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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/semi-batch processes, it is vital to monitor and control product quality throughout the batch duration. The ideal strategy is to achieve end-product quality specifications through trajectory tracking control during a batch run. However, due to the lack of in-situ sensors for continuous monitoring of batch product quality, the measurements are usually implemented by laboratory assays and are inherently intermittent. Therefore, direct trajectory tracking of batch product quality is challenging in such applications. This paper proposes a practical approach to realise trajectory tracking control of batch product quality in those situations where only intermittent measurements are available. The first step of the approach consists in identifying a projection to latent structures (PLS) model to identify a relationship between readily measured process variable trajectories and intermittently measured batch product quality. Then the identified PLS-based prediction model is transformed into recursive formulation by utilising missing data imputation algorithms. Such recursive formulation allows identified PLS-based model to be readily incorporated as a predictor into standard model predictive control (MPC) framework. Case study employing simulated fed-batch fermentation process used to manufacture penicillin was employed to illustrate the principle and the effectiveness of the proposed approach.

Keywords: Batch process control, projection to latent structures, intermittent measurements, disturbance rejection, model predictive control.

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1. Introduction

Batch processes are widely used in industry for the manufacturing of low-volume, high-value added products such as specialty chemicals, polymers and pharmaceuticals [1]. Their popularity is frequently attributed to the following two reasons [2]: one is that batch process operation can be continuously improved using information from previous batch runs; the other is that batch operation is more efficient than continuous operation for those processes that experience frequent product changes and/or focus on the production of small quantities, which is particularly attractive for initial commercial productions of novel materials. For such materials it may be critical to recover research and development costs before competing products affect prices.

The ultimate objective for batch processes is to ensure consistent and desirable product quality is attained for each batch. This is not easy to fulfil in practice as chemical batch processes are usually described by complex time-varying and non-linear dynamics. Also, batch-to-batch variations resulting from changes in raw material properties and operating conditions render robust control of batch product quality more challenging. Technically, the main operational difficulty for the feedback control of batch processes lies in the lack of in-situ sensors to measure product quality [3]. Many process monitoring and control schemes have been proposed in the literature to overcome the issues encountered in batch operations. Initial control approaches for batch processes were based on mechanistic models and traditional control methods [4]. However, the identification of accurate mechanistic or first-principle models for batch processes is often difficult and time-consuming [5].

In recent years, multivariate statistical methods have been increasingly employed to identify models that describe batch process behaviour by using historical data. These models can then be used for monitoring and/or control purposes [6]. One of the key advantages of such data-driven models is that they do not require deep theoretical understanding of a given process and are, therefore, relatively easy to identify and keep up to date. Amongst the multivariate statistical methods used to identify models, principal component analysis (PCA) and projection to latent structures (PLS) have received considerable attention over the past two decades. These methods were initially employed in condition monitoring applications involving continuous processes [7]. Once the procedure of unfolding inherently three-dimensional data arrays found in batch processes into more ubiquitous two-dimensional form was introduced in [8] and [9], development of batch process monitoring applications involving PCA [10] and PLS [11] followed. In particular, the use of PLS models to monitor batch processes and predict product quality at the batch end-point were initially reported in [11].

In order to enable multivariate methods to capture dynamic relationships between various process variables several modifications of PCA and PLS were also proposed. In [12] it was demonstrated how the PCA technique can be employed to model the dynamic behaviour of chemical processes by simply appending 'time lag duplicates' to the data matrix, and then applying PCA to such matrix. As a result, a dynamic PCA model can be identified and used to monitor chemical processes. Similar procedure used to build a dynamic PLS model was proposed in [13]. Such dynamic PLS modelling consists in identifying ARX or Hammerstein models between the input and output scores, instead of a linear static model. The method presented in [13] requires continuous measurements of the output. However, in typical chemical batch process applications, the main technical difficulty lies in the lack of on-line sensors that can readily measure product quality. Batch product quality measurements are typically obtained by laboratory assays and are inherently intermittent. In [14] a multi-block PLS algorithm was proposed, such algorithm employs intermittent measurements of product quality within its formulation. The approach presented in [14] allows identification of either multiple models, the number of which is equal to the number of intermittent measurements used, or alternatively a single model for which outputs' intermittent measurements are stacked together. This method was proposed as a tool to monitor batch processes and to analyse the effects that process' variables have on mid-course and end-point quality. However, the algorithm presented in [14] requires the intermediate measurements of product quality to be taken at the same time during every training batch. Recently, a batch monitoring procedure similar to the one presented in [14], was introduced in [15]. In [15] an evolving PLS model method is proposed to predict intermediate values of batch product quality. This method is based on identifying a model at every single sample instant for every single intermittent measurement. Therefore, this method is computationally expensive, although the authors argue that it provides a more accurate monitoring tool when compared to other approaches, such as the one presented in [14]. The PLS model method proposed in [15] can only predict quality at those intermediate sample instants used in the training data.

Another approach that employs intermediate measurements in order to devise a dynamic PLS-based estimator of batch product quality was introduced in [16]. This modelling method does not require intermittent measurements to be taken at the same instants during each training batch nor does it rely on the usage of computationally intensive multiple-model architecture. This modelling method constructs time-windows of readily measured batch process data and appends them with the intermittent measurements of product quality that are collected at the end of each of these time-windows. Each pair of the time-window and the corresponding intermittent measurement represents the so-called pseudo-batch. Therefore, there can be as many pseudo-batches as there are intermittent measurements. Also, note that data related to different pseudo-batches may actually have been collected from a single batch run during which several intermittent measurements were taken. The time-windows of readily measured process variables' values form the input matrix, while the intermittent measurements collected at the end of each of the time-windows form the output matrix. These data structures can then be readily used to identify a corresponding PLS model, which can make on-line estimation of the difficult-to-measure product quality variables. However, it is formulated as an estimator rather than predictor and so is not suitable for forecasting future evolution of either readily measured process variables or batch product quality at a particular instant during a batch progression.

Models identified using statistical methods can be integrated within a model based control framework, with the objective of ensuring satisfactory batch product quality is attained [17]. In general, batch process control approaches can be classified in two main categories [18]:

1. Batch end-point control.
2. Trajectory tracking control.

Batch end-point control aims to ensure that the controlled variables, which are assumed to be measured at the very end of the batch, are as close to their target values as possible by adjusting manipulated variables' trajectories (MVTs). The controller is based on a PLS model that relates readily measured process variable trajectories to batch end-product quality. Initial development of the batch end-point control scheme was reported by Yabuki and MacGregor in [19], where a PLS model is used to provide a long-term estimate of product quality at the batch end-point. If, at the mid-way point of the batch, the estimate is significantly different from the target, then suitable corrective action is calculated and then implemented. This method was extended in [20] with the inclusion of several decision points during a batch progression at which prediction of batch end-product quality is made and the required adjustments are computed and then implemented. The key drawback of the batch end-point control scheme is the fact that the controlled variables are assumed to be measured only at the very end of a batch at which point it is no longer possible to perform any corrective action. Therefore, there is no direct feedback of the product quality properties during the batch run and, consequently, performance of the batch end-point control is likely to be affected by unanticipated disturbances and the inevitable plant-model mismatch. This is a particularly acute issue if disturbances and model inaccuracies directly impact controlled variables throughout the batch duration but are not observed in the readily-measured process variables. Some work has been published that attempts to overcome this issue, e.g. by constructing different models for each disturbance case-scenario [21], such approach is heavily dependent on having the knowledge and stored information for every type of perturbation, which is generally not the case. Also, the inclusion of a disturbance model to offset future measured variables' predictions has been proposed in [22]. However, such approach assumes that disturbances directly affect measured process variables rather than product quality.

The typical trajectory tracking approach was addressed in [23], where a control framework based on a dynamic PCA model embedded in a model predictive control (MPC) architecture was proposed. This approach was further investigated in [24], where the authors proposed a multi-phased PCA model, and in [25], where different data unfolding methods for PCA modelling were compared. The resulting controller then uses a PCA model to predict trajectories of the controlled variables in order to determine appropriate MVTs. However, the requirement for continuously measured controlled variables may in many practical applications prevent difficult-to-measure product quality-related quantities to be considered as viable controlled variable candidates. Instead, trajectory tracking approaches rely on the assumption that batch product quality can be guaranteed if some key process variables that are readily measured, such as reactor temperature or pressure, follow their pre-determined trajectories. However, that assumption is not generally true [26], especially if the disturbance or plant model mismatch affects the relationship between readily measured controlled variables and the product quality variables. Also, disturbances such as raw materials composition may significantly affect product quality but have insignificant impact on other readily measured process variables, such as reactor temperature. In those cases the loss of optimality of a given desired trajectory would lead immediately to the loss of optimality attained by the trajectory tracking controller.

The approach proposed in this paper aims to address the shortcomings of both batch end-point control and trajectory tracking by utilising intermittent measurements directly related to product quality. This intermittent feedback of controlled variables improves the controller's ability to reject the disturbances and attenuate the impact of plant-model mismatch on the product quality attained at the batch end-point. This approach is based on the method proposed originally in [16] that described how to devise an estimator of a difficult-to-measure product quality for which only intermittent measurements are available. However,the PLS model obtained using the method proposed in [16] is given in estimator form with inputs that are not necessarily independent manipulating and/or disturbance variables. Instead, many of the input variables, such as reactor temperature or pressure, are related dynamically not only to each other but also to the manipulated variables. Therefore, the resultant PLS model given in the form of finite impulse response model structure that incorporates dependent process variables as inputs is inappropriate for control applications. This paper describes how to transform the PLS model obtained using the approach described in [16] into the recursive formulation that can be readily incorporated into a MPC control framework. Such transformation is achieved by employing missing-data estimation capability offered by multivariate statistical methods in order to make future predictions of readily measured process variables. These predictions of process variables are then used to calculate future values of product quality.

It is highly beneficial for the effectiveness of the proposed control system if the desired trajectory of product quality, i.e. the *golden batch*[1], is known a priori. This desired trajectory can be obtained off-line using stored experimental data and well-established interpolation techniques [27]. However, the knowledge of a golden batch is not necessary to realise the proposed controller. In fact, the proposed controller's objective function could be formulated with a single end-point target value of the product quality. Note that in such cases the intermittent measurements of product quality would still be utilised for prediction purposes but they would not be explicitly considered in the objective function. Intermittent measurements would, however, be considered implicitly since they influence the predicted mismatch between the actual and desired batch end-product quality.

The remainder of the paper is organised as follows. Section 2 details the methodology of identifying a PLS model and transforming it into predictor form as well as incorporating it into trajectory tracking control system. Section 3 documents the results of applying the proposed approach to simulated fermentation process. These include the results detailing ability of the PLS-based predictor to forecast future evolution of batch process and also the assessment of the proposed trajectory tracking controller's ability to ensure product quality remains within specification in the presence of unmeasured disturbances. Finally, concluding remarks are provided in Section 4.

[1] The *golden batch* refers to the best batch profile achieved, which is based on theory an experimentation.

2. Trajectory tracking control of batch product quality

The proposed methodology of developing a PLS-based model, converting it into prediction form and then incorporating it into trajectory tracking MPC control scheme is described in this section. More specifically, Subsection 2.1 details the approach of identifying a PLS model using batch process data. This data is comprised of intermittently measured values of the product quality as well as the continuously measured values of other process variables and manipulating variables. Modelling approach described in Subsection 2.1 utilises the concept of pseudo-batches in order to use intermittent measurements of product quality for PLS model identification. Developed PLS model, however, is initially given in estimator rather than predictor form. Therefore, in order to incorporate it into the control scheme, the PLS model needs to be transformed into a predictor form, which is accomplished using moving window estimation procedure, as detailed in Subsection 2.2. The resulting PLS model-based predictor can be integrated into the trajectory tracking controller, which is described in Subsection 2.3. Finally, in Subsection 2.4 it is shown how to ensure that the trajectory tracking controller is able to reject unmeasured and un-modelled disturbances that affect product quality.

2.1. Model identification

Firstly, the model structure has to be defined, which specifies the variables that are used as inputs and the variables that are predicted using the model and are termed as outputs. Input variables used in the approach proposed in this paper correspond to the trajectories of the readily measured process variables and of the manipulated variables. The output variables are directly related to batch product quality and are assumed to be intermittently measured. The proposed method for identifying a PLS model is similar to the approach proposed in [16], where a pseudo-batch is created for every intermittent measurement of product quality. These pseudo-batches are then aligned with respect to their end-points for identifying a PLS model based on a selected modelling window (K_w).

Fig. 1 illustrates this data alignment using an example of two batch runs, each having three intermittent measurements for product quality. Therefore, a total of six pseudo-batches are created and they are aligned with respect to their end-points as shown in Fig. 1. Following the creation of pseudo-batches and their alignment, a modelling window is selected to identify the PLS model with the intermittent measurements representing outputs and all the other process variable measurements, including those of the manipulated variables, as inputs.

Batch process data is typically arranged in 3-dimensional arrays of size I by J by K, where I is the number of batches, J is the number of input variables[2] and K is the number of samples collected during a batch run. Several different methods have been suggested in the literature that 'unfold' original 3-dimensional data structure into a more familiar 2-dimensional data matrix, denoted as X. A well established method known as batch-wise unfolding [25] is used in this paper. Using this method the resulting input data matrix X_w is of dimensions I_w by JK_w, where I_w represents the number of pseudo-batches created following the procedure depicted in Fig. 1. Note that by considering the time-lagged input data the resulting PLS model is expected to capture dynamic behaviour of the batch process.

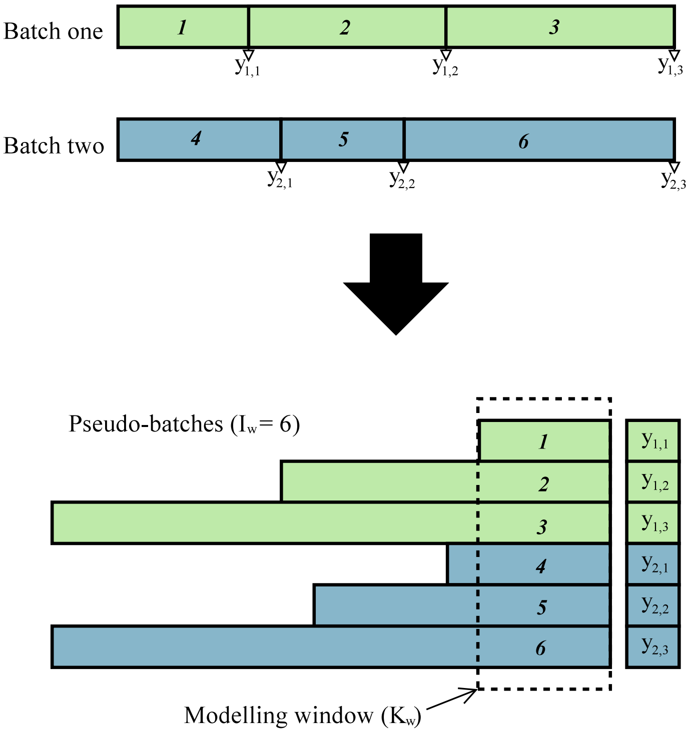


Figure 1: Proposed unfolding for batch data containing intermittent measurements. Data from two different batch runs are displayed, where two intermediate measurements and one final measurement are considered.

Obtained data can then be analysed using multivariate statistical methods such as PLS in order to develop causal input/output models. A PLS model is typically obtained using the non-linear iterative partial least squares (NIPALS) algorithm [28]. This algorithm iteratively decomposes the input X_w and output Y_w data matrices into the input and output scores and their corresponding input and

[2] $J = n_x + n_u$, where n_x is the number of readily measured variables, and n_u is the number of manipulated variables.

output loading matrices[3]:

$$\begin{aligned} X_w &= TP^T + E && (1) \\ Y_w &= UQ^T + F && (2) \end{aligned}$$

where $T \in \mathbb{R}^{I_w \times n_{pc}}$, $P \in \mathbb{R}^{JK_w \times n_{pc}}$, $E \in \mathbb{R}^{I_w \times JK_w}$ are the input scores matrix, input loadings matrix and input residuals matrix, respectively; and $U \in \mathbb{R}^{I_w \times n_{pc}}$, $Q \in \mathbb{R}^{n_y \times n_{pc}}$, $F \in \mathbb{R}^{I_w \times n_y}$ represent the output scores, output loadings and output residuals matrices, respectively. n_y represents the number of outputs, and n_{pc} is the number of latent variables or principal components (column vectors in the loadings matrices) retained by the PLS model. n_{pc} is commonly chosen by means of cross-validation techniques [30]. In this work leave-one-out cross-validation [31] was used. Note that usually $n_{pc} \ll JK_w$ due to the presence of high correlation amongst the process variables. Residuals matrices E and F contain negligible information that is not captured by the statistical models. Discarding these matrices, the estimated input and output matrices denoted by $\widehat{X}_w$ and $\widehat{Y}_w$, respectively, are given by the following two equations:

$$\begin{aligned} \widehat{X}_w &= TP^T && (3) \\ \widehat{Y}_w &= UQ^T && (4) \end{aligned}$$

A least square regression is then carried out to identify the so-called 'inner relationship' between the input and output score vectors:

$$U = TB \tag{5}$$

where $B \in \mathbb{R}^{n_{pc} \times n_{pc}}$. However, in order to improve the numerical stability of the inner relationship model given in Eq.(5), an additional weighting matrix $W \in \mathbb{R}^{JK_w \times n_{pc}}$ is employed to ensure orthogonality of the input scores. Resulting relationship between the input variables and scores is given as follows[4]:

$$T = X_w W \left(P^T W\right)^{-1} \tag{6}$$

[3] The PLS regression method is applied to the mean centred and scaled (unit variance) data [29].

[4] A detailed description of the NIPALS algorithm, including the corresponding Matlab® code, can be found in [32].

In practice, the PLS model is often expressed as a predictive model directly relating the input and output variables [33]. Such model form can be obtained by substituting Eq.(6) and Eq.(5) into Eq.(4):

$$Y_w = X_w \underbrace{W\left(P^T W\right)^{-1} B Q^T}_{\Theta^T} + F^* \tag{7}$$

where the PLS model coefficients are stored in the matrix $\Theta \in \mathbb{R}^{n_y \times JK_w}$ and $F^* \in \mathbb{R}^{I_w \times n_y}$ is the residuals matrix. If an appropriate number of retained latent variables is chosen, the residual matrix F^* contains negligible information. Consequently, after discarding F^*, the multi-way PLS model becomes:

$$\widehat{Y}_w = X_w \Theta^T \tag{8}$$

2.2. Moving window estimation

Once the PLS model is identified, it can be used to predict future batch product quality for a new batch run by employing the strategy of moving window estimation. The principle of moving window estimation is illustrated in Fig. (2), where the length of the modelling window for the identified PLS model is equal to K_w. Consider that the current time instant of a new batch run is k. The first step for moving window estimation is to place the modelling window to cover the measured $K_w - 1$ past samples of the input variables. As a result an input vector ξ_k is formed:

$$\xi_k = \left[x^T_{me|k-K_w+2\to k} \quad u^T_{mv|k-K_w+2\to k}\right]^T \tag{9}$$

$$x_{me} = \left[x_1 \cdots x_{n_x}\right]^T \tag{10}$$

$$u_{mv} = \left[u_1 \cdots u_{n_u}\right]^T \tag{11}$$

where $x_{me} \in \mathbb{R}^{n_x \times 1}$ and $u_{mv} \in \mathbb{R}^{n_u \times 1}$ are the readily measured process variables and manipulated variables, respectively.

Assuming that the future manipulated variables $u_{mv|k+1}$ are available after solving an optimisation problem (described in the next subsection), then the future measured process variables $x_{me|k+1}$ can be estimated using the PLS model and missing data algorithms.

Several missing data imputation methods have been proposed in the literature [34, 35], such as single component projection (SCP), projection to the model plane (PMP), conditional mean replacement (CMR) and trimmed score regression (TSR). The common idea behind them is to make use of

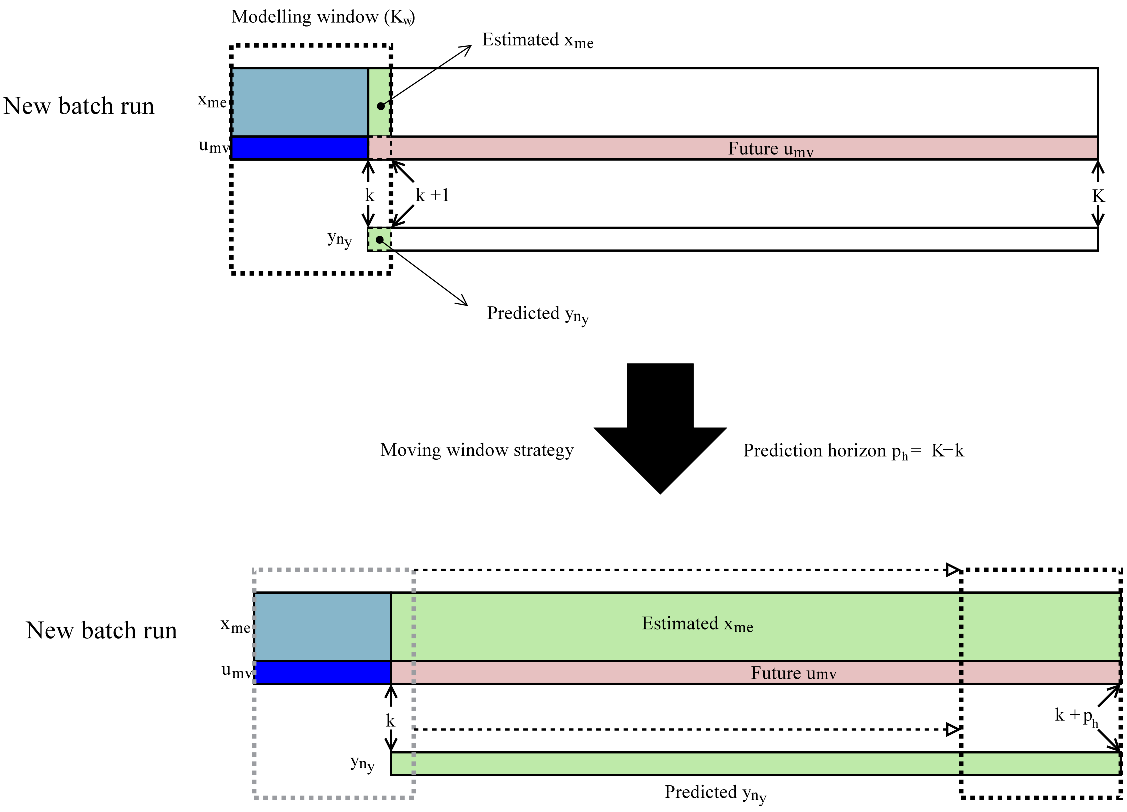


Figure 2: Moving window estimation using intermittent measurements

the underlying data pattern to deduce the missing part from the known part. In this paper the PMP method was selected due to its ability to estimate all the missing data at once, which is not possible in the case of SCP. Additionally, it was found out after several simulation tests that PMP was less computationally expensive than CMR and TSR.

The PMP method consists of partitioning the predictor variables, denoted as χ, into $\chi^T = [\chi^{*^T} \;\; \chi^{\sharp^T}]$, where χ^* contains the known data and $\chi^\sharp$ contains the missing data. The loading matrix P from identified PLS model, given in Eq. (3), can also be partitioned into two corresponding parts P^* and $P^\sharp$. Then, the missing data can be estimated as follows [34]:

$$\chi^\sharp = P^\sharp \left(P^{*^T} P^*\right)^{-1} P^{*^T} \chi^* \tag{12}$$

Therefore, at sample instant k, the prediction of the future measured variables $x_{me|k+1}$, denoted as $\widehat{x}_{me|k+1}$, can be expressed as a function of the past $K_w - 1$ measured and manipulated variables, contained in ξ_k, and the future manipulated variables $u_{mv|k+1}$ as follows:

Consider the future measured variables as missing information. Then, employing the PLS model, Eq.(3), and the missing data algorithm PMP, described in Eq.(12), results in the following expression:

$$\widehat{x}_{me|k+1} = P^{\sharp} \left(P^{*T} P^{*}\right)^{-1} P^{*T} \left[\xi_k^T \quad u_{mv|k+1}^T\right]^T \tag{13}$$

where:

$$\Gamma \triangleq P^{\sharp} \left(P^{*T} P^{*}\right)^{-1} P^{*T} \tag{14}$$

Substituting Eq.(9) and Eq.(14) in Eq.(13):

$$\widehat{x}_{me|k+1} = \Gamma \underbrace{\left[x_{me|k-K_w+2\to k}^T \quad u_{mv|k-K_w+2\to k+1}^T\right]^T}_{\left[\xi_k \quad u_{mv|k+1}^T\right]^T} \tag{15}$$

where Γ can be partitioned in accordance to $\left[x_{me|k-K_w+2\to k}^T \quad u_{mv|k-K_w+2\to k+1}^T\right]^T$ in two matrices:

$$\Gamma \triangleq [\Gamma_x \ \Gamma_u] \tag{16}$$

Finally, substituting Eq.(16) in Eq.(15):

$$\widehat{x}_{me|k+1} = \Gamma_x x_{me|k-K_w+2\to k} + \Gamma_u u_{mv|k-K_w+2\to k+1} \tag{17}$$

where $\Gamma_x \in \mathbb{R}^{n_x \times n_x(K_w-1)}$ and $\Gamma_u \in \mathbb{R}^{n_x \times n_u K_w}$

A similar approach is applied for the prediction of future output variables, y_{k+1}, denoted as $\widehat{y}_{k+1}$. Using Eq.(17) and the PLS model, given in Eq.(8), the future output variables can be expressed as a function of past $K_w - 1$ measured variables, and the future manipulated variable trajectories $u_{mv|k+1}$. Using the transposed version of the PLS model described in Eq.(8), the future output, $\widehat{y}_{k+1}$, is given by:

$$\widehat{y}_{k+1} = \Theta \left[x_{me|k-K_w+2\to k}^T \quad \widehat{x}_{me|k+1}^T \quad u_{mv|k-K_w+2\to k+1}^T\right]^T \tag{18}$$

Θ can be partitioned in two matrices:

$$\Theta \triangleq [\Theta_x \ \Theta_u] \tag{19}$$

where $\Theta_x \in \mathbb{R}^{n_y \times n_x K_w}$ and $\Theta_u \in \mathbb{R}^{n_y \times n_u K_w}$.

Then by substituting Eq.(19) in Eq.(18):

$$\widehat{y}_{k+1} = \Theta_x \left[x^T_{me|k-K_w+2\to k} \;\; \widehat{x}^T_{me|k+1}\right]^T + \;\Theta_u u_{mv|k-K_w+2\to k+1} \tag{20}$$

Similarly to Eq.(19), Θ_x can be partitioned in two matrices according to $\left[x^T_{me|k-w+2\to k} \;\; \widehat{x}^T_{me|k+1}\right]^T$:

$$\Theta_x \triangleq [\Theta_{x1} \;\; \Theta_{x2}] \tag{21}$$

where $\Theta_{x1} \in \mathbb{R}^{n_y \times n_x(K_w-1)}$ and $\Theta_{x2} \in \mathbb{R}^{n_y \times n_x}$. Then, by substituting Eq.(17) and Eq.(21) in Eq.(20):

$$\widehat{y}_{k+1} = \Theta_{x_1} x_{me|k-w+2\to k} + \;\Theta_{x_2}\left[\Gamma_x x_{me|k-w+2\to k} + \Gamma_u u_{mv|k-w+2\to k+1}\right] + \;\Theta_u u_{mv|k-w+2\to k+1} \tag{22}$$

$$\widehat{y}_{k+1} = \left[\Theta_{x_1} + \Theta_{x_2}\Gamma_x\right] x_{me|k-w+2\to k} \;+\; \left[\Theta_u + \Theta_{x_2}\Gamma_u\right] u_{mv|k-w+2\to k+1} \tag{23}$$

Defining:

$$\Phi \triangleq \left[\Theta_{x_1} + \Theta_{x_2}\Gamma_x\right] \tag{24}$$

$$\Psi \triangleq \left[\Theta_u + \Theta_{x_2}\Gamma_u\right] \tag{25}$$

results in:

$$\widehat{y}_{k+1} = \Phi x_{me|k-K_w+2\to k} \;+\; \Psi u_{mv|k-K_w+2\to k+1} \tag{26}$$

where $\Phi \in \mathbb{R}^{n_y \times n_x(K_w-1)}$ and $\Psi \in \mathbb{R}^{n_y \times n_u K_w}$.

After the measured variables, $\widehat{x}_{me|k+1}$, and the product quality variables, $\widehat{y}_{k+1}$, have been estimated using Eq.(17) and Eq.(26), the modelling window is to be moved forward as shown in Fig. 2. Then the measured variables and the product quality values at the time instant $k+2$ can be deduced in the same way using $u_{mv|k+2}$ and the formerly calculated value of $\widehat{x}_{me|k+1}$. The whole estimation process is repeated recursively up to the end of the prediction horizon (p_h). Note that during the evaluation of the PLS model at time instant k it is the vector ξ_k that is updated with measured values. On the other hand, matrices Γ_x, Γ_u, Φ and Ψ remain constant since the PLS model is assumed to be time-invariant.

2.3. Trajectory tracking control

The proposed trajectory tracking control is performed in a shrinking horizon manner [36], such that at sample instant k, p_h is equal to the remaining batch time (i.e. $p_h = K - k$, where K is equal to the total batch duration). The future manipulated variable trajectories, $u_{mv|k+1 \to k+p_h}$, are optimised in order to minimise the difference between the predicted future quality trajectory, $\widehat{y}_{k+1\to k+p_h}$, and the target future quality trajectory, $\overrightarrow{y}_{k+1\to k+p_h}$, at each control decision point. The optimised future manipulated variable trajectories are then implemented up to the next control decision point. Then the entire procedure is repeated until the batch process ends.

Hence, assuming that the current control decision point is at the time instant k and the target future quality trajectory is $\overrightarrow{y}_{k+1\to k+p_h}$, the predicted future quality trajectory, $\widehat{y}_{k+1\to k+p_h}$, can be obtained using the moving window strategy depicted in Fig. 2. According to such strategy, the predicted future quality trajectory can be expressed as a function of the future manipulated variable trajectories $u_{mv|k+1 \to k+p_h}$. Therefore, the corresponding optimisation of the future manipulated variable trajectories can be formulated as follows:

$$\begin{aligned} \min_{u_{mv|k+1 \to k+p_h}} \quad & (\widehat{y}_{k+1\to k+p_h} - \overrightarrow{y}_{k+1\to k+p_h})^T \; Q_1 \; (\widehat{y}_{k+1\to k+p_h} - \overrightarrow{y}_{k+1\to k+p_h}) + \\ & \Delta u^T_{mv|k+1 \to k+M} \; Q_2 \; \Delta u_{mv|k+1 \to k+M} \end{aligned} \tag{27}$$

$$\text{s.t.}$$

$$\begin{aligned} \widehat{x}_{me|k+1} &= \Gamma_x x_{me|k-K_w+2\to k} \; + \; \Gamma_u u_{mv|k-K_w+2\to k+1} \\ \widehat{y}_{k+1} &= \Phi x_{me|k-K_w+2\to k} \; + \; \Psi u_{mv|k-K_w+2\to k+1} \\ U_{lb} &\leq \; u_{mv} \; \leq \; U_{ub} \\ \Delta u_{mv} &\leq \; \Delta u_{max} \end{aligned}$$

where $Q_1 \in \mathbb{R}^{n_y \cdot p_h \times n_y \cdot p_h}$ and $Q_2 \in \mathbb{R}^{M \cdot n_u \times M \cdot n_u}$ are the symmetric and positive definite weighting matrices for trajectory tracking errors, $\left(\widehat{y}_{k+1\to k_p} - \overrightarrow{y}_{k+1\to k_p}\right)$, and control change rates ,$\Delta u_{mv|k+1 \to k+M}$, respectively. M is the control horizon, Δu_{max} represents the maximum change rate allowed for the manipulated variables. $U_{lb} \in \mathbb{R}^{n_u \times 1}$ and $U_{ub} \in \mathbb{R}^{n_u \times 1}$ are the vectors conformed by the lower (lb) and upper (ub) bounds of each manipulated variable, respectively. U_{lb} and U_{ub}, are normally derived from the saturation constraints imposed on the actuation equipment. Alternatively, these bounds may be set by the process engineers who aim to reduce the chances of erratic controller action and wear-and-tear of actuation equipment by imposing artificial constraints on the manipulating variables.

However, the predictions used in the optimisation problem described in Eq. (27) do not account for the impact of unmeasured disturbances and plant-model mismatch on the trajectory tracking controller performance. This is addressed in the following subsection.

2.4. Disturbance rejection using intermittent measurements

In order to account for the inevitable presence of unmeasured disturbances and plant-model mismatch, the target quality trajectory, $\overrightarrow{y}_{k+1 \to k+p_h}$, can be adjusted using the difference between the predicted and the measured values of product quality whenever its intermittent measurements are available. This approach is typically used in standard MPC control implementation, in which any mismatch between the predicted and the actual value of the control variable is attributed to constant output disturbance, which is then propagated to the end of prediction horizon [37]. An end-point controller using a 'disturbance model' was presented in [22]. However, in [22] intermittent measurements of product quality are not considered, and the 'disturbance model' is built based on the mismatch between measured and predicted values of readily measured process variables instead. Therefore, such disturbance model is not effective in applications where the disturbances directly affect product quality and have little or no impact on other readily measured process variables. The controller proposed in this paper employs intermittent measurements of product quality in order to estimate the impact of unmeasured disturbances and inherent plant-model mismatch and modify the target trajectory accordingly. By using the intermittent measurements of batch product quality, the controller is able to reject un-modelled disturbances affecting batch product quality, even if such disturbances have little or no effect on the readily measured process variables.

In order to reject disturbances, intermittent measurements of product quality are used to calculate the difference (offset) between the predicted and the actual product quality. This offset is then used to adjust the target quality trajectory. The method for calculating the offset (Δy) is described next: Suppose that a sample of batch quality, denoted as $\Upsilon_{k_s} \in \mathbb{R}^{ny \times 1}$, is taken at a sample instant k_s. This measurement is scaled using the mean, $\mu_{Y_w} \in \mathbb{R}^{1 \times n_y}$, and standard deviation, $\sigma_{Y_w} \in \mathbb{R}^{1 \times n_y}$, vectors calculated from the training data used for model identification:

$$y_{k_s}^T = \left(\Upsilon_{k_s}^T - \mu_{Y_w}\right) \oslash \sigma_{Y_w} \tag{28}$$

where $\oslash$ represents the Hadamard or element by element division.

Using the PLS model defined in Eq.(8), and the past K_w values of both the readily measured variables, x_{me}, and the manipulated variables, u_{mv}, the estimated output at sample instant k_s can be obtained as follows:

$$\widehat{y}_{k_s}^T = \left[x_{me|k_s-K_w+1 \rightarrow k_s}^T \quad u_{mv|k_s-K_w+1 \rightarrow k_s}^T \right] \Theta^T \tag{29}$$

The offset for the trajectory is then defined as:

$$\Delta y = \widehat{y}_{k_s} - y_{k_s} \tag{30}$$

After Δy has been calculated, it can be used to update the target quality trajectory:

$$\overrightarrow{y} = y^* + \mathbf{1} \cdot \Delta y^T \tag{31}$$

where $\mathbf{1}$ represents a $K \times 1$ vector of ones and y^* is the scaled desired quality trajectory: $y^* = (Y^* - \mathbf{1} \cdot \mu_{Y_w}) \oslash \mathbf{1} \cdot \sigma_{Y_w}$.

The target quality trajectory is used for the optimisation of Eq.(27) and if an un-modelled disturbance is present and an intermittent measurement has been taken, the control algorithm will be able to cope with the disturbance by incorporating the offset Δy. An example of this is shown in the next section using a fed-batch fermentation of penicillin as benchmark simulation.

However, during the initial stage of batch progression and before the first intermittent measurement of product quality is available, the estimate of the offset, Δy, cannot be computed by using Eq. (30). During this initial time period Δy is estimated using the approach similar to that proposed in [22]. In particular, it is obtained by calculating mismatch between the prediction of product quality obtained using only information available at time $k-1$, denoted as $\widehat{y}_{a|k}$, and its estimate obtained using all the information available at time k, denoted as $\widehat{y}_{b|k}$. Both $\widehat{y}_{a|k}$ and $\widehat{y}_{b|k}$ are obtained using the PLS model. However, $\widehat{y}_{a|k}$ is computed using Eq.(26) that relies on the prediction of $\widehat{x}_{me|k}$ whereas $\widehat{y}_{b|k}$ is computed using Eq. (8) that does not require predictions of readily measured process variables. Therefore, effects not captured by the model will be less observable in $\widehat{y}_a$ when compared to $\widehat{y}_b$ and can be at least partially quantified by differencing these two estimates:

$$\Delta y = \widehat{y}_{a|\,k} - \widehat{y}_{b|\,k} \tag{32}$$

Estimate of Δy obtained using Eq.(32) is, however, based on the assumption that the un-modelled effects of disturbances and plant-model mismatch will directly impact readily measured process variables and be therefore revealed as their prediction errors. Therefore, it is considered sub-optimal. On the other hand, the offset computed according to Eq.(30), which is used once intermediate measurement of product quality is available, takes into account the direct impact of unmeasured disturbances and plant-model mismatch on the product quality. Therefore, it facilitates, albeit intermittently, closed-loop control of product quality.

3. Case studies

In order to assess the proposed approach for trajectory tracking control of product quality, a benchmark simulation of a fed-batch fermentation process used to produce penicillin is employed. This simulation, called PenSim, is based upon a series of detailed mechanistic models that describe the fermentation process [38]. Although the PenSim simulator considers various process variables, such as the concentration of substrate in the feed, many of these cannot be readily measured in most real-world applications. Therefore, only the variables listed in Table 1 were assumed to be measured hourly in order to ensure that the case study considered in this paper is realistic. It was also assumed that white noise, with a signal-to-noise ratio[5] (SNR) of 40 dB, affected the measurements of the eight process variables listed in Table 1.

The quality-related variable is the biomass concentration, which was assumed to be measured intermittently through laboratory assay during a batch run. For all the simulated batches it was assumed that the desired specification for the batch end-point biomass concentration was 12.2 g/l ± 0.3 g/l (i.e. specification allows a ± 2.5% variability around the desired batch end-product quality).

The manipulated variable which has significant impact on the biomass is the substrate feed rate, which was also measured and stored hourly. The manipulated variable, and the eight readily measured process variables listed in Table 1 form the input data matrix of the PLS model that was used to predict biomass concentration.

The assessment of the proposed modelling and control approaches is documented in the following 4 subsections. Subsection 3.1 details development of the PLS model. Subsection 3.2 documents assessment of the prediction capability of the developed PLS model when applied to validating batches.

[5] $\mathrm{SNR} = 20\log\left(\frac{\mathrm{RMS}_{signal}}{\mathrm{RMS}_{noise}}\right) dB$

Table 1: Readily measured process variables.

1. Aeration rate.
2. Agitation power.
3. Substrate feed temperature.
4. Dissolved Oxygen (DO) concentration.
5. Culture volume.
6. Carbon dioxide (CO_2) concentration.
7. pH.
8. Fermenter temperature.

Subsection 3.3 focuses on the ability of the MPC controller that utilises PLS model and moving window estimation to perform adequate trajectory tracking of the batch product quality in the absence of any intermittent measurements. Finally, Subsection 3.4 demonstrates the ability of the proposed trajectory tracking MPC control scheme to reject the disturbances by utilising intermittent measurements of batch product quality.

3.1. PLS model identification

Data from 30 simulated batches was collected for the identification of the PLS model, with each batch having a duration time of K = 200 hours. Sampling time of the eight readily measured process variables and the manipulated variable was set to one hour. In order to excite process dynamics and generate realistic batch to batch variation, filtered pseudo-random binary signal (PRBS) was appended to the nominal substrate feed rate of 0.045 l/hr as well as to aeration rate and agitator power for each batch [39].

It was further assumed that during each batch run some samples were taken in order to obtain biomass concentration measurements. A single sample was randomly taken between the 45^{th} and 55^{th} hour, another one between the 95^{th} and 105^{th} hour, a third one between the 145^{th} and 155^{th} hour and the last one at the end of each batch run. Therefore, four measurements were taken during each batch run, resulting in the total of 120 pseudo-batches aligned according to the procedure depicted in Fig. 3.

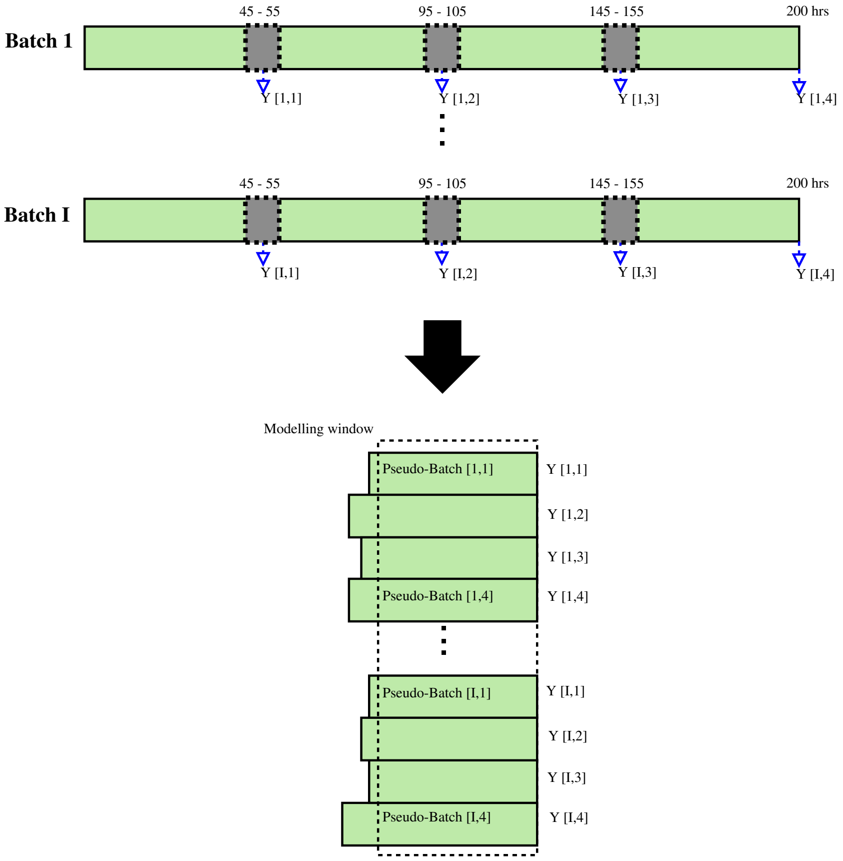


Figure 3: Unfolding of the data from $I = 30$ batches used for modelling the fermentation process.

A PLS model was identified using the data arrangement depicted in Fig. 3, where the length of the modelling window, K_w, was selected to be 45 hours, which is equal to the length of the smallest pseudo-batch. The number of latent variables for the PLS model was chosen to be 10 by using leave-one-out cross-validation procedure.

3.2. Prediction of product quality using the moving window strategy

In order to demonstrate the prediction capability of the identified PLS model, 50 new (validating) batches were simulated. During the simulations a filtered PRBS was appended to the nominal substrate feed rate in order to introduce batch-to-batch variability. The PLS model, identified according to the procedure outlined in Subsection 3.1, was then evaluated using the data from these 50 validating batches in terms of its ability to predict both the biomass concentration and the readily measured process variables.

For each validating batch run the prediction of the future trajectories of the readily measured process variables as well as the biomass concentration was obtained at $k = K_w = 45$. From this instant the future variable trajectories were predicted by means of the moving window methodology described in Subsection 2.2 under the assumption that the future trajectory of the manipulating variable, i.e. substrate federate, is known. As discussed in Subsection 2.2, this assumption is considered to be realistic because manipulating variable trajectories are pre-computed by the control algorithm.

Two statistical measures were used to analyse model accuracy when predicting the biomass concentration. These are the mean absolute percentage error (MAPE) and the R^2 statistic:

$$\mathrm{MAPE} = \frac{100}{K - K_w + 1} \sum_{k=K_w}^{K} \left| \frac{\widehat{y}_k - y_k}{y_k - y_k^{(nom)}} \right| \tag{33}$$

$$\mathrm{R}^2 = 1 - \frac{\sum\limits_{k=K_w}^{K} \left(\widehat{y}_k - y_k\right)^2}{\sum\limits_{k=K_w}^{K} \left(y_k - y_k^{(nom)}\right)^2} \tag{34}$$

where $y^{(nom)}$ denotes nominal trajectory. Nominal trajectory is obtained by running a single batch run under nominal constant feed conditions and in the absence of any variation. Such information may not be available in realistic applications but in this case it is used to properly assess the capability of the PLS model-based predictor. Note that both MAPE and R^2 are obtained by normalising prediction error with the variation of the biomass concentration from its nominal trajectory rather than simply its mean value. Such normalisation was done in order to assess the ability of the prediction model to identify batch-to-batch variation of biomass concentration. Therefore, R^2 statistic in particular describes the percentage of batch-to-batch variation of biomass concentration that is captured by the prediction model. The values of R^2 and MAPE statistics calculated for 50 validating batches are shown in histogram form in Figs. 4 and 5, respectively.

Fig. 4 indicates that for the great majority of the validating batches the percentage of batch-to-batch variation in biomass concentration captured by the prediction model was greater than 80%. For only nine validating batches prediction model captured less than 80% of the biomass variation. Even in those nine cases the percentage of captured batch-to-batch variation of biomass concentration was greater than 60%.

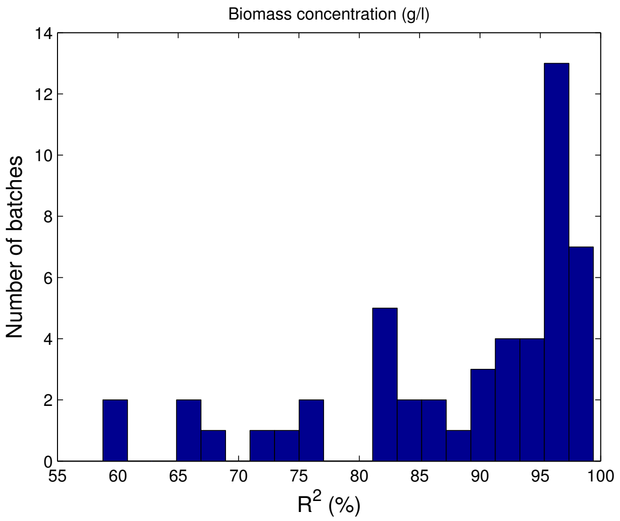


Figure 4: R^2 of the variability around a nominal biomass trajectory obtained with the PLS model. Results correspond to 50 simulated batches.

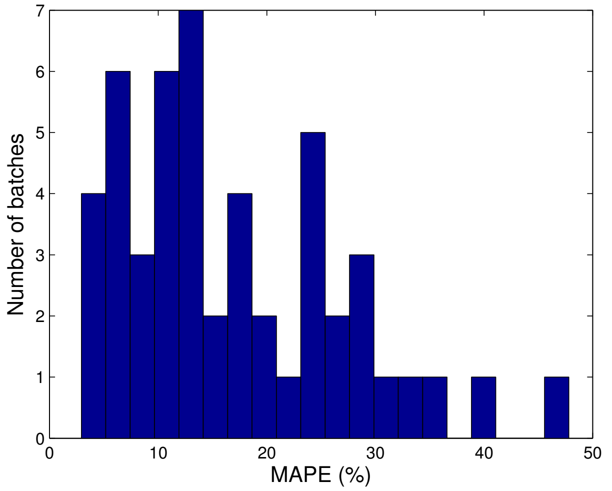
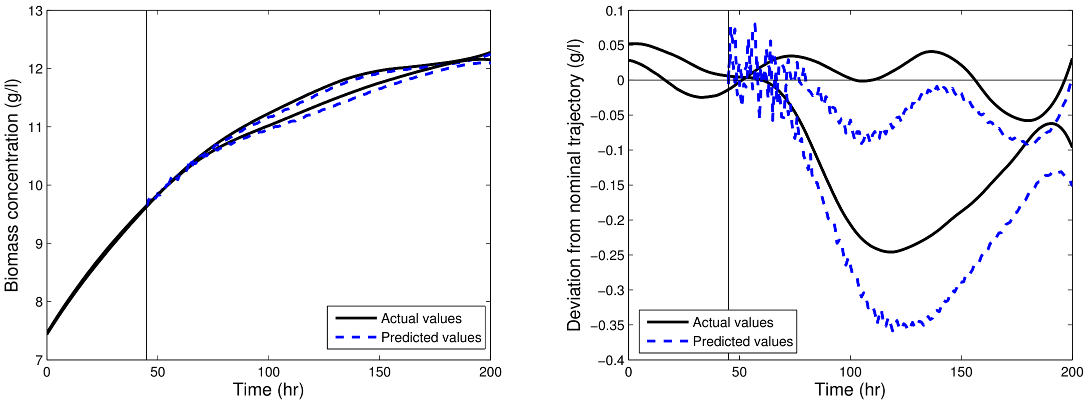


Figure 5: MAPE of the variability around a nominal biomass trajectory obtained with the PLS model. Results correspond to 50 simulated batches.

In terms of MAPE metric it is observed in Fig. 5 that for a majority of the validating batches the mean of the relative prediction error is less than 30% of the variation of biomass concentration. Seemingly large values of MAPE statistic do occur, as observed in Fig. 5. However, this is primarily due to the fact that the normalisation is done by dividing the error with the deviation of biomass concentration from its nominal trajectory rather than its mean value. In order to show that the model is able to capture sufficient amount of variation even in those cases where MAPE statistic is relatively large, Fig. 6 plots the biomass concentration trajectory along with its prediction for the two validating batches with the worst MAPE values. Trajectories of the actual biomass concentration are shown using solid lines whilst the predictions are shown using dashed lines.



(a) Biomass trajectory

(b) Variability around nominal trajectory

Figure 6: Plot of biomass concentration and its predictions for 2 worst-case batches.

Whilst Fig. 6(a) shows the absolute trajectories of the actual and the predicted biomass concentration, Fig. 6(b) shows these trajectories in terms of their deviations from the nominal biomass concentration trend. Plot in Fig. 6(b) allows user to more clearly inspect the ability of the prediction model to characterise batch-to-batch variation of the product quality. Even though MAPE statistic for these two batches was found to be greater than 40% it can be observed in Fig. 6 that the model is still able to sufficiently capture batch-to-batch variation of biomass concentration.

The ability of the PLS model to predict the readily measured process variables' trajectories was assessed using MAPE metric, which was calculated as follows:

$$\text{MAPE}^{(x_{me})} = \frac{100}{K - K_w + 1} \sum_{k=K_w}^{K} \left| \frac{\widehat{x}_{n_k} - x_{n_k}}{x_{n_k} - \overline{x}_n} \right|, \quad where \;\; \overline{x}_n = \frac{\sum\limits_{k=K_w}^{K} x_{n_k}}{K - K_w + 1} \tag{35}$$

Note that the statistic represented by Eq.(35) takes into account the variation of each measured variable around its mean value. Therefore, Eq.(35) scales the prediction error for each of the readily measured process variables by their actual variation. Fig. 7 displays MAPE$^{(x_{me})}$ metric calculated for each readily measured variable and expressed in percentage form.

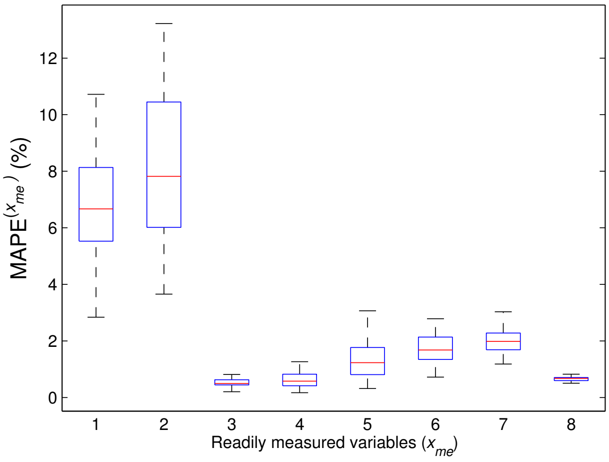
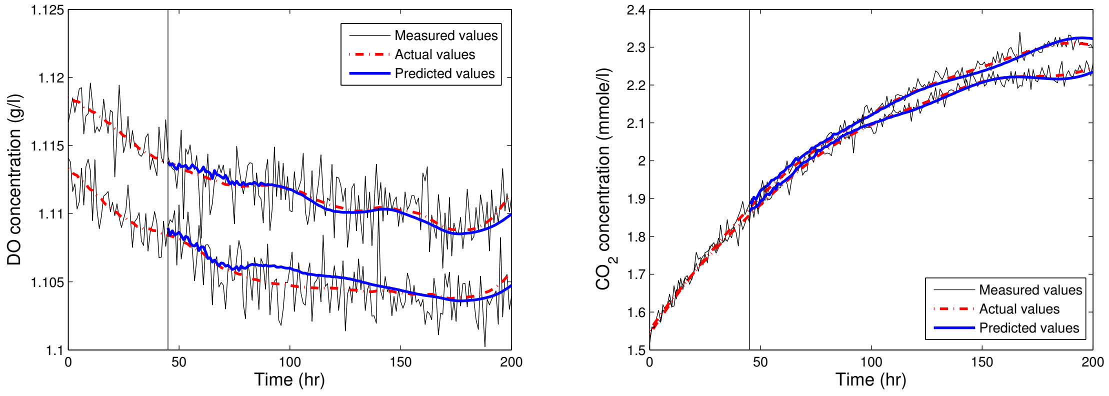


Figure 7: MAPE$^{(x_{me})}$ obtained from 50 validating batches

Each box in Fig. 7 corresponds to one of the measured variables listed in Table 1 (i.e. variable '1' is the aeration rate, variable '2' is the agitation power, etc.). For each box, the central red mark represents the median value whilst the edges of the boxes denote the 25th and 75th percentiles and the whiskers extend to the most extreme data points. Fig. 7 shows that the percentage of estimation error corresponding to measured process variables was less than approximately 14% for all the readily measured process variables across all of the 50 validating batches.



(a) Trajectory of DO

(b) Trajectory of CO$_2$

Figure 8: Trajectories of DO and CO$_2$ corresponding to two different batches.

Fig. 8 (a) and (b) are also included to give a visual comparison between the predicted and the actual values of two readily measured process variables, namely dissolved oxygen (DO) and carbon dioxide (CO_2) concentration, respectively. These variables were chosen because they are related to the product quality and also exhibit considerable batch-to-batch variation. Fig. 8 (a) and (b) show three trends. The true values of DO and CO_2 are represented by red traces whereas the measured values are represented by black traces. Blue trends denote predictions made using the PLS model in conjunction with moving window estimation procedure. The vertical black line at the 45^{th} hour represents the sample instant at which the predictions of the future trajectories were made. It is clear from Fig. 8 that the PLS model is able to produce accurate predictions of DO and CO_2, which clearly appear to be much closer to the true values of these two process variables when compared to their noisy measurements.

In summary, the results displayed in Figs. 4 to 8 demonstrate the ability of the proposed modelling approach to accurately predict future trajectories of both readily measured process variables and intermittently measured product quality-related variable. These results indicate suitability of the proposed prediction model to be utilised for the trajectory tracking MPC control of batch product quality.

3.3. Trajectory tracking control using the identified model

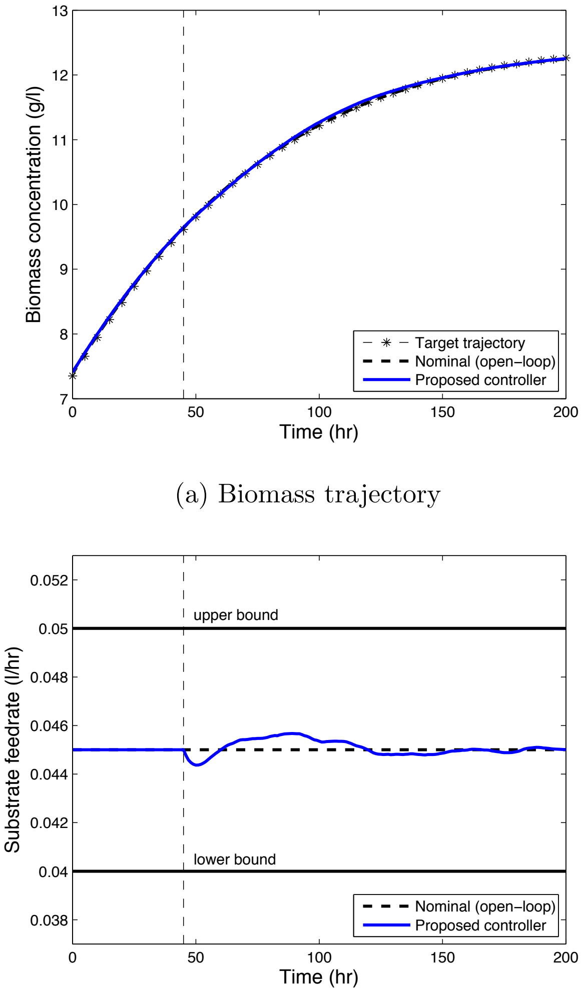
This subsection details the results obtained when the proposed controller, utilising the PLS model, was used to track target trajectory of biomass concentration. The results presented in this subsection assumed that no intermittent measurements were available during any of the batch runs. For all the subsequent simulations, the control parameters displayed in Table 2 were selected:

Table 2: Controller parameters

K_w	Decision points	M	Q_1	Q_2	U_{lb} (l/hr)	U_{ub} (l/hr)	Δu_{max} (l/hr)
45	$\{K_w,\ K_w+1,\ \cdots\ ,\ K-1\}$	10	$\mathbf{I}$	$0.1{\cdot}\mathbf{I}$	0.04	0.05	0.005

$\mathbf{I}$ denotes the identity matrix

In order to ensure satisfactory closed-loop system performance the controller was tuned by choosing appropriate values of the control horizon M and cost function weights Q_1 and Q_2. As discussed in Subsection 2.3, U_{lb} and U_{ub}, are normally derived from the saturation constraints imposed on the actuation equipment. Alternatively, they are introduced to reduce the chances of erratic controller action and wear-and-tear of actuation equipment. In this particular case study the actuation limits were selected to ensure that the process remains fairly close to the nominal operating regime which, in turn, would also ensure that the simulation remains realistic.



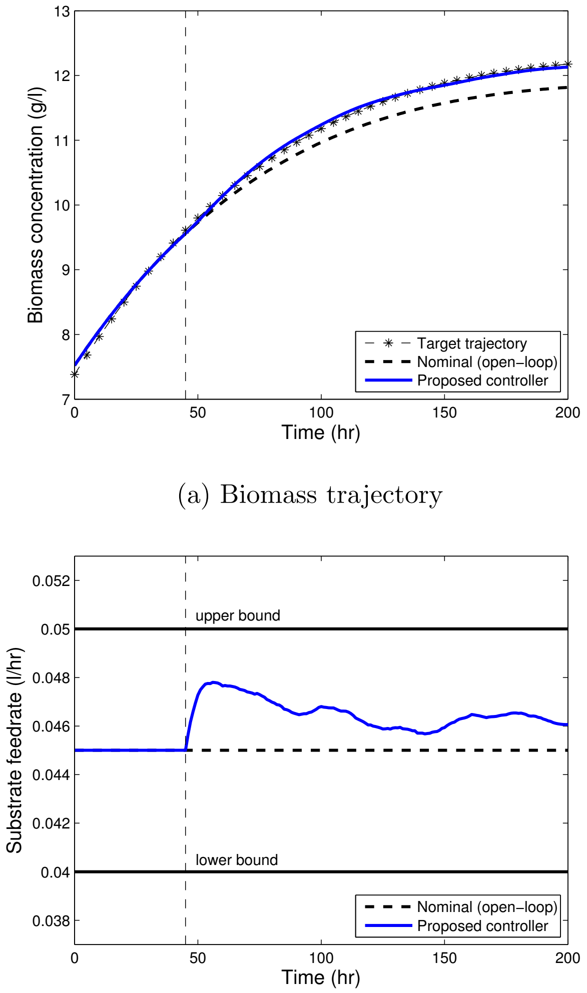
(a) Biomass trajectory

(b) Manipulated variable trajectory

Figure 9: Performance of the trajectory tracking controller considering noisy measurements and assuming that no disturbances affected the batch.

To demonstrate the capability of the proposed controller to perform trajectory tracking of product quality, the results of three simulated batch runs are shown in Fig. 9, Fig. 10 and Fig. 11. The desired biomass trajectory was assumed to be known and obtained by applying a nominal substrate feed rate of 0.045 l/hr in the absence of any disturbances. The vertical dashed line shown in each of the figures represents the sample instant $k = K_w = 45$ at which the trajectory tracking MPC controller becomes active. These figures show both the biomass concentration and the substrate feed rate trajectories.

The results displayed in Fig. 9 correspond to the batch during which noise with SNR equal to 40 dB was added to all measurements. The results displayed in Fig. 9 show the robustness of the proposed controller to the presence of measurement noise. Most notably, the computed manipulated variable shown in Fig. 9(b) remains close to its nominal trend and does not appear to be significantly affected by the measurement noise.

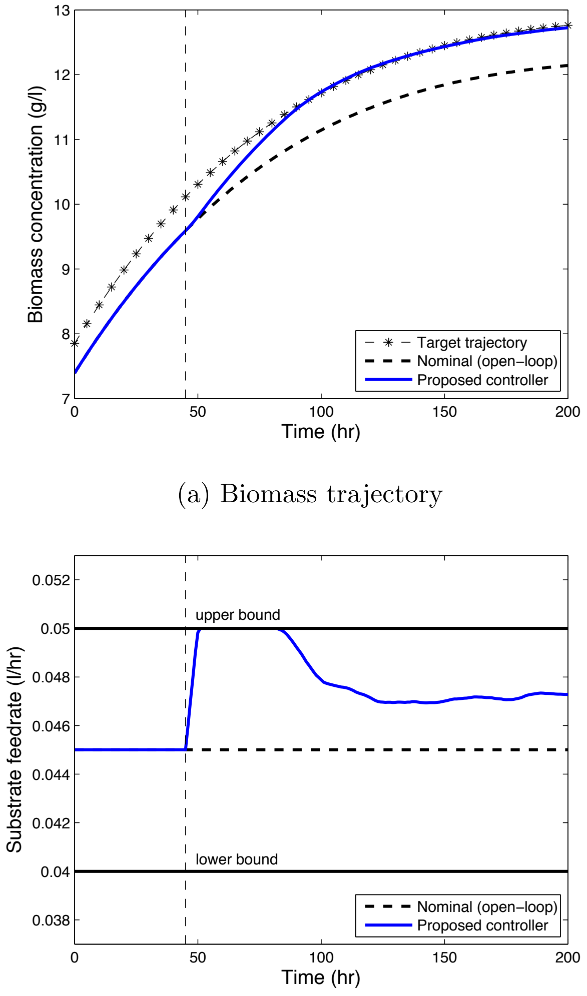


(a) Biomass trajectory

(b) Manipulated variable trajectory

Figure 10: Performance of the trajectory tracking controller considering noisy measurements and a small change in batch initial conditions.

Fig. 10 shows the trajectories of biomass concentration and substrate feed rate obtained from the second simulated batch. For this batch, measurement noise with SNR equal to 40 dB was added and the substrate feed concentration was changed from nominal 600 g/l to 590 g/l through the entire batch. This change of the substrate feed concentration represents constant un-modelled and unmeasured disturbance that has a considerable impact on biomass concentration. It is clearly shown in Fig. 10(a) that the desired biomass concentration was not reached using the nominal substrate feed rate of 0.045 l/hr. On the other hand, the proposed controller was capable of achieving the desired end-quality as well as adequate tracking of the desired biomass concentration trajectory. The adjustments made by the proposed controller to the manipulated variable are displayed in Fig. 10(b).



(a) Biomass trajectory

(b) Manipulated variable trajectory

Figure 11: Controller performance considering noisy measurements and a slightly different target trajectory.

Simulation results from a third batch are displayed in Fig. 11. For this batch the target trajectory of biomass concentration was increased uniformly from its nominal trend by 0.5 g/l. Furthermore, measurement noise and a slightly different initial substrate concentration (595 g/l) were also applied. It can be seen in Fig. 11(a) that the proposed controller was able to track the desired product quality trajectory by adding the offset $\Delta y = 0.5$, calculated using Eq. (30). The adjustments made by the controller to the substrate feed rate are shown in Fig. 11(b), which notably did not violate any of the actuation constraints (i.e. $U_{lb} \leq u_{mv} \leq U_{ub}$).

The results shown and discussed in this subsection demonstrate the capability of the proposed controller to track the desired trajectory of the product quality. These results were obtained under the assumption that no intermittent measurements of the biomass concentration are available. Although it may often be unfeasible to continuously measure product quality, it is reasonable to assume that a few laboratory assays could be carried out during a new batch. The data obtained from those laboratory assays can then be utilised by the proposed controller in order to reject unmeasured disturbances, as will be demonstrated in the following subsection.

3.4. Controller performance with intermittent quality measurements

This subsection considers the case in which intermittent measurements of biomass concentration are available and are utilised as feedback information by the proposed controller in order to reject the unmeasured disturbances. The proposed controller is compared with the end-point controller proposed in [22] which does not utilise intermittent measurements of product quality. Also, the comparison is made with the so-called open-loop scheme which simply implements constant nominal substrate feed rate equal to 0.045 l/h throughout a batch duration.

In order to demonstrate the benefits of considering intermediate product quality values rather than just the batch end-product quality, the simulated batch process was subjected to an un-measured disturbance represented by a change in substrate feed concentration from its nominal constant value of 600 g/l. Also, it was assumed that two intermittent measurements were taken at $k = 50$ and $k = 150$.

The results obtained from a single batch run are shown in Figs. 12 and 13, which correspond to the product quality and manipulated variable trajectories, respectively. In this case disturbance took form of a single step change of substrate feed concentration from its nominal value of 600 g/l to 550 g/l occurring at $k = 30$. By looking at Fig. 12 it can be noted that both the proposed controller and the endpoint controller increase the substrate feed rate in order to cope with the disturbance.

However, the proposed controller achieves a much better tracking performance and ensures biomass concentration at the end-point is closer to its desired value, when compared to the batch end-point controller.

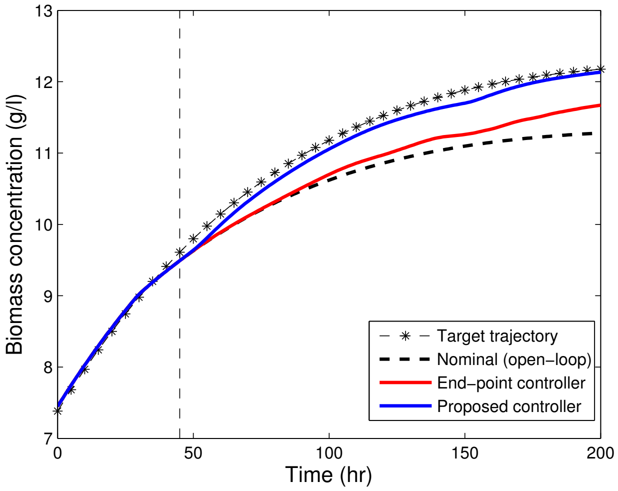


Figure 12: Comparison of the trajectory tracking performance in the presence of an un-modelled disturbance (step change in substrate concentration at the 30^{th} hr).

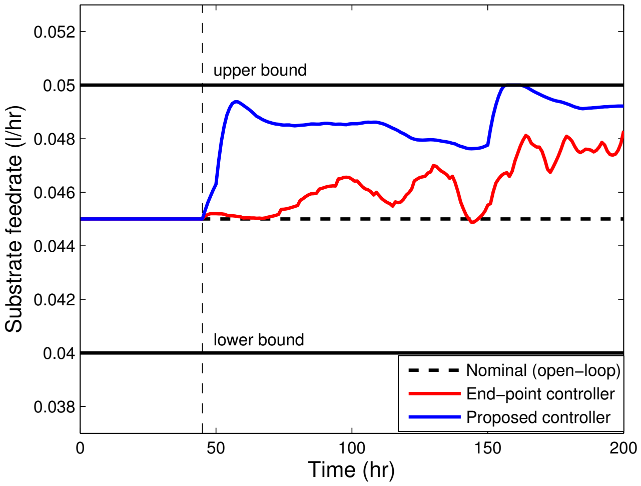


Figure 13: Comparison of the manipulated variable trajectories computed by the controllers in the presence of an un-modelled disturbance (step change in substrate concentration at the 30^{th} hr).

Controller performance was also assessed by employing two different metrics that quantify the tracking error of the biomass concentration. Firstly, root mean squared error (RMSE) metric is used to compare the actual and the desired biomass concentration trajectories and is calculated using the following equation:

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{k=1}^{K} \left(\frac{y_k - y_k^*}{y_k^* - \overline{y}^*} \right)^2}{K}} \tag{36}$$

Also, relative end-point error (EPE) is calculated using the following formula:

$$\mathrm{EPE} = 100 \cdot \left| \frac{(y_K - y_K^*)}{y_K^*} \right| \tag{37}$$

Note that the RMSE is scaled by the variation of the desired biomass concentration trajectory in order to clearly specify the controller's performance in the context of the actual variability of the product quality. Also, end-point error is given as a percentage of the desired biomass concentration attained at the batch end-point.

Table 3 presents a summary of the RMSE and the relative end-point error that correspond to the proposed trajectory tracking MPC controller, batch end-point controller and open-loop scheme. These metrics are calculated using the biomass concentration trajectories shown in Fig. 12

Table 3: Trajectory tracking performance comparison in the presence of un-modelled disturbance.

Index	Nominal feed rate	End-point controller	Proposed controller
RMSE	8.26	7.67	2.48
EPE (%)	7.3	4.8	0.4

The results summarised in Table 3 show quantitatively that the proposed controller provides an improved performance when compared to both the end-point controller and open-loop operation, which confirms the results presented in Figs. 12 and 13.

In addition to the results shown in Figs. 12 and 13, further 50 batch runs were simulated. During each of these 50 testing batches substrate feed concentration, which is the dominant unmeasured disturbance, was varied by applying a filtered PRBS signal of ± 30 g/l to a non-nominal substrate feed concentration of 580 g/l. The values of RMSE and relative end-point error that correspond to proposed trajectory tracking MPC controller, batch end-point controller and open-loop scheme are shown in Figs. 14 and 15 for each of the 50 testing batches.

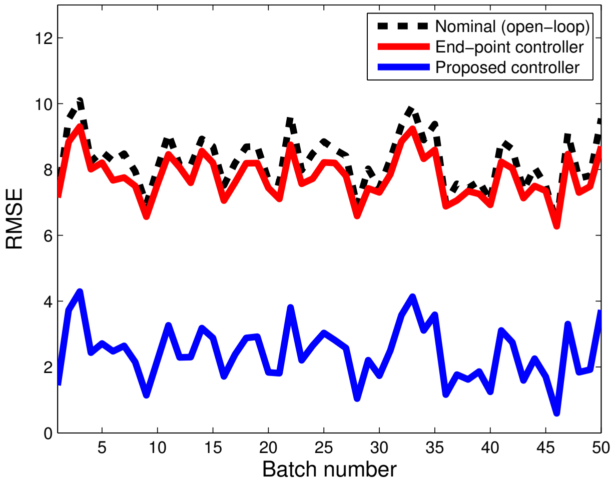


Figure 14: RMSE obtained after simulating 50 batches subject to changes in substrate concentration.

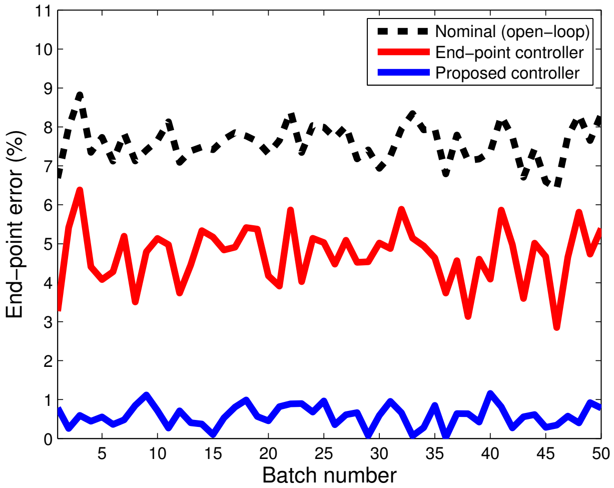


Figure 15: End-point error obtained after simulating 50 batches subject to changes in substrate concentration.

Figs. 14 and 15 do indicate that the end-point controller was able to provide some improvement over simple open-loop scheme by employing a disturbance model within its formulation. This disturbance model is used to calculate the difference between the predictions and the actual values of the readily measured process variables and then use that difference to estimate the impact that the disturbance will have on the controlled variable. However, the manner in which disturbance affects readily measured process variables may be significantly different from its impact on the product quality. Hence, it is much more appropriate to estimate the impact of the disturbance by measuring, albeit intermittently, the actual product quality and compare it with its predicted value, which is the methodology employed by the proposed controller. This is confirmed by the results shown in Figs. 14 and 15 where the RMSE and relative end-point error are both shown to be consistently much lower in the case of the proposed trajectory tracking MPC controller for every single one of the 50 testing batches.

4. Conclusions

This paper described the approach of incorporating intermittent measurements of product quality in order to deliver satisfactory trajectory tracking of desired product quality. This methodology uses the PLS approach to identify a model that relates readily measured process variables and manipulating variables, all of which are considered as inputs, to batch product quality, which is considered as output. Developed was then transformed into autoregressive format by using data imputation and moving window estimation. Resulting autoregressive model can then be recursively evaluated in order to predict future trajectories of both readily and product quality. Hence, the developed model can be readily incorporated into trajectory tracking control of batch product quality.

Case study employing simulated fed-batch fermentation process used to manufacture penicillin was employed to illustrate the principle and the effectiveness of the proposed approach. In particular, it was shown that the developed PLS model was able to accurately predict future trajectories of both the readily measured process variables and product quality. Also, proposed trajectory tracking controller was able to ensure satisfactory trajectory tracking of batch product quality, assumed to be biomass concentration, whilst ensuring manipulated variable constraints were not violated. Furthermore, it was demonstrated that the proposed control scheme can reject disturbances during a batch progression by utilising intermittent measurements whilst ensuring minimal sensitivity to measurement noise. Finally, it was shown that the proposed controller outperforms end-point controller, especially in the presence of inevitable un-modelled disturbances, which makes it a viable candidate for controlling batch/semi-batch processes when intermittent quality measurements are available.

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