{W}^* = [\mathbf{0}^T \quad \Delta \mathbf{x}^T_2]\begin{bmatrix}\mathbf{W}_1^* \\ \mathbf{W}_2^*\end{bmatrix} \qquad (14)$$

where $\Delta \mathbf{x}^T_2 = [\Delta \mathbf{x}^T_{\mathbf{m,missing}} \quad \Delta \mathbf{u}^T_{\mathbf{c,future}}]$ is the vector representing the change in future measurements and remaining MVT (θ_i ≤ θ ≤θ_f), and $\mathbf{W}_2^*$ its corresponding projection matrix. Then,

$$\Delta \mathbf{t}^T = [\Delta \mathbf{x}^T_2]\mathbf{W}_2^* \qquad (15)$$

Furthermore, in order for the MVT and missing values to keep their correlation structure according to the PLS model (equation 12) the following condition must hold:

$$\Delta \mathbf{x}^T_2 = \boldsymbol{\alpha}^T \mathbf{P}_2^{\mathbf{T}} \qquad (16)$$

This ensures that the relationship among all the process and manipulated variables trajectories that are being computed, will respect the nature of those trajectories in the data used to build the PLS model.

a can be estimated by substituting (16) in (15) according to:

$$\Delta \mathbf{t}^T = (\boldsymbol{\alpha}^T \mathbf{P}_2^{\mathbf{T}})\mathbf{W}_2^*$$
$$\boldsymbol{\alpha}^T = \Delta \mathbf{t}^T (\mathbf{P}_2^{\mathbf{T}} \mathbf{W}_2^*)^{-\mathbf{1}} \qquad (17)$$

and by substituting (17) in (16), the MVT are obtained (θ_i ≤ θ ≤θ_f):

$$\Delta \mathbf{x}^T_2 = \Delta \mathbf{t}^T (\mathbf{P}_2^{\mathbf{T}} \mathbf{W}_2^*)^{-\mathbf{1}} \mathbf{P}_2^{\mathbf{T}} \qquad (18)$$

It is easy shown that this reduces to the relationship in (12) when θ_i =0 where there are no previous trajectory measurements or manipulated variables.

The final control algorithm, in the case of linear models and no constrains, is obtained by substituting (11) in (18):

$$\Delta \mathbf{x}_2^T = -\delta(\hat{\mathbf{t}}_{\mathbf{present}}^T \mathbf{Q}^{\mathbf{T}})(\mathbf{Q}\mathbf{Q}^{\mathbf{T}})^{-1}\mathbf{Q}(\mathbf{P}_2^{\mathbf{T}}\mathbf{W}_2^{*})^{-1}\mathbf{P}_2^{\mathbf{T}} \quad (19)$$

This inferential algorithm (19) is then repeated at every decision point (θ_i) until completion of the batch. Inversion of the ($A \times A$) matrix $\mathbf{P}^{\mathbf{T}}\mathbf{W}^{*}$ is nearly always well conditioned.

3. SIMULATION STUDIES

In the batch condensation polymerisation of nylon 6,6 the end product properties are affected by disturbances in the water content of the feed. In plant operation feed water content disturbances occurs because a single evaporator usually feeds several reactors (Russell et al., 1998). The non-linear model used in this work for data generation and model performance evaluation was developed by Russell et al., (1998). For a complete description of the model, and model parameters the reader is referred to the original publication.

Russell et al., (1998) studied this system and proposed several control strategies including conventional control (PID and gain schedule PID), non-linear model based control and empirical control based in linear state-space models. In their data-base approach, control of the system is achieved by reactor and jacket pressure manipulation. These two manipulated variables were segmented and characterised by slope and level (stair-case parameterisation) leading to 10 control variables. A total of 7 intervals (decision points) were used. The empirical state space model was identified from 69 batches arising from an experimental design. Several differences between the control strategy used by Russell et al., and the one proposed here can be noticed, the two most important being that: (*i*) the control is computed in the reduce latent variable space rather than in the real space of the MVT's, and that (*ii*) a much finer MVT reconstruction is achieved without increasing the complexity and number of experiments to be used in model building.

Control objectives and Trajectory segmentation.
The control objective is to obtain nylon 6,6 with an end-amine concentration (NH_2) of 49.33 and number averaged molecular weight (MWN) of 13533 (total reaction time 200 min), when the system is affected by changes in the initial water content (W). The MVT's used to control the end-qualities are the jacket and reactor pressure trajectories. These trajectories are finely segmented every 5 min. starting at 35 min. (of the beginning of the reaction) until 30 min. before the completion of the batch, giving a total of 40 control variables. Two control decision points at 38 and 75 min. were found to be necessary to yield adequate control for the conditions used in this example. In order to predict NH_2 and MWN, on-line measurements of the reactor temperature (Tr) and venting (v) are considered available every two minutes.

Data Generation: In the example that follows, a PLS model with 5 latent variables (determined by cross-validation) was built from a data set consisting of 15 batches in which *W* was randomly varied and 30 batches in which some movement in the MVT (at the two decision points) was performed (some of this data set may be available from historical data). However, adequate control performance has been achieved using only a total of 15 batches (Flores-Cerrillo, 2003).

3.1 Results

To illustrate the control performance of the algorithm, some results are presented. The first step is to determine if the prediction of the PLS model at the decision points is adequate. In Figure 3, the final qualities are shown for the case in which the water content randomly varies for 15 batches in the range of ±10%. The end quality property prediction should be performed at every decision point to determine if the next control action should be implemented or not. In Figure 3 prediction results at 38 min are shown. As can be seen in this figure, the predicted quality properties (□) using the PLS model are in good agreement with the observed values (o). Slight improvement in the predictions at high MWN and NH_2 values could be obtained with a non-linear PLS model (Flores-Cerrillo, 2003). However, the linear PLS model is very good in the target region (mid-values) and adequate in the extremes.

In Figure 4 is shown the performance of the controller algorithm (equation 19 with d=1.0) to the end-properties when the process is affected by the disturbances in the initial water concentration discussed above. In this Figure (o) represents what would happen if control action were not taken and (□) the qualities obtained after control is performed. As can be seen in this Figure, the proposed control scheme tracks on target all bad batches (inside the dotted box of quality specifications). Figure 5a and 5b show the jacket and reactor pressure MVT respectively for runs 1 and 15 together with their nominal conditions.

4. CONCLUSIONS

A novel control strategy for final product quality control in batch and semi-batch processes is proposed. The strategy recomputes on-line the entire remaining trajectories for the MV's at several decision points. However, in spite of the fact that the resulting controller consist of high dimensional manipulated variable trajectories (MVT's) the control algorithm involves only the solution for a small number of latent variables in the reduced dimensional space of a PLS model. The strategy uses empirical PLS models identified from historical data and a few complementary experiments. The strategy is illustrated using a simulated condensation polymerisation process. Since smooth and continuous MV trajectories can be obtained, the approach seems well suited for use in processes and mechanical systems (robotics) where such smooth changes in the MV's are desirable.

5. ACKNOWLEDGMENTS

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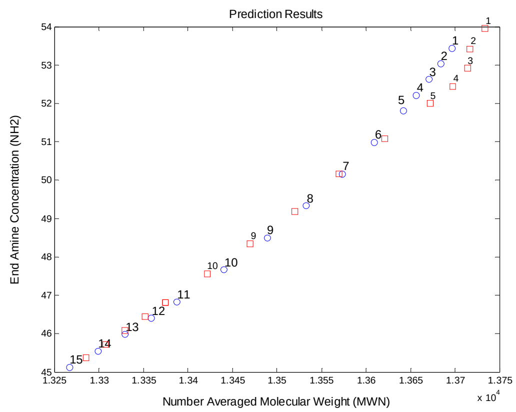


Fig. 3. Observed (o) and predicted (□) end-quality properties using PLS model.

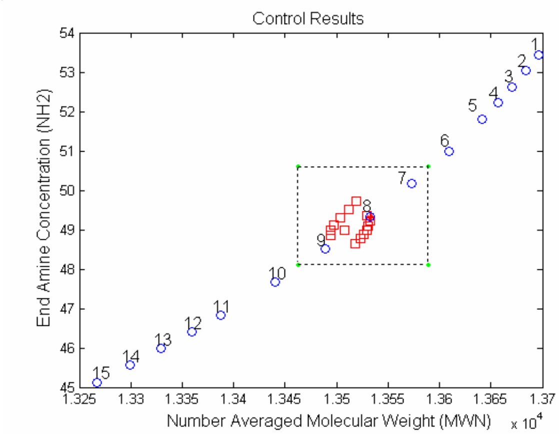
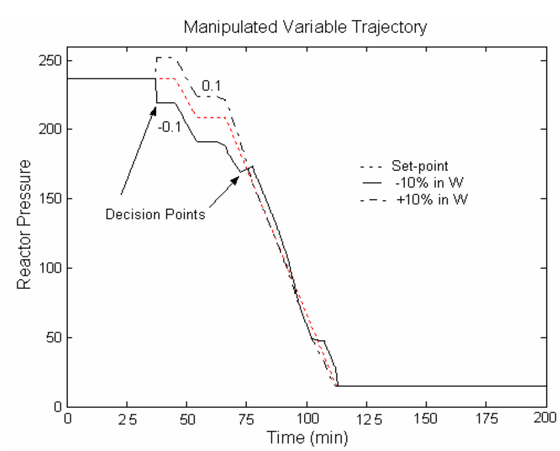
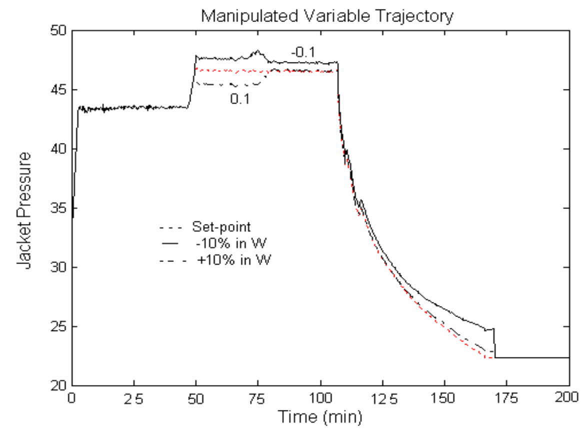


Fig. 4. Control results. (o) End-quality properties without control and (□) after control is taken.



a)



b)

Fig. 5a, 5b. Manipulated Variable Trajectories. (- - -) set-point, (—) when the disturbance is –10% in W, and (- – -) when disturbance is +10% in W. Reaction time 200min.

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