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Trajectory tracking of batch product quality using intermittent measurements and moving window estimation

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***Abstract*—In order to meet tight product quality specifications for batch/fed-batch processes, it is vital to monitor and control batch product quality throughout the batch duration. The ideal strategy is to control batch product quality through trajectory tracking of a desirable batch product quality evolution during the batch run. However, due to the lack of in-situ sensors for continuous measurements of batch product quality, the measurement of batch product quality is usually implemented by laboratory assay of samples and thus these measurements are generally intermittent. Therefore direct trajectory tracking of batch product quality is not feasible for such scenarios with intermittent measurements. This paper proposes an approach to use intermittent measurements to realize trajectory tracking control of batch product quality through moving window estimation. The first step of the approach is to identify a partial least squares (PLS) model using intermittent measurements to relate process variable trajectories and batch product quality. Then the identified PLS model is further applied to predict product quality trajectory during the batch run so as to realize trajectory tracking of a desirable product quality evolution. An example from fed-batch fermentation for penicillin production is used to illustrate the principle and the effectiveness of the proposed approach.**

I. Introduction

Batch processes are widely used in industry for manufacturing low-volume and high-value added products such as specialty chemicals, polymers and pharmaceuticals [1]. The popularity of batch operation in industry has two main reasons [2]: one is that batch processes are easier to set up and operate with the possibility of continuous improvements from earlier batch runs; the other is that batch operation is more efficient than continuous operation for frequent product changes and the production of small quantities with little or no hardware modification at all, which is especially attractive for starting commercial productions of novel materials to recover research and development costs before competing products affect prices.

The ultimate task for batch processes is to ensure consistent and desirable batch end-product quality for each batch run. This is not easy to fulfil in practice as batch processes are usually complex physical-chemical processes with time-varying and nonlinear dynamics. Furthermore, there still lack reliable in-situ sensors to monitor batch product quality during the batch run. Batch-to-batch variations resulting from changes to raw material properties and operating conditions also render robust control of batch end-product quality even more challenging. Many process monitoring and control schemes have been proposed in the literature to confront the issues encountered in batch operations [3], [4], [5], [6], [7]. Initial studies for the control of batch processes were based on mechanistic process models and traditional control methods [8], [9], [10], [11], [12], [13]. However, the identification of an accurate mechanistic model for a batch process is often difficult and time-consuming. Therefore multivariate statistical process control methods, which are based on process history data to develop empirical models, become a popular technique for modern process monitoring and control [14], [1], [15], [4], [16], [7], [17]. Among them, multi-way principal components analysis (PCA) and multi-way projection to latent structures (PLS), which are the extensions of PCA and PLS, enabling them handle three-dimensional matrices, are most widely used [18], [19], [20], [21], [7].

Using latent variable models such as multi-way PCA and PLS, currently there are two control approaches for batch processes: batch end-product quality control and trajectory tracking. The typical batch end-product quality control approach is addressed in [19], [22], where a PLS model relates process variable trajectories to batch end-product quality. Manipulated variable trajectories (MVTs) are determined such that they minimize the difference between the predicted and the target batch end-product quality. Since there is no measurement of batch product quality during the batch running period, the effectiveness of the approach relies heavily on the accuracy of the identified PLS model. The typical trajectory tracking approach is addressed in [21], [7], where a PCA model is identified to model the process dynamics of all process variable trajectories and MVTs are deduced from feeding future process variable trajectories with the target trajectories. Due to the difficulty of on-line measurements of batch product quality during the batch run, the target trajectories are usually some key process variable trajectories such as temperature set-points rather than the target batch product quality trajectories and thus the assumption is that the batch end-product quality can be guaranteed if these key process variable trajectories follow their pre-determined set-points. However, such an assumption is not always true as the batch end-product quality can deteriorate in the case of disturbances even if the pre-determined process variable trajectories are perfectly tracked.

Although batch product quality cannot typically be measured continuously along with other process variables due to the lack of in-situ sensors for quality measurement, it can often be measured intermittently through laboratory assay of samples taken during the batch run. Making use of the intermittent measurement data, a PLS model can be identified according to the method proposed in [5], where a series of created pseudo batches are synchronized to their batch endpoints and a PLS model is identified upon the synchronized pseudo batch data. The identified PLS model can further be applied to predict future batch product quality trajectories using moving window estimation. Thus it is possible to realize trajectory tracking of a pre-determined product quality trajectory directly rather than trajectory tracking of other process variable trajectories for a new batch run.

This paper proposes a practical approach to realize trajectory tracking control of batch product quality using intermittent measurements and moving window estimation. The paper is organized as follows: Section 2 details the methodology of the proposed trajectory tracking control of batch product quality; a case study of penicillin fermentation is described in Section 3; some conclusions and remarks are provided in Section 4.

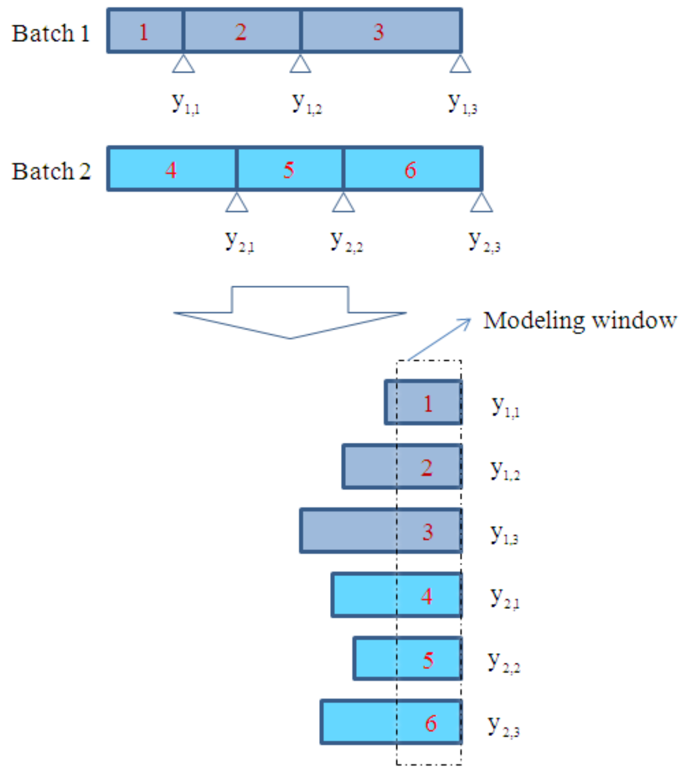

Fig. 1. Model building using intermittent measurements

II. Trajectory Tracking Control of Batch Product Quality

In order to realize trajectory tracking control of batch product quality using intermittent measurements and moving window estimation, three steps are to be fulfilled: the first step is to identify a PLS model using intermittent quality measurements and a PCA model without any data from intermittent quality measurements; the second step is to predict future quality trajectories using the identified PCA&PLS models and the strategy of moving window estimation; and the third step is to compute the MVTs and implement them in a receding horizon manner. These three steps are to be described in detail in the following subsections.

A. Model identification

For PLS, process variables are divided into two groups: the predictor values such as measured process variable trajectories and manipulated variable trajectories; the response values such as measured batch product quality variables. The method for identifying the PLS model using intermittent measurements is similar to the approach proposed in [5], where pseudo batches are created at those measurement points and they are further aligned toward their end-points for identifying the PLS model based on a selected modeling window.

Taking two batches shown in Figure 1 as an example, each batch has three intermittent measurements for product quality during the batch run. Therefore a total of six pseudo batches are created and they are aligned toward their end-points as shown in Figure 1. Then a modeling window is selected to identify the PLS model with the intermittent measurements as the response values and all other process variable measurements including the manipulated variables as the predictor values. The predictor and response values are generally three-dimensional matrices of size $I \times J \times K$, where I is the number of pseudo batches for which data are available, J is the number of variables that are measured and K is the number of samples collected during the time period of the modeling window. These three dimensional matrices of data can be unfolded in a batch-wise way to model differences among batches [7]. The batch-wisely unfolded data are further mean-centered and scaled to be unit variance and performing PLS on the obtained data results in a latent variable model of the form:

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

$$\mathbf{Y} = \mathbf{U}\mathbf{Q}^T + \mathbf{F}, \tag{2}$$

where $\mathbf{X}$ is a matrix of $I \times J_x K_x$ for the predictor variables, $\mathbf{Y}$ is a matrix of $I \times J_y K_y$ for the response variables, $\mathbf{P}$ of $J_x K_x \times A$ and $\mathbf{Q}$ of $J_y K_y \times A$ are the loading matrices, respectively. Here A is the number of latent variables. The scores $\mathbf{T}$ and $\mathbf{U}$ are related by a diagonal matrix $\mathbf{B}$ of proper dimensions with $\mathbf{U} = \mathbf{TB}$. $\mathbf{T} = \mathbf{XW}(\mathbf{P}^T\mathbf{W})^{-1}$, where $\mathbf{W}$ is the weight matrix. Finally, $\mathbf{E}$ and $\mathbf{F}$ are residual matrices. In practice, the PLS model is often expressed as a predictive model relating the predictor variables and the response variables directly [23]:

$$\mathbf{Y} = \mathbf{XW}(\mathbf{P}^T\mathbf{W})^{-1}\mathbf{B}\mathbf{Q}^T + \mathbf{F}^*, \tag{3}$$

where $\mathbf{F}^*$ is a residual matrix.

Without considering the intermittent measurements for product quality variables, multi-way PCA can be identified instead to model the correlation structure for all predictor variables:

$$\mathbf{X} = \mathbf{T}_c \mathbf{P}_c^T + \mathbf{E}_c. \tag{4}$$

B. Moving window estimation

Once the PCA and PLS models have been identified from past batch data, they can be further used to predict future batch product quality for a new batch run through the strategy of moving window estimation. The principle of moving window estimation can be described in Figure 2, where the length of the modeling window for the identified PCA&PLS models is assumed to be l and the current time instant is θ_i. The first step for moving window estimation is to place the modeling window to cover the measured $l-1$ samples of predictor variables, which are $\mathbf{u}_{\theta_i - l+1 \to \theta_i - 1}$ for the manipulated variable $\mathbf{x}_{\theta_i - l+2 \to \theta_i}$ and for all other measured process variables. Assume that the future manipulated variable trajectory is known in advance, then the future process variables $\mathbf{x}_{\theta_i+1}$ can be estimated using the identified PCA model and missing data algorithms. Several missing data imputation methods have been proposed in the literature [24], [25]. The common idea of them is to make use of the underlying data pattern to deduce the missing part from the known part. Taking the missing data algorithm called Projection to the Plane as an example, the predictor variables $\mathbf{x}$ are grouped into two parts $\mathbf{x}^T = [\mathbf{x}^{*T} \mathbf{x}^{\sharp T}]$, where $\mathbf{x}^{*T} = [\mathbf{x}_{\theta_i - l+2 \to \theta_i}^T \;\; \mathbf{u}_{\theta_i - l+1 \to \theta_i}^T]$ contains the known data and $\mathbf{x}^\sharp = \mathbf{x}_{\theta_i+1}$ contains the missing data. The loading matrix $\mathbf{P}$ from the identified PCA model can also be grouped into two corresponding parts $\mathbf{P}_c^*$ and $\mathbf{P}_c^\sharp$. Then the missing data can be deduced from the optimal score vector $\hat{\tau}$, which is obtained from minimizing the following objective function [21]:

$$J = \frac{1}{2}(\mathbf{x}^* - \mathbf{P}_c^* \tau)^T (\mathbf{x}^* - \mathbf{P}_c^* \tau). \tag{5}$$

The optimal solution for Eq. (5) is $\hat{\tau} = (\mathbf{P}_c^{*T} \mathbf{P}_c^*)^{-1} \mathbf{P}_c^{*T} \mathbf{x}^*$ and thus the missing data $\mathbf{x}^\sharp$ can be deduced from it straightforwardly:

$$\mathbf{x}^\sharp = \mathbf{P}_c^\sharp \hat{\tau}. \tag{6}$$

Therefore the estimation of the future process variable $\mathbf{x}_{\theta_i+1}$, denoted as $\hat{\mathbf{x}}_{\theta_i+1}$, can be expressed as a function of the measured process variable trajectories $\mathbf{x}_{\theta_i - l+2 \to \theta_i}$ and the manipulated variable trajectories $\mathbf{u}_{\theta_i - l+1 \to \theta_i}$:

$$\hat{\mathbf{x}}_{\theta_i+1} = \mathbf{P}_c^\sharp (\mathbf{P}_c^{*T} \mathbf{P}_c^*)^{-1} \mathbf{P}_c^{*T} [\mathbf{x}_{\theta_i - l+2 \to \theta_i}^T \;\; \mathbf{u}_{\theta_i - l+1 \to \theta_i}^T]^T. \tag{7}$$

Using the estimated $\hat{\mathbf{x}}_{\theta_i+1}$ and the identified PLS model, the product quality at the time instant $\theta_i + 1$, denoted as $\hat{\mathbf{y}}_{\theta_i+1}$, can be predicted as follows according to Eq. (3):

$$\hat{\mathbf{y}}_{\theta_i+1} = [\mathbf{x}_{\theta_i - l+2 \to \theta_i}^T \;\; \hat{\mathbf{x}}_{\theta_i+1}^T \;\; \mathbf{u}_{\theta_i - l+1 \to \theta_i}^T] \mathbf{W} (\mathbf{P}^T \mathbf{W})^{-1} \mathbf{B} \mathbf{Q}^T. \tag{8}$$

After the process variable values and the product quality value at the time instant $\theta_i + 1$ have been estimated using

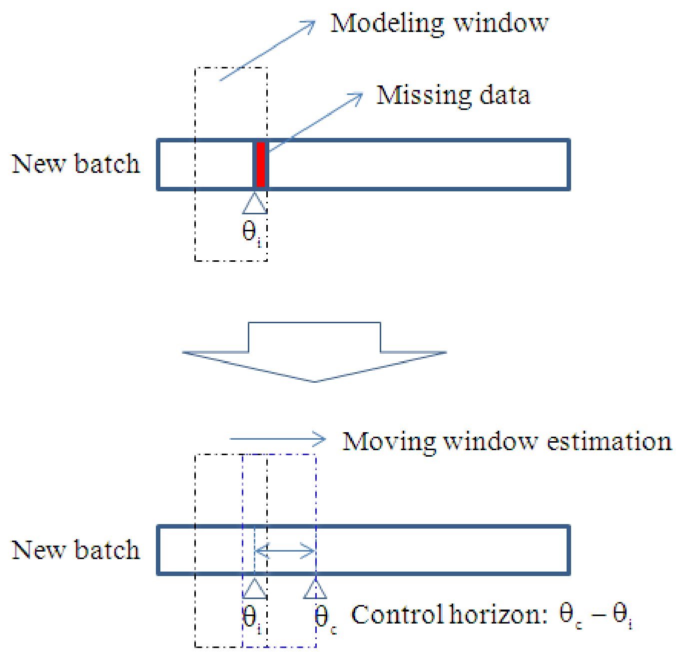

Fig. 2. Moving window estimation

the identified PCA&PLS models, the modeling window is to be moved forward as shown in Figure 2. Then the process variable values and the product quality value at the time instant $\theta_i + 2$ can be deduced in a similar way, where the value of $\mathbf{x}_{\theta_i+1}$ is assumed to be known in advance as the formerly estimated value $\hat{\mathbf{x}}_{\theta_i+1}$. The whole estimation process is repeated sequentially up to the end of the control horizon θ_c. So the estimated process variable trajectories $\hat{\mathbf{x}}_{\theta_i+1 \to \theta_c}$ and the estimated product quality trajectories $\hat{\mathbf{y}}_{\theta_i+1 \to \theta_c}$ can both be expressed as a function of the future manipulated variable trajectories $\mathbf{u}_{\theta_i \to \theta_c - 1}^T$.

C. Trajectory tracking control

The proposed trajectory tracking control is performed in a typical receding horizon manner: the future manipulated variable trajectories with the horizon of c are optimized to minimize the difference between the predicted future quality trajectory and the target future quality trajectory at each control decision point; the optimized future manipulated variable trajectories are implemented into the process up to the next control decision point and the whole process is repeated until the operation ends. Assume that the control decision point is at the current time instant θ_i and the target future quality trajectory is $\bar{\mathbf{y}}_{\theta_i+1 \to \theta_i+c}$, the predicted future quality trajectory $\hat{\mathbf{y}}_{\theta_i+1 \to \theta_i+c}$ can be obtained using moving window estimation. According to the moving window estimation procedure described in Eqs. (7-8), the predicted future quality trajectory $\hat{\mathbf{y}}_{\theta_i+1 \to \theta_i+c}$ can be illustrated as a function of the future manipulated variable trajectory $\mathbf{u}_{\theta_i \to \theta_i+c-1}$, i.e.,

$$\hat{\mathbf{y}}_{\theta_i+1 \to \theta_i+c} = \mathbf{f}(\mathbf{x}_{\theta_i - l+c+1 \to \theta_i}, \mathbf{u}_{\theta_i \to \theta_i+c-1}). \tag{9}$$

The corresponding optimization for the optimal future manipulated variable trajectory $\tilde{\mathbf{u}}_{\theta_i\to\theta_i+c-1}$ can then be formulated as follows:

$$\begin{aligned}\min_{\mathbf{u}_{\theta_i\to\theta_i+c-1}} \quad & (\hat{\mathbf{y}}_{\theta_i+1\to\theta_i+c} - \bar{\mathbf{y}}_{\theta_i+1\to\theta_i+c})^T \mathbf{Q}_1 \\ & (\hat{\mathbf{y}}_{\theta_i+1\to\theta_i+c} - \bar{\mathbf{y}}_{\theta_i+1\to\theta_i+c}) + \\ & \Delta\mathbf{u}^T_{\theta_i\to\theta_i+c-1}\mathbf{Q}_2\Delta\mathbf{u}_{\theta_i\to\theta_i+c-1}, \\ s.t. \quad & \mathbf{U}_{lb} \le \mathbf{u}_{\theta_i\to\theta_i+c-1} \le \mathbf{U}_{ub} \end{aligned} \tag{10}$$

where $\mathbf{Q}_1$ and $\mathbf{Q}_2$ are the weight matrices for trajectory errors and control rates, respectively; $\mathbf{U}_{lb}$ and $\mathbf{U}_{ub}$ are the lower and upper bound for $\mathbf{u}_{\theta_i\to\theta_i+c-1}$, respectively.

III. Case Study

In order to assess and validate the proposed approach for trajectory tracking control of product quality, a benchmark simulation for fed-batch fermentation of penicillin is used. The simulator, called Pensim, is based upon a series of detailed mechanistic models that describe the fermentation process [26]. The following process variables are collected hourly during the fermentation process: aeration rate, agitator power, substrate feed temperature, substrate concentration, dissolved oxygen concentration, culture volume, carbon dioxide concentration, pH, fermenter temperature, generated heat and substrate feed rate. The substrate feed rate is the manipulated process variable and the batch product quality is the biomass concentration that is measurable intermittently through laboratory assay during the batch run. Ten batch data are collected for model building and each batch has a duration time of 200 hours. It is further assumed that the biomass concentration is measured four times at a time interval of 50 hours during the batch running for each batch and therefore a total of 40 pseudo batches are created according to Figure 1. The validation of the proposed approach is performed in two steps: the first step is focused on building the PCA&PLS models and validating their accuracy for the strategy of moving window estimation; the second step is focused on realizing trajectory tracking control of batch product quality using the identified PCA&PLS models and the strategy of moving window estimation. These two steps are detailed in the following two subsections.

A. Building the PCA&PLS models and validating their accuracy using moving window estimation

The PCA&PLS models are identified using the created 40 pseudo bath data, where the length for the modeling window is selected to be 50 hours and the number of latent variables for the identified PCA&PLS models is selected to be 12 through cross-validation [27]. Taking a new batch run for an example, the control decision point is set at 50th hour and the future substrate feed rate is also assumed to be known. Then the future process variables such as the future carbon dioxide concentration can be estimated recursively using the identified PCA model according to Eq. (7). The estimated future carbon dioxide concentration from 50th hour to 90th hour is shown in Figure 3, where the estimated values are compared with their actual values. It can be seen that the estimated values are close to their actual values and thus the identified PCA model can be used to estimate the future process variable trajectories using the strategy of moving window estimation.

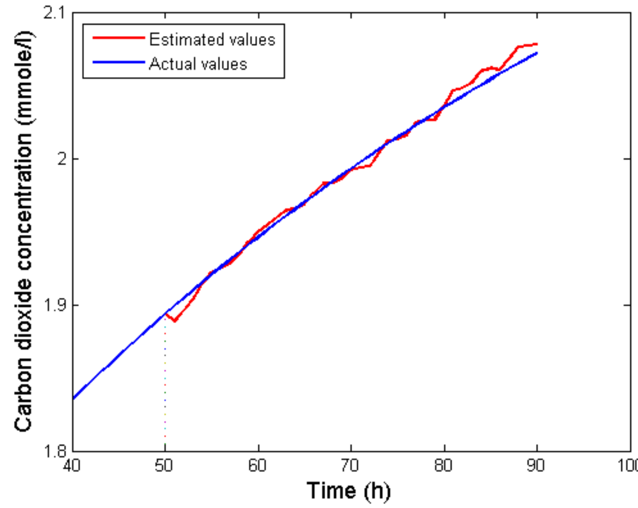

Fig. 3. Moving window estimation of the future carbon dioxide concentration

Using the same known future substrate feed rate and the estimated future process variable trajectories, the future biomass concentration can also be predicted using the identified PLS model and the strategy of moving window estimation according to Eq. (8). The predicted future biomass concentration from 50th hour to 90th hour is shown in Figure 4, where the predicted values are compared with their actual values. It can be seen that the identified PLS model can also successfully apply to predict the future product quality trajectory. These results shown in Figures 3 and 4 have demonstrated the accuracy of the identified PCA&PLS models as well as the effectiveness of moving window estimation and therefore they can be used for the following trajectory tracking control of batch product quality.

B. Trajectory tracking control using the identified PCA&PLS models and moving window estimation

For the same new batch run, the task of the proposed controller is to track a pre-determined product quality trajectory during the batch run. Taking a pre-determined biomass concentration trajectory under nominal conditions as an example, the control result of tracking the predetermined trajectory is shown in Figure 5, where the control horizon is selected to be 10 hours and the controller is switched on at 50th hours. It can be seen that the target product quality trajectory has been tracked approximately. However, there are some oscillations for the controlled quality trajectory. This is due to the oscillatory trajectory of the computed substrate feed rates, as shown in Figure 6. Additional measures such as adding extra constraints on control input sequences are to be taken to reduce such oscillatory behavior for a smoother trajectory tracking in the

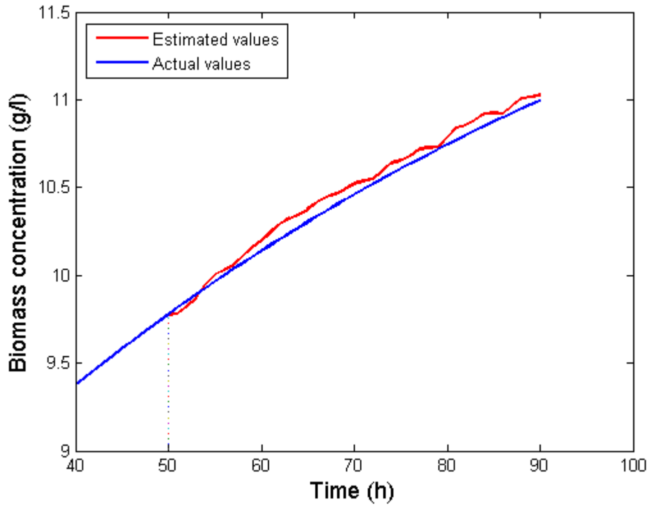

Fig. 4. Moving window prediction of the future biomass concentration

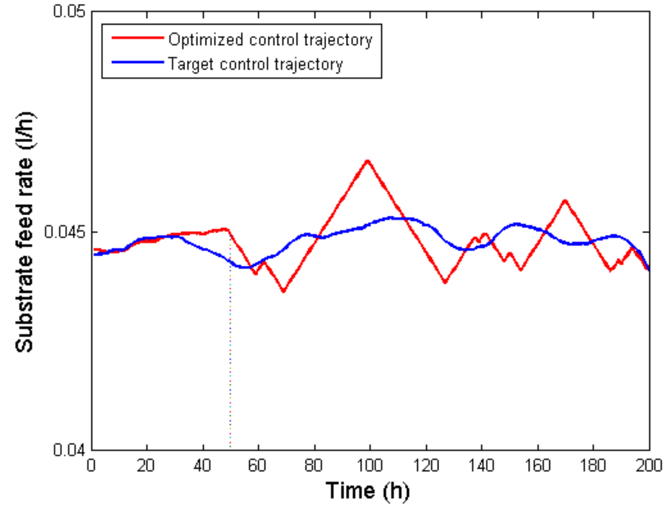

Fig. 6. The computed manipulated variable trajectory from the controller

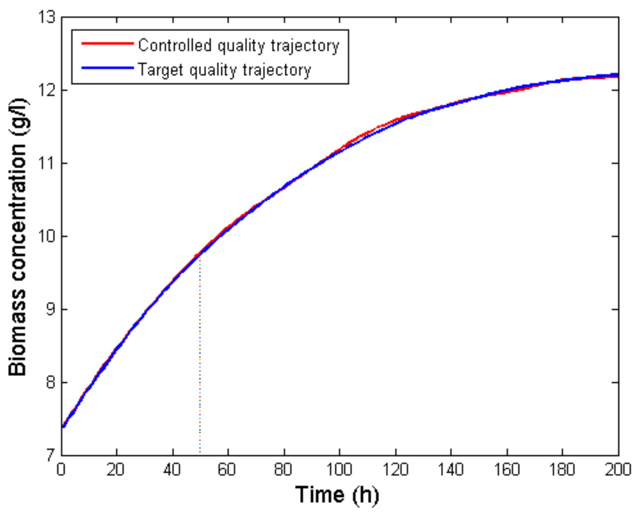

Fig. 5. Tracking an ideal product quality trajectory using the controller

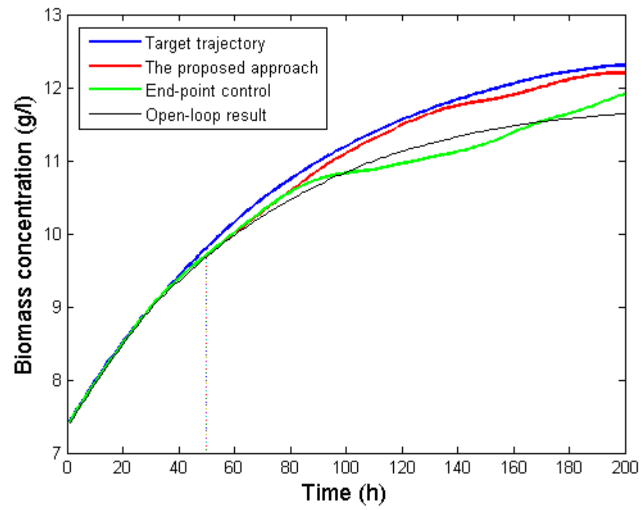

Fig. 7. Tracking product quality trajectory subject to un-modeled disturbances

future work [22].

The proposed control approach for trajectory tracking of batch product quality is further compared to the traditional end-point control approach of batch product quality [19]. In order to demonstrate the benefits of considering intermediate product quality trajectory rather than just the batch end-product quality, the fed-batch process is assumed to be subject to un-modeled disturbances. The added disturbance is chosen to be a step change in the concentration of the substrate feed from its nominal value of 600 g/l to 570 g/l occurring at the 30th hour. As shown in Figure 7, the traditional batch end-product quality control approach lacks the capability to detect the occurred disturbance and thus generates a much lower batch end-product quality than the proposed control approach. The proposed control approach manages to track the target product quality trajectory approximately despite the occurrence of the added disturbance and thus it can generate a much better batch end-product quality as well.

IV. Conclusions

Due to the lack of in-situ sensors for continuous measurements of batch product quality, it is hard to realize trajectory tracking control of product quality directly. Making use of intermittent measurements for batch product quality, this paper proposes a practical approach for tracking a desirable quality trajectory during the batch runs. The proposed approach is based on the strategy of moving window estimation for online prediction of future product quality trajectory. The benchmark simulation results have demonstrated the accuracy of the identified PCA&PLS models using intermittent measurements and

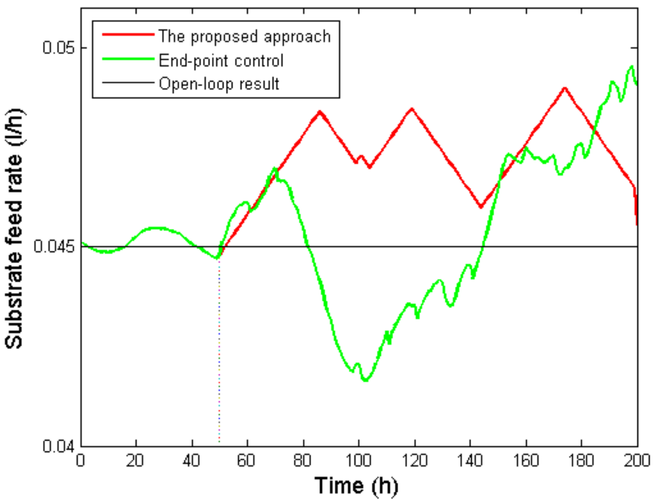

Fig. 8. The computed manipulated variable trajectories subject to un-modeled disturbances

the effectiveness of the proposed trajectory tracking scheme for batch product quality control, especially in the case of un-modeled disturbances. The obtained manipulated variable trajectory tends to be oscillatory and measures are to be taken to reduce such oscillatory behavior in the future work.

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