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Latent Variable MPC and its Consistency in Temperature Control of Batch Processes

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Abstract: In this work, an investigation has been made in to the performance of latent variable MPC (LV-MPC) in the specific application of reactor temperature control of an exothermic batch process. The paper analyzes the LV-MPC control law derivation and its performance within a batch application. The article considers both constrained and unconstrained applications.

Keywords: Batch process, adaptive control, model predictive control.

1. INTRODUCTION

Batch control is a vast research field, and it has been discussed extensively in the literature. For many batch processes, the regulation of reactor temperature is the primary requirement. Thermal control is often not a trivial task, because the operating conditions vary with time, and therefore the chemical state may change over the batch period. dual-mode control utilizing standard PID (proportional-integral-derivative) was an early approach that was used to perform the desired control profile for batch processes Shinskey and Weinstein (1965).

Iterative learning dual-mode control was proposed by Lee. et al. (2000). Although it has met with some success, the optimal switching time of this approach must normally be defined a priori, hence its performance can be substantially affected when the operating conditions are changed Cott and Macchietto (1989) and Shinskey (1996). Cascade control is widely applied in industrial chemical systems. It was proposed as a technique to address the shortcoming of conventional feedback loops, where the corrective action following a disturbance does not start until deviation from the process set-point is measured. Although Feedforward techniques offer some disturbance rejection capability, they require an explicit model of the disturbance. In contrast, cascade control does not require a model of the disturbance Seborg et al. (2004).

Adaptive control has been successfully applied in many fields including batch processing, where a good knowledge of reactor state can be obtained on-line by using recursive real time estimation techniques. Kiparissides and Shah (1983) promoted adaptive control for batch reactors and compared their performance with fixed gain PID regulators. An adaptive pole-assignment algorithm was proposed by Tzouanas and Shah (1989), which was applied experimentally. Although the idea of the adaptive control is theoretically attractive, it encountered several practical problems such as the sampling rate selection and constraints of the manipulated variables.

Jutan and Uppal (1984) utilized a model-based approach to estimate the heat being released in a reactor at any given time. This information was then used in the feedforward loop to correct the resultant plant-model mismatch. The feedback loop used a Dahlin's algorithm Dahlin (1968) to compensate for the process dead time, and considered tuning the two algorithms (feedforward-feedback) separately. Despite the fact that this technique improved the system performance compared with the open loop strategy, it did not effectively address the problem of thermal overshoot at the beginning of the feed cycle or the drop at the end of this cycle.

Generic Model Control (GMC) developed by Lee and Sullivan (1988), represents an important contribution in this area of research. The approach suggested a general framework for process controllers, where a single-loop PI control, feedforward, decoupling control and model-based control over a finite horizon can be efficiently performed by proper selection of a performance index and an approximate plant model without resorting to linearization.

Bonvin et al. (1989) and Valliere and Bonvin (1989) discussed the necessity for a model to be accurate around the optimal operating conditions in a batch reactor. The issues associated with obtaining all the necessary information regarding the chemical process (due to changes in concentration, viscosity, temperature, etc.) during the reaction was discussed, and it was proposed that where necessary these be inferred using other readily available on-line measurements. In their study, Bonvin et al. (1989) proposed a non-linear or extended Kalman filter (EKF) to estimate the thermal and chemical effects in the reactor.

Rafalimanana et al. (1992) implemented linear Generalized Predictive Control (GPC) to control the temperature profile of a semi batch jacketed pilot reactor based on the pioneering work of Clark et al. (1987). To track the time-varying dynamics of the process, on-line adaptation of a linear SISO model was performed at each sampling instant. The adaptation was carried out using a recursive least squares (RLS) algorithm. The authors concluded that the results from their study encouraged the use of GPC to regulate the temperature in batch reactors.

Chylla and Haase (1993) introduced a mathematical model for a multi-product exothermic semi-batch reactor as a benchmark to test control formulation for batch processes. The process consists of a stirred tank reactor with a jacket that can cool and heat the reactor. The reactor temperature is controlled using a master controller (PID) that manipulates the jacket temperature set-point. The slave controller (PI) is responsible for manipulating the valves, which regulate the jacket temperature. The authors showed that the controlling mechanism could cool and heat the reactor by injecting cold water or high pressure steam into the jacket. The model considers reaction kinetics variability in viscosity and heat transfer mechanisms. The challenge for the control system is to maintain the reactor temperature at a particular set-point while there are changes in raw material properties, heat transfer coefficients, and ambient temperature.

Clarke-Pringle and MacGregor (1997) proposed a nonlinear adaptive controller for the Chylla-Haase process. The article focused on the design of a master controller with PI control being used in the salve loop. A nonlinear controller was designed based on differential geometric control theory. The control formulation involved identifying the time varying factors, such as the heat transfer coefficient using an EKF, where the uncertainty was assumed to be a random walk signal.

Aziz et al. (2000) proposed the use of a neural network model to update the GMC when regulating the temperature in an exothermic batch reactor. Later, Mujtaba et al. (2006) compared three types of nonlinear control strategy. In this work, Mujtaba et al. (2006) compared the performance of a dynamic neural network (NN) estimator coupled, with GMC, direct inverse control (DIC), and internal model control (IMC) for controlling the temperature of an exothermic batch reactor. The results highlighted that all the controllers gave comparable performance, however in the case of DIC and IMC, the NN estimator required more training to achieve similar accuracy to GMC.

Implementation of control by projection to the latent dimensional space was presented by Flores-Cerrillo and MacGregor (2005) for tracking set-point trajectories in batch processes and was named Latent Variable Model Predictive Control (LV-MPC). In LV-MPC, a dynamic PCA model was utilized to determine the control moves. The authors argued that the proposed control law could provide a control action similar to the standard MPC strategy.

In the following subsection the LV-MPC framework is reviewed and examined in detail as a method for controlling the reactor temperature of a batch reactor. The main objective of this study was to highlight certain problems which can exist when implementing this technique to regulate the temperature of a batch process.

The remainder of this paper is organized as; section 2 reviews the design of the LV-MPC. In section 3, results with appropriate analysis are demonstrated, and finally section 4 summaries the study.

2. LV-MPC DESIGN

2.1 Control Law Derivation and Design Considerations

LV-MPC was proposed by Flores-Cerrillo and MacGregor (2005) for batch process trajectory tracking. The control law is essentially obtained using the projection to the model plane (PMP) technique Nelson et al. (1996). Although some studies have presented analogous techniques before, the authors argued that the suggested controller was a more direct approach to integrating process data and MPC through latent variable methods. This multivariate control algorithm exploits the space of a dynamic principle component analysis (PCA) model for set-point trajectory tracking and disturbance rejection. This technique employs a matrix of data, which contains the process variable measurements and the desired output set-point trajectories, in the PCA model construction. Flores-Cerrillo and MacGregor (2005) used data collected from three batches to build the model. During each of the three "training batches", a PRBS sequence was added to the manipulated variable to ensure a rich set of data was collected. The authors mentioned that based on a cross validation principle that was discussed by Wold (1978), 30 latent variables were retained in the PCA model and 17 and 15 past and future horizons were selected for the variables, respectively. Therefore, the LV-MPC approach relies on the assumption that the correlation structure during the current batch matches that obtained in the training batches.

This paper will not present the technique details due the space limitations. Instead the focus will be directed to the final formula of the control law that is used to evaluate the control moves. Flores-Cerrillo and MacGregor (2005) proposed a controller which minimized the following cost function

$$\begin{aligned} &\min\,(\hat{\mathbf{t}} - \mathbf{x_1^T P}_1 - \mathbf{x_2^T P}_2)\mathbf{Q}(\hat{\mathbf{t}} - \mathbf{x_1^T P}_1 - \mathbf{x_2^T P}_2)^{\mathrm{T}} \\ &\text{s.t}\ \ \mathbf{x_2^T} = \hat{\mathbf{t}}^{\mathrm{T}}\mathbf{P}_2^{\mathrm{T}} \end{aligned} \tag{1}$$

where $\mathbf{Q}$ is the weighting matrix, the missing data vector ($\mathbf{x}_2^{\mathrm{T}}$) will be used to drive the process output to match their set-points over the future period. $\mathbf{x}_1^{\mathrm{T}}$ contains all the known variable information up to a time where the current data was collected. Meanwhile $\hat{\mathbf{t}}^{\mathrm{T}}$ denotes the required score vector for the current batch. Corresponding to the data vector partition ($\mathbf{x}_1^{\mathrm{T}}, \mathbf{x}_2^{\mathrm{T}}$), the loadings can be decomposed into two sub-matrices as follows:

$$\mathbf{P} = \begin{bmatrix} \mathbf{P}_1 \\ \mathbf{P}_2 \end{bmatrix} \tag{2}$$

The control objective is to predict the missing data vector $\mathbf{x}_2^{\mathrm{T}}$ that will then drive the process output to match their set-points over the future period. If $\mathbf{Q}$ is an identity matrix, $\mathbf{x}_2^{\mathrm{T}}$ is then explicitly computed as follows:

$$\mathbf{x_2^T} = \mathbf{x_1^T P}_1(\mathbf{I} - \mathbf{P}_2^{\mathrm{T}}\mathbf{P}_2)^{-1}\mathbf{P}_2^{\mathrm{T}} \tag{3}$$

From the orthogonal property, the loading matrix can be rewritten as:

$$\mathbf{P}_1^{\mathrm{T}}\mathbf{P}_1 = (\mathbf{I} - \mathbf{P}_2^{\mathrm{T}}\mathbf{P}_2) \tag{4}$$

and equation (3) then can be further simplified as:

$$\mathbf{x}_2^{\mathbf{T}} = \mathbf{x}_1^{\mathbf{T}}\mathbf{P}_1(\mathbf{P}_1^{\mathrm{T}}\mathbf{P}_1)^{-1}\mathbf{P}_2^{\mathrm{T}} \tag{5}$$

In the case of constrained control, a nonlinear programme routine must be employed to obtain the optimum solution. Under these conditions the following cost function is applied:

$$\begin{aligned} &\min\,(\hat{\mathbf{t}} - \mathbf{x}_1^{\mathbf{T}}\mathbf{P}_1 - \mathbf{x}_2^{\mathbf{T}}\mathbf{P}_2)\mathbf{Q}(\hat{\mathbf{t}} - \mathbf{x}_1^{\mathbf{T}}\mathbf{P}_1 - \mathbf{x}_2^{\mathbf{T}}\mathbf{P}_2)^{\mathrm{T}} \\ &\qquad + \nabla\mathbf{u}_c^{\mathrm{T}}\mathbf{R}\nabla\mathbf{u}_c \\ &\text{s.t}\ \ \mathbf{x}_2^{\mathbf{T}} = \hat{\mathbf{t}}^{\mathrm{T}}\mathbf{P}_2^{\mathrm{T}} \\ &\qquad \mathbf{x}_{c,\min}^{\mathrm{T}} \le \mathbf{x}_c^{\mathbf{T}} = \hat{\mathbf{t}}^{\mathrm{T}}\mathbf{P}_c^{\mathrm{T}} \le \mathbf{x}_{c,\max}^{\mathrm{T}} \\ &\qquad \hat{\mathbf{t}}_{\min}^{\mathrm{T}} \le \hat{\mathbf{t}}^{\mathrm{T}} \le \hat{\mathbf{t}}_{\max}^{\mathrm{T}} \end{aligned} \tag{6}$$

In this equation, all the variables belonging to the missing data vector ($\mathbf{x}_2^{\mathrm{T}}$) that may violate the constraints are represented by $\mathbf{x}_c^{\mathrm{T}}$ in equation (6). $\mathbf{R}$ signifies a control suppression matrix, while $\nabla\mathbf{u}_c^{\mathrm{T}}$ is the vector of manipulated variable moves $[\nabla\mathbf{u}_c^{\mathrm{T}} = (\nabla\mathbf{u}_{c,j}^{\mathrm{T}}, \nabla\mathbf{u}_{c,j+1}^{\mathrm{T}}, \ldots, \nabla\mathbf{u}_{c,j+M}^{\mathrm{T}})\ ]$.

This technique proposed decomposing the loading matrix, $\mathbf{P}$, into $\mathbf{P}_1$ and $\mathbf{P}_2$ corresponding to the known and unknown data, denoted by $\mathbf{x}_1^{\mathrm{T}}\mathbf{x}_2^{\mathrm{T}}$ respectively. Since the missing data algorithm has an impact on the original loading matrix, then the orthogonality of the loading matrix will no longer exist Arteaga and Ferre (2002). With the loss of orthogonality $\mathbf{P}_1$ and $\mathbf{P}_2$ can become ill-conditioned, which can be verified by the norm test (condition number test). The condition number is always greater than or equal to one. If it is close to one, then the data matrix is said to be well conditioned which means that its inverse can be computed accurately. If the condition number is large, then the matrix is said to be ill-conditioned, and inversion can be difficult. Flores-Cerrillo and MacGregor (2005) invert $\mathbf{P}_1^{\mathrm{T}}\mathbf{P}_1$ when solving equation (5) at each sampling period and with $(\mathbf{P}_1^{\mathrm{T}}\mathbf{P}_1)$ being ill-conditioned then problems can results, even when iterative techniques are used to solve the equation.

The mechanistic description of an exothermic batch reactor that was described by Cott and Macchietto (1989) and later by Flores-Cerrillo and MacGregor (2005) is used in this work as a benchmark simulation of a batch process and as a test-bed for the developed control system. For the sake of consistency with the original work of Flores-Cerrillo and MacGregor (2005), all the design considerations (number of latent variables, past and future horizons, etc.) that were proposed by these authors were applied here. Therefore, a dynamic PCA model was constructed from the data collected from three PID controlled batches, sampled at 0.5 min with PID settings of $K_c = 13.5381$, $\tau_I = 28.75$, $\tau_D = 0.406$. The duration of each batch was 150 min. PRBS excitation was added to the PID output to ensure sufficient excitation of the process. Flores-Cerrillo and MacGregor (2005) suggested that the amplitude of the PRBS signal be chosen to be quite small so that operation of the batch was not significantly upset.

To make quantitative comparison, a mean absolute error (MAE) statistic is used to track the performance of the implemented controllers This statistical index is derived from the following equation Flores-Cerrillo and MacGregor (2005):

$$\mathrm{MAE} = \sum_{i=1}^{N} \frac{|y_{cv,i} - y_{sp,i}|}{N} \tag{7}$$

where $y_{cv,i}$ is the controlled variable, $y_{sp,i}$ represents its corresponding set-point, and N denotes the number of samples.

When testing LV-MPC it was found that its performance was inconsistent, with instability resulting during some tests. To thoroughly test the controller, data was collected from 60 batches operating under PID control. Three batches of data were taken from these 60 batches and a dynamic PCA model identified. Again to be consistent with the original work of Flores-Cerrillo and MacGregor (2005), the dynamic model was then utilized by LV-MPC to control an on-line batch. In the simulation, normally distributed random noise with a standard deviation of 0.2 was added to the reactor temperature measurement. This process was repeated 20 times. The LV-MPC solution was evaluated by comparing the direct solution (DR) approach, equation (5), with the optimization of equation (6), which considers constraints. In this work equation (6), was solved using a quadratic programming routine, which it was anticipated would be more robust to the ill-conditioning. This method is referred to as the QP solution.

To further determine the reliability of the controller, tests were conducted with increased PRBS amplitude. The MAE index was used to assess the magnitude of the PRBS exactions. In the excitation assessment, the MAE index was calculated firstly for the reactor temperature controlled by PID without PRBS excitation, and then compared with others, which were subjected to the PRBS excitation. Three types of excitation were considered:

1. Low excitation (LOW) with MAE = 34% Flores-Cerrillo and MacGregor (2005) higher than when no PRBS was added.
2. High excitation (HIGH) with MAE = 486.1% higher than when no PRBS was added.
3. Very high excitation (VHIGH) with MAE = 731.14% higher than when no PRBS was added).

The results are classified as:

1. Direct solution with low excitation (DR-LOW).
2. Direct solution with high exaction (DR-HIGH).
3. Direct solution with very high exaction (DR-VHIGH).
4. QP solution with low excitation and $\mathbf{R} = 0$ (QP-LOW, $\mathbf{R} = 0$).
5. QP solution with low excitation and $\mathbf{R} = 0.001$ (QP-LOW, $\mathbf{R} = 0$).
6. QP solution with high excitation and $\mathbf{R} = 0$ (QP-HIGH, $\mathbf{R} = 0$).
7. QP solution with very high excitation and $\mathbf{R} = 0$ (QP-VHIGH,).
8. QP solution with very high excitation and $\mathbf{R} = 0.001$ (QP-VHIGH, $\mathbf{R} = 0.001$).
9. QP solution with very high excitation and $\mathbf{R} = 3 \times 10^{-7}$ (QP-VHIGH, $\mathbf{R} = 3 \times 10^{-7}$)
10. QP solution with very high excitation and $\mathbf{R} = 3 \times 10^{-7}$, $\sigma = 0.25$ (QP-VHIGH, $\mathbf{R} = 3{\times}10^{-7}$, $\sigma = 0.25$).

Note that not all the mentioned results will be presented here due to the space shortage. However, the discussion will consider all of them.

3. SIMULATION RESULTS AND INTERPRETATIONS

Figures (1) to (6) show the training data, performance of the LV-MPC technique, and MAE indices based on the DR technique of low and high excitation (case studies 1 and 2) respectively. The results of the quadratic programming approach (case study 10) are provided in Figures (7) through (9). The results in Figures (2), (5), and (8) show the inconsistency of LV-MPC when the excitation was low and high for both DR and QP. The tests also reveal that the control signal tends to have an aggressive action. The performance of the LV-MPC controller improved with very high excitation as shown in figure (5) but with control behaviour that would be unsuitable for real application. In each application, the MAE index highlights the instability associated with LV-MPC. By applying the direct solution (DR), on some occasions a stable controller did result, as illustrated in Figure (2), however most tests were poor. The reason for the poor control performance is that the matrix $\mathbf{P}_1^{\mathrm{T}}\mathbf{P}_1$ is ill-conditioned (as showed by the norm tests, the condition number of $\mathbf{P}_1^{\mathrm{T}}\mathbf{P}_1$ varied from 2.2×10^4 to 5.1×10^4.

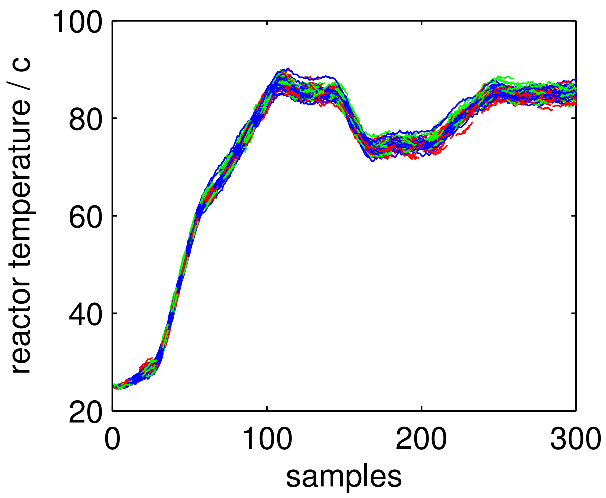

Fig. 1. Training data (60 batches, LOW)

At the first trial using the QP solution, $\mathbf{Q}$ and $\mathbf{R}$ in equation (6) were set to $\mathbf{I}$ and 0 respectively and hard constraints of 15 and 140C were applied to the values of the control action. This should produce results that are comparable to the direct solution obtained earlier. However, this time the QP should be better able to cope with the matrix inversion problem.

The obtained results indicate that the control is significantly improved when high excitation in the training data was applied. However, some of the controllers still resulted in very poor performance. One of the poor performing controllers was then tested with varying weightings imposed on to $\mathbf{R}$. The results obtained with weightings show accurate control can be achieved but with unusual excitation. The results also showed improved stability when

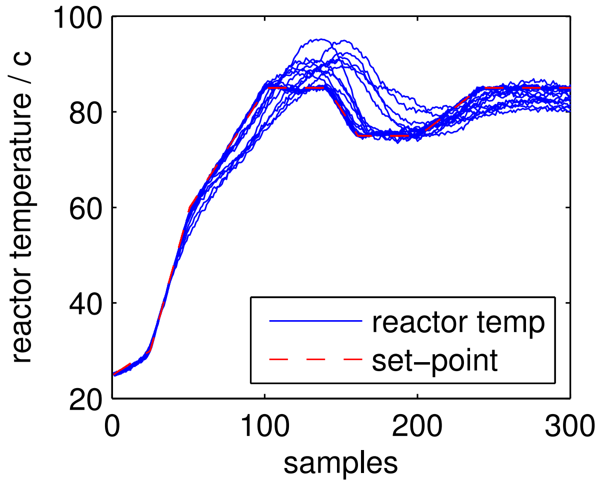

Fig. 2. Reactor temperature (20 batches, DR- LOW)

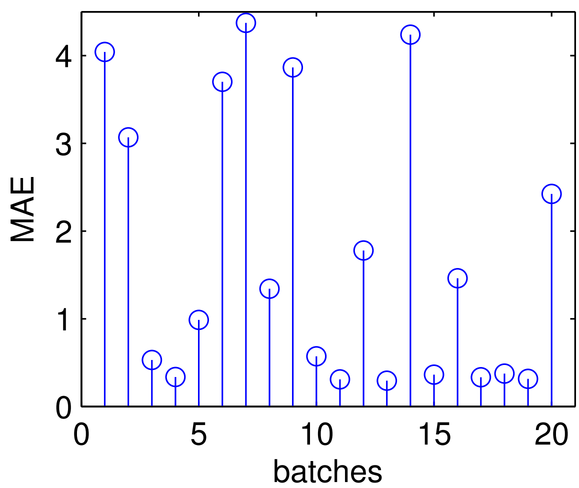

Fig. 3. MAE (20 batches, DR-LOW)

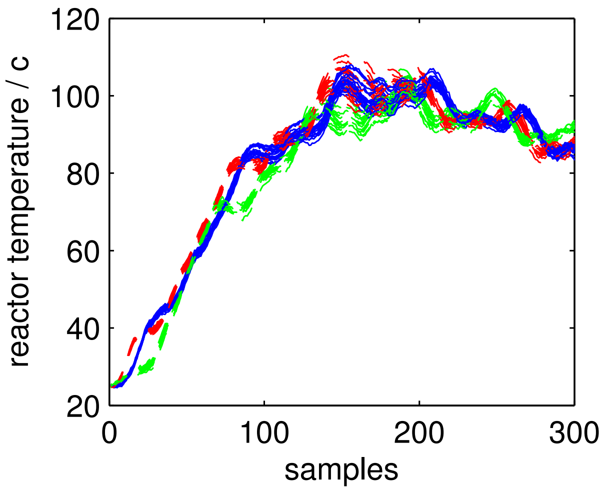

Fig. 4. Training data (60 batches, HIGH)

a very high level of excitation was applied in the case of QP solution. However, when the noise applied to the

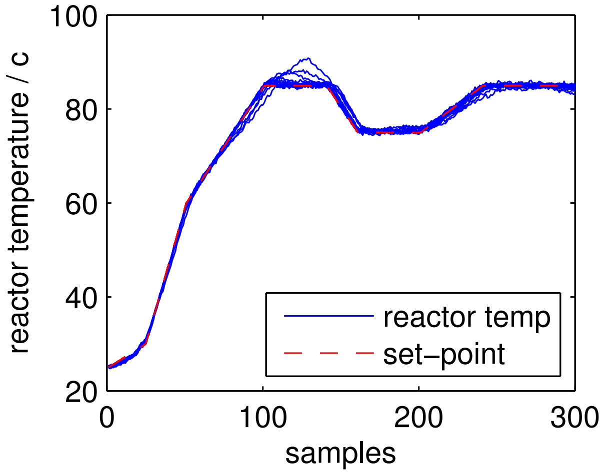

Fig. 5. Reactor temperature(20 batches, DR-HIGH)

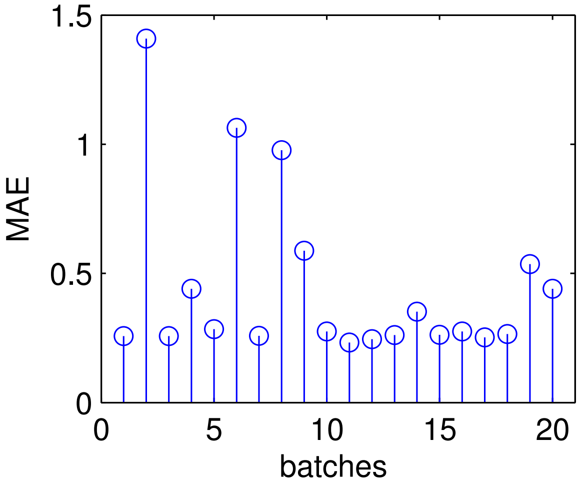

Fig. 6. MAE (20 batches, DR- HIGH)

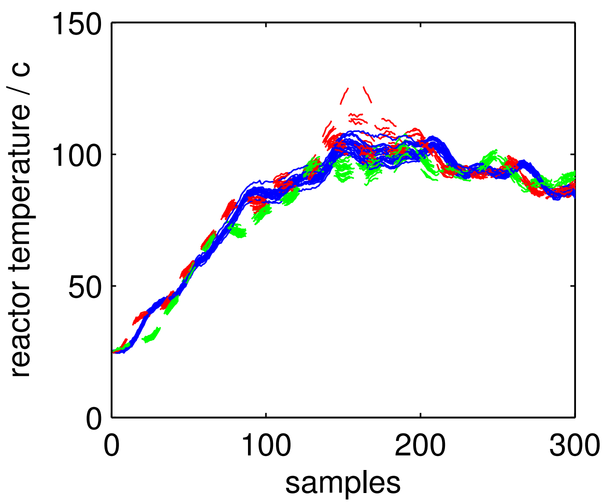

Fig. 7. Training data (60 batches, VHIGH)

output measurements was increased the controller became inconsistent again as illustrated in Figure (8).

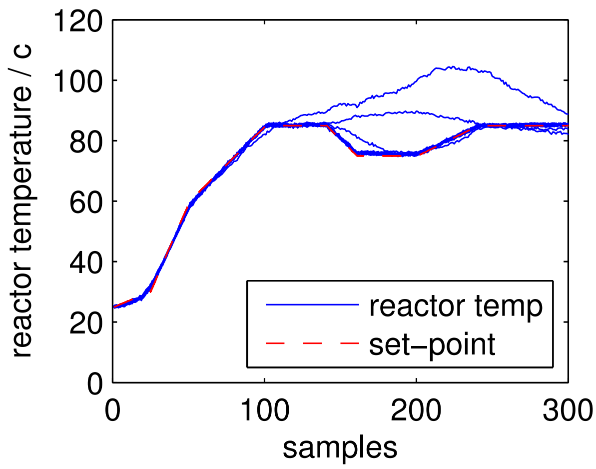

Fig. 8. (20 batches, QP-VHIGH, $\mathbf{R} = 3 \times 10^{-7}$,$\sigma = 0.25$)

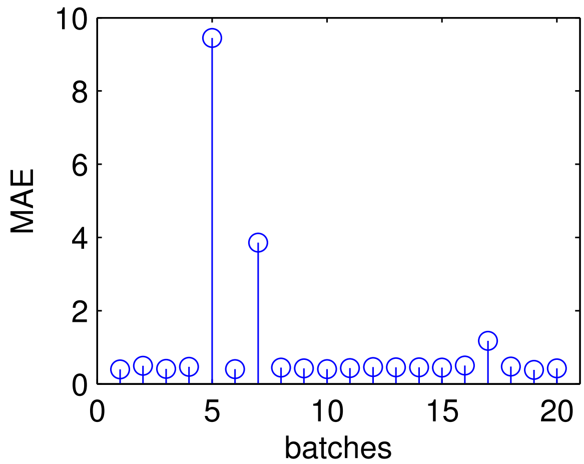

Fig. 9. (MAE (20 batches, QP-VHIGH, $\mathbf{R} = 3 \times 10^{-7}$,$\sigma = 0.25$)

A major problem with LV-MPC is that it requires the solution of an extremely ill-conditioned matrix ($\mathbf{P}_1^T\mathbf{P}_1$). Flores-Cerrillo and MacGregor (2005) stated that this may cause problems, however they suggested that standard control mechanisms could be applied to prevent it being a problem. The analysis reported here shows that this can cause problems even for a QP formulation. Despite the fact that high excitation can partially improve the controller stability for both DR and QP, this comes at the price of an aggressive control signal.

The results highlight the following points:

1. LV-MPC does not appear to be robust for this particular process due to the fact that highly weighted latent variables are ignored. Therefore significant estimation errors may result.
2. The results indicated that a very high level of excitation was required to improve the controller performance. Although high excitation could moderately address the controller stability, it could not eliminate the ill-conditioning problem. However, such excitation is unlikely to be practical in real applications.

4. CONCLUSION

In this paper the LV-MPC technique has been investigated in order to show its suitability for the considered case study. From the control move evaluations, which were based on inferred data, it has been shown that when the missing data has significant weight in the loading matrix the estimate can be generated with very large error, which can result in controller instability.

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