Inferential Product Quality Control of a Multistage Batch Plant

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A modeling framework is developed that addresses the connectivity of a particular, but commonplace, batch plant configuration. Traditional inferential model building techniques such as partial least squares (PLS) and subspace identification are modified to allow for the identification of models that capture the correlation structure across the plant, so that when a disturbance or deviation is detected in one reactor, such information can be shared with other reactors to improve overall control performance. The ability to use information from other running reactors, as well as from previous batch runs, translates into more informed control decisions leading to better overall plant performance. The developed modeling strategy will be applied using data generated from simulating a rigorous model of the Nylon 6,6 process. © 2004 American Institute of Chemical Engineers *AIChE J,* 50: 136–148, 2004

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Introduction

Many batch plants are composed of several batch reactors operating in parallel, of which the primary goal is to produce a product of uniform quality despite persistent disturbances occurring in the plant. An interesting aspect of such plants is that the reactors oftentimes share a common feed source, as well as common utility sources. Hence, disturbances that occur in the feedstream or in the utility supply for one reactor are likely to repeat in adjacent reactors. Yet, it is a common practice to control each reactor in the plant independently of how the other reactors are operating. The traditional control approach involves the sequential execution of recipe steps and the tracking of certain process variables according to product recipe. Often, no attempt is made to adjust the batch condition until a statistical process control (SPC) algorithm like CUSUM or EWMA charts (formed based on the off-line quality measurements) indicate an abnormality. One drawback to this approach is that, when a persistent change occurs in the feedstream and disturbs all of the reactors, the independent SPC charts can be slow in indicating a problem, quickly leading to a large amount of off-spec product.

The focus of this article is on improving existing, as well as developing, new data-based modeling techniques that allow the quality predictor to take into direct consideration the conditions of neighboring reactors operating in parallel. The developed models can help alleviate a common problem in batch process control that control decisions have to be made based on limited information. In the developed approach, control algorithms can be formulated to make use of measurements from previous

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batches, as well as measurements from other running reactors in the plant-wide configuration. The added complexity involved in identifying the plantwide model may be justified by the importance of more informed and, hence, more effective quality control decisions. Much of the discussion and developments that follow will be built around the nylon 6,6 example, but the general configuration of the nylon plant is common to many batch plants.

Overview of nylon 6,6 example

The production of nylon 6,6 involves the polycondensation reaction between hexamethylene diamine (HMD) and adipic acid, which produces water as a byproduct. The reaction is carried out in an autoclave, which is shown in Figure 1. The autoclave is designed to maintain a predefined pressure profile throughout the reaction sequence by venting the produced water. The heat for the vaporization is delivered from a steam supply into the jacket surrounding the vessel. In an industrial setting, several autoclaves are positioned together and their feeds come from a single evaporator, which is used to concentrate the solution of adipic acid and HMD and deliver an equimolar solution of the monomer salts into the autoclaves. There can be several such banks of autoclaves depending on the size of the overall plant. The configuration is depicted in Figure 2. The cycle time of the batch evaporator is roughly one-third of the total autoclave cycle time. Therefore, each of the three autoclaves is charged sequentially after each evaporator cycle. Upon the completion of the reaction in the autoclave, the polymer is cast, cut into pellets, and transferred directly into a product blender.

For this study, it is assumed that each reactor is producing a same grade of nylon and, thus, the polymer of each autoclave is blended together to produce the overall final product, which is put into containers at the exit of the blender. The quality of the product from each autoclave is measured in a laboratory periodically, as well as for every container produced from the blender. The two main quality variables are the amine ends concentration and the average molecular weight. It is important for both quality variables to be maintained at the customers' specifications, because changes in the end concentration and/or the average molecular weight can dramatically change the polymer's ability to accept dye or be further processed.

The primary challenge in maintaining the produced polymer at consistent quality levels are changes occurring in the feed condition, utility quality, and individual reactor behavior. Many of the difficulties for controlling the autoclave were addressed by Russell et al. (1998a), who considered several different control strategies for rejecting disturbances occurring in a *single* autoclave. The behavior of the disturbances in the multiunit plant configuration depicted in Figure 2 takes on a more complex nature and has not been looked at, however.

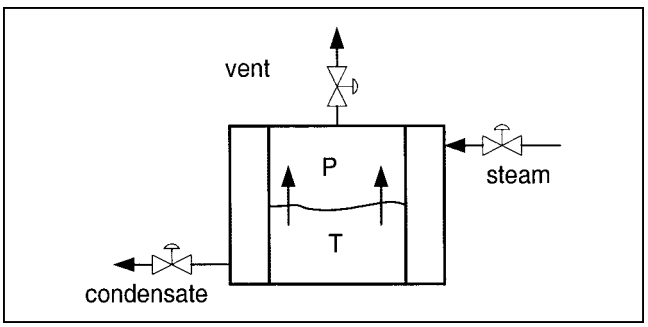

Figure 1. Typical nylon autoclave.

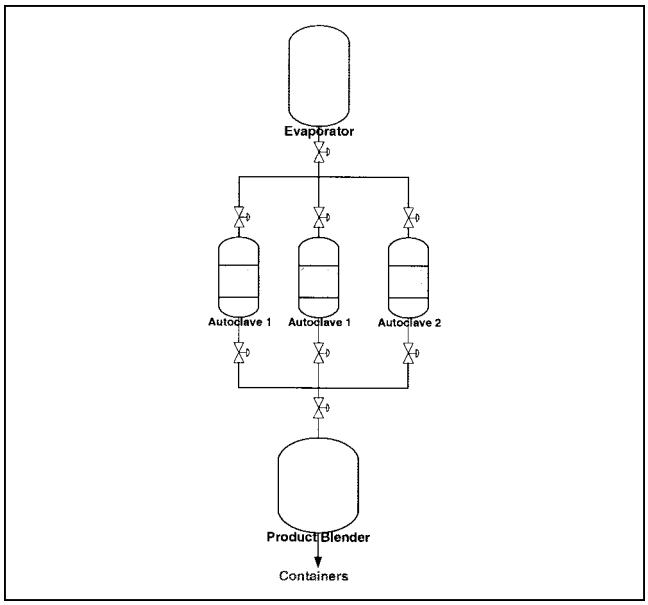

Figure 2. Typical industrial configuration of nylon autoclaves.

An interesting implication of this particular industrial configuration is how disturbances propagate through the plant. When disturbances occur either in the feed of diamine and adipic acid or in the operation of the evaporator, they propagate to each autoclave in a sequential manner. Thus, significant dynamic correlation can exist in the various autoclaves in the bank due to changes in the feed and operating performance of the evaporator. This can lead to significant drifts in the product quality in all the individual autoclaves and in the blender.

The blender can only be effective in reducing short-term random variability of the polymer properties, which are the result of high frequency disturbances. The blender is ineffective in reducing long-term drifts in the product quality, which are the result of low frequency disturbances. Hence, variations that are correlated across the parallel reactor units can have a strong impact on the performance of the product blender. Existing control strategies do not adequately complement the blender's ability to filter out the higher frequency changes in the polymer quality, and they are not efficient in reducing or removing the low frequency drifts in the product quality, which will ultimately be observed in the exit of the blender.

Current SPC methods, which are in place to detect sustained drifts in the process, are sluggish in performance primarily because of the dependence on laboratory quality measurements which are typically available only after long delays. As an example, consider a situation when the SPC algorithm does not detect a drift in the product quality until 7 batches have passed due to a combination of conservativeness of the bounds (for a low false alarm rate) and delays of the quality measurements. If the particular disturbance has occurred as a result of a step change in the concentration of salts charged to the reactors,

then roughly 21 batches of off-spec product will result before a control change is signaled for each of the individual reactors. However, if the connection of the reactors in the plant-wide scheme can be directly considered, a much faster detection may be possible. For example, if the detection scheme required measurements of 7 separate batches regardless of which autoclaves they came from, it would have resulted in only seven batches of off-spec product.

Inferential modeling methods

The main difficulty in making control moves in a batch plant is caused by the measurements of controlled quality variables becoming available only well after the completion of the batch. A potential solution is to build data-based detection or quality prediction models with available *on-line measurements* that correlate well with the off-line quality variables. For the nylon 6,6 example considered here, there are several on-line measurements that correlate well with the final polymer properties: The temperature history of the batch, as well as the vent rate from the process, are good indicators for the extent of the reaction and, thus, of the final polymer properties. In Russell et al. (2000) it was proposed to use the available on-line measurements to predict the quality variables by designing an Extended Kalman Filter (EKF) based on a fundamental model of the autoclave. Others have proposed identifying data-based models of the process to infer the product quality or monitor the on-line measurements' space. Nomikos and MacGregor (1995) used real industrial data to demonstrate how the partial least squares (PLS) method can be used for this purpose. The data-based approach is more realistic in practice because of the considerable time and effort often needed to develop an accurate fundamental model of the process in real industrial situations.

One shortcoming of the previous applications of the multivariate statistical methods is that they do not attempt to use information from previous batches or from surrounding units that make up the plant in predicting the product quality of an ongoing batch. They also require in principle that full measurements from an entire batch be available for prediction, even though ways to fill in the missing measurements for a mid-course prediction have been proposed. In order to control an ongoing batch successfully, however, accurate predictions of the quality variables are usually required early in the batch. This can be difficult since, at the start of a batch, only a few measurements would have been collected. Hence, with the approach of treating each batch independently, the control of an ongoing batch can be fundamentally limited by the lack of measurement and batch-to-batch control may be the only possibility. For some applications, this is the best that can be hoped for, since on-line adjustment of batch recipe parameters is difficult once the batch has been initialized. However, the approach is limiting in overall since batch-to-batch variations, which cannot be controlled by a batch-to-batch control approach, can be significant and there may be opportunities to change the remaining recipe at some midpoint of a batch. An indication of a quality problem early in the batch can also be useful for a potential product release decision.

The fact that the amount of measurements are limited in the initial phase of the batch, however, does not mean that accurate early predictions cannot be made at all; one may be able to complement on-line measurements with the information gathered from other running batches or from previous batch runs, if there exist strong correlations. For example, in the nylon 6,6 industrial example highlighted earlier, the operation of each autoclave in the bank is staggered by the cycle time of the evaporator. So, at the start of one autoclave's cycle, the two other autoclaves are well into their production. Measurements from these other running autoclaves can be valuable since they may indicate that a significant change in the feed quality has occurred to raise concerns for the current reactor. Development of modeling and control methods that support such plantwide control decisions is the objective of this article.

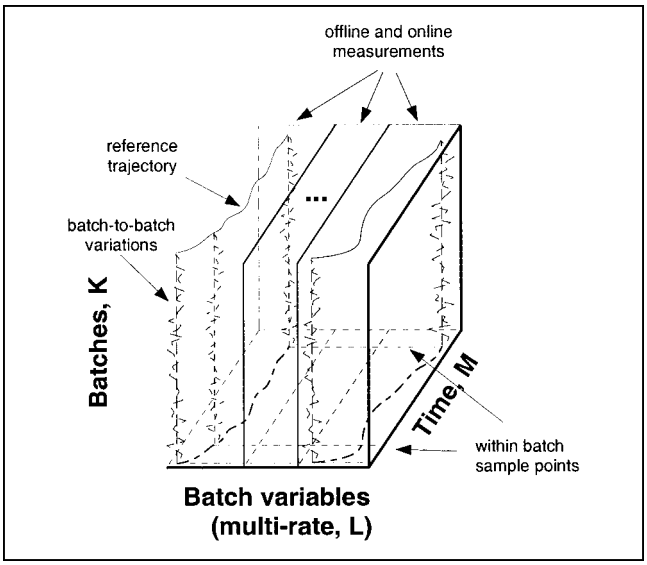

Figure 3. Description of batch data array $\underline{X}$.

Model Development: PLS Approach

The two techniques considered for developing quality prediction models in this article are the PLS method (Wise and Gallagher, 1999) and the subspace identification method (Van Overschee and De Moor, 1994; Dorsey and Lee, 2003). In this section we explore how the PLS method may be used to develop models that capture dynamic correlations among various operational units in the plant. To help understand the modeling approach in the multibatch plant's context, we first discuss the method in the context of a single batch reactor.

Single reactor case

A single batch reactor's process data can be represented by a three-dimensional (3-D) data array containing the different process variables (index = 1, . . . , L) sampled across both the batch dimension (index = 1, . . . , K) and time dimension (index = 1, . . . , M) as depicted in Figure 3. Let $X(K \times L \times M)$ represent this 3-D data array. The application of the PLS method to the batch data begins by first unfolding this 3-D data array into a 2-D matrix. The typical choice for unfolding this array is to preserve the batch dimension and rearrange each resulting batch slice by collapsing the "within-batch" dimensions (L and M). This unfolding process creates a large data matrix $X(K \times LM)$ whose columns contain the batch-to-batch history of a certain variable at a certain sample point within the

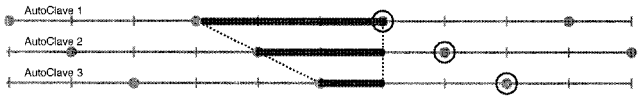

Figure 4. Description of three autoclave cycles.

Solid circles indicate the start of each batch, tick marks indicate the time points within the batch when another autoclave is starting, and the dark solid lines indicate the window of measurements that will be used for prediction of the quality variables (the open circles).

batch. Each row of this matrix is the "lifted" measurement vector for each batch, which contains all of the measurements of batch k ordered in time and will be denoted by $\mathcal{Y}_k^T$

$$\mathcal{Y}_k^T = [\, y(1)_k^T \quad y(2)_k^T \quad \cdots \quad y(M)_k^T] \tag{1}$$

The off-line end quality measurement vectors q_k are then collected in a similar manner in the matrix Q. For the application of the PLS algorithm, the columns of X and Q are first mean-centered and scaled to unit variance. The PLS algorithm is then applied, the result of which can be expressed as the following linear relationship between the lifted batch vector and offline quality measurements

$$\hat{q}_k = B^T \mathcal{Y}_k \tag{2}$$

The above can be used to predict the batch quality variables q_k based on a new observation of the lifted measurement vector $\mathcal{Y}_k$. Here, B is obtained from the matrices of the weighting vectors W, the loading vectors P, and the scores T from the PLS algorithm along with the original Y block of data used in model building (Wise and Gallagher, 1999)

$$B = W(P^TW)^{-1}(T^TT)^{-1}T^TY \tag{3}$$

One difficulty in using the PLS model for quality prediction is that the full data for $\mathcal{Y}$ need to be collected before the prediction can be made. If a batch-to-batch control scheme is implemented, then all of the process measurements from the previous batch can be included in $\mathcal{Y}$. However, if some mid-course control adjustment is desired, then $\mathcal{Y}$ can include only the measurements available up to the control time point. Alternatively, Russell et al. (1998b) demonstrated a recursive formulation that can deliver predictions at every sample time throughout the batch based on a single PLS model. In the context of a multiunit batch plant, we want to develop a model that can allow us to take advantage of the correlation existing across the different reactors for the prediction. For the nylon plant, it is the intent here to exploit the particular production sequence of the plant so that when disturbances pass through the reactors in sequence, measurements from the reactor experiencing the disturbance the first time can be relayed to the other reactors' control algorithms for accurate early-phase predictions.

Multiple reactor case

This section will cover how PLS can be used to build a prediction model capturing dynamic correlations among multiple reactors in a parallel configuration. It will be helpful here to return to the nylon example to explain the application of the PLS modeling approach in such context. As explained in the Overview of Nylon 6,6 section, the three autoclaves in the production configuration are served by a single evaporator. Thus, the batch cycles of the different autoclaves are staggered by the cycle time of the evaporator. When the plant is operating under nominal conditions, this cycle will be more or less uniform and is illustrated by the time line in Figure 4. The solid circles in the illustration represent the start and the end of each autoclave cycle. The tick marks indicate a point in time when another autoclave in the bank is being charged and its cycle is beginning. The position of the tick marks for each reactor will be denoted by $t_{1/3}$, $t_{2/3}$, and t_f. It is desired to make predictions for each of the autoclaves at these points, as well as at the batch's end to allow for the adjustment of operating conditions for the next batch. As described above, it is of interest to take into account the conditions of the other running autoclaves in the control calculation so that any developing trends seen in the other running reactors can be compensated for when choosing the operating conditions for the next batch. The conventional approach is to develop individual PLS models for each autoclave at each of the three time points. This would provide predictions at each of the three points in the production cycle for control adjustment. However, the individual models will not capture the correlation among the variables of the different reactors in the reactor bank. A model that captures such a correlation can potentially give better predictions, especially during the initial phase of the batch when information is limited.

To develop such a model with the PLS technique, we make use of a moving window of process measurements. The darker lines in Figure 4 indicate the window of measurements that will be used from the reactors to predict the quality variables of the reactors at the terminal points (indicated by the open circles). Let $\mathcal{Y}_k^{1^T}$, $\mathcal{Y}_k^{2^T}$, and $\mathcal{Y}_k^{3^T}$ be the full lifted measurement vector from autoclaves 1, 2, and 3, respectively, for batch k. Furthermore, we adopt the notation $\mathcal{Y}^1(1 : t_{1/3})_k^T$ to denote all the measurements up to the end of the first phase or 1/3 of the total batch length, $\mathcal{Y}^1(1 : t_{2/3})_k^T$ to denote all the measurements up to the end of the second phase or 2/3 of the total batch length, and, accordingly, the total batch measurements are denoted as $\mathcal{Y}^1(1 : t_f)_k^T$. There are three possible window configurations depending on which autoclave has just finished its production. The measurements for the three window configurations will be designated as Y_{mw}^1, Y_{mw}^2, and Y_{mw}^3 with the superscript for the respective autoclave that has just finished. Hence

$$Y_{mwk}^{1^T} = [\mathcal{Y}^1(1 : t_f)_k^T \quad \mathcal{Y}^2(1 : t_{2/3})_k^T \quad \mathcal{Y}^3(1 : t_{1/3})_k^T] \tag{4}$$

$$Y_{mwk}^{2^T} = [\mathcal{Y}^2(1 : t_f)_k^T \quad \mathcal{Y}^3(1 : t_{2/3})_k^T \quad \mathcal{Y}^1(1 : t_{1/3})_{k+1}^T] \tag{5}$$

$$Y_{mwk}^{3^T} = [\mathcal{Y}^3(1 : t_f)_k^T \quad \mathcal{Y}^1(1 : t_{2/3})_{k+1}^T \quad \mathcal{Y}^2(1 : t_{1/3})_{k+1}^T] \tag{6}$$

In forming the historical data matrix (X_{mw}), each row is formed by rotating through these as the production would have proceeded, so that the full measurement vector for each autoclave is used at least once. Each row in this matrix will act as an independent observation of this window as it moves through the various autoclaves

$$X_{mw} = \begin{bmatrix} \mathcal{Y}^1(1:t_f)_{k-K+1}^T & \mathcal{Y}^2(1:t_{2/3})_{k-K+1}^T & \mathcal{Y}^3(1:t_{1/3})_{k-K+1}^T \\ \mathcal{Y}^2(1:t_f)_{k-K+1}^T & \mathcal{Y}^3(1:t_{2/3})_{k-K+1}^T & \mathcal{Y}^1(1:t_{1/3})_{k-K+2}^T \\ \mathcal{Y}^3(1:t_f)_{k-K+1}^T & \mathcal{Y}^1(1:t_{2/3})_{k-K+2}^T & \mathcal{Y}^2(1:t_{1/3})_{k-K+2}^T \\ \mathcal{Y}^1(1:t_f)_{k-K+2}^T & \mathcal{Y}^2(1:t_{2/3})_{k-K+2}^T & \mathcal{Y}^3(1:t_{1/3})_{k-K+2}^T \\ \vdots & \vdots & \vdots \\ \mathcal{Y}^1(1:t_f)_k^T & \mathcal{Y}^2(1:t_{2/3})_k^T & \mathcal{Y}^3(1:t_{1/3})_k^T \end{bmatrix} \tag{7}$$

Hence, the first lifted vector in each row corresponds to the reactor that has just finished its production, the second lifted vector of measurements in each row corresponds to the autoclave that will finish next, which is two-thirds of the way into its production, and so on. Some of the measurements will repeat from row to row, but the relative positions within the window will have shifted.

The matrix of quality variables is created in the same manner. Let q_k^1, q_k^2, and q_k^3 denote the quality measurements for autoclaves 1, 2, and 3, respectively, for batch k. Then, collecting these quality measurements into the same form of the moving window used for the on-line measurements gives

$$\mathcal{Q}_{mwk}^{1^T} = [q_{k+1}^{1^T} \quad q_k^{2^T} \quad q_k^{3^T}] \tag{8}$$

$$\mathcal{Q}_{mwk}^{2^T} = [q_{k+1}^{2^T} \quad q_k^{3^T} \quad q_{k+1}^{1^T}] \tag{9}$$

$$\mathcal{Q}_{mwk}^{3^T} = [q_{k+1}^{3^T} \quad q_{k+1}^{1^T} \quad q_{k+1}^{2^T}] \tag{10}$$

$$Q_{mw} = \begin{bmatrix} q_{k-K+2}^{1^T} & q_{k-K+1}^{2^T} & q_{k-K+1}^{3^T} \\ q_{k-K+2}^{2^T} & q_{k-K+1}^{3^T} & q_{k-K+2}^{1^T} \\ q_{k-K+2}^{3^T} & q_{k-K+2}^{1^T} & q_{k-K+2}^{2^T} \\ q_{k-K+3}^{1^T} & q_{k-K+2}^{2^T} & q_{k-K+2}^{3^T} \\ \vdots & \vdots & \vdots \\ q_{k+1}^{1^T} & q_k^{2^T} & q_k^{3^T} \end{bmatrix} \tag{11}$$

The PLS model would then be developed based on the historical data matrices X_{mw} and Q_{mw} to create a model of the following form

$$\mathcal{Q}_{mwk}^i = B^T Y_{mwk}^i \tag{12}$$

where B is obtained from the outputs of the PLS algorithm as described earlier. The model can then used at the end of each batch based on the measurement arranged in the form of Y_{mw}^i to obtain predictions of the respective quality variables within $\mathcal{Q}_{mw}^i$.

To show the benefit of this proposed formulation, data for 400 batch cycles of the three reactors were generated by simulating a fundamental model of the nylon autoclave. To simulate disturbances from the evaporator, changes were introduced across the reactor bank by changing the feed concentrations of adipic acid and hexamethyldiamine in a correlated manner. The data from the first 200 cycles were used for the model building, and the remaining data were used to compare the prediction performance. A single PLS model was built using data from 200 cycles according to the procedure explained above. In contrast, the conventional approach involved building a total of 9 individual PLS models for the three time points and the three separate autoclaves. In Figure 5, the prediction performance of these two methods is compared for autoclave 1 with the remaining 200 batch data. The comparison shown is for the time point where autoclave 1 is only 1/3 of the way through its production. This means the PLS predictions for the moving window formulation are based on Y_{mw}^3, while the PLS predictions shown for the conventional approach are based only on the measurements in autoclave 1 up to $t_{1/3}$. The mean-squared error for the prediction of the average molecular weight over the 200 batches shown in Figure 5 was 0.2975 for the conventional multiple PLS model approach vs. 0.0602 for the moving window PLS formulation. Hence, significant improvement in the quality prediction is achieved by including measurements from the ongoing batches of the other reactors, especially since the prediction is made near the start of the batch when information is limited.

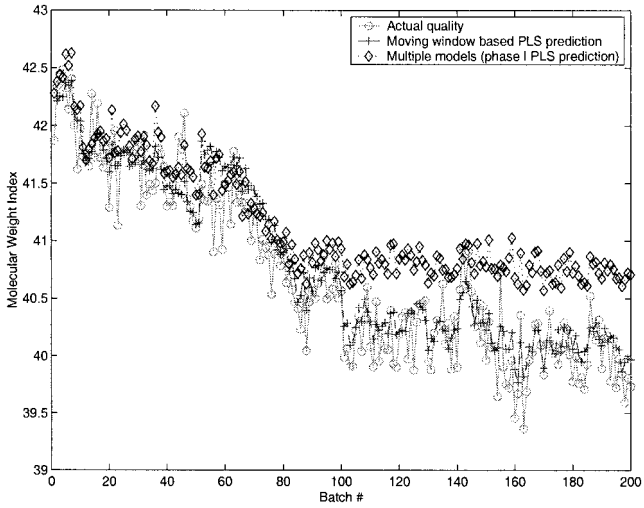

Figure 5. Comparing moving window based prediction performance against multiple model approach in the presence of correlated changes from the feed evaporator.

Note that, for the sake of simplicity, we have not discussed the effect of input (recipe parameter) manipulations that may be present in the historical data. One can certainly include them in the PLS model, or, if a causal model is available, their effect can be subtracted out before the PLS model is developed.

Model Development: Subspace Identification Approach

A drawback of the PLS approach is that the manipulation of the data needed for developing the multireactor moving window-based model can be tedious. Another drawback is that any correlations that exist along the batch number dimension (that is, correlations among successive batches) are ignored. Subspace identification is a technique used to build a state space model directly from available data from the process. It has been used primarily for identifying discrete-time process models for continuously run processes. Recently, Dorsey and Lee (2003) showed how the method can be used on batch process data to derive a model capturing batch-to-batch dynamics or correlations. The main advantage of having a model capturing batch-

to-batch dynamics is that measurements of previous batches such as delayed laboratory measurements of the quality variables can be used directly in the model for improved predictions. In this section, we will first review the application of subspace identification to single reactor process data and then present extensions to the multiple reactor system studied in this article.

Single reactor case

The model identified through subspace identification is typically in the so-called innovation form of

$$x_{k+1} = Ax_k + K\mathscr{E}_k$$

$$\mathscr{Y}_k = Cx_k + \mathscr{E}_k \tag{13}$$

where $\mathscr{E}_k$ represents the model's prediction error and is a white noise sequence. In the continuous process setting, the index k refers to the current sample time. On the other hand, in the batch process setting, the index k refers to the current batch number. Hence, the dynamic correlations captured in the identified state space model are those that are present from batch to batch. Intrabatch dynamics or correlations are captured through the covariance matrix of $\mathscr{E}_k$, which is typically nondiagonal. As before, we don't include the input manipulation effect in the model. One can include their effect in the usual way if the causal model is given, or include the changed input parameters in the output vector.

The application of the algorithm to batch process data begins by first defining a lifted output vector $\mathscr{Y}$ containing all the measurements throughout the batch. Letting the outputs measured throughout the batch be denoted as y and creating the time index $t = 0 \cdots N$, $\mathscr{Y}$ can be expressed as

$$\mathscr{Y}_k^T = [\, y(1)_k^T,\, y(2)_k^T,\, \ldots,\, y(N)_k^T] \tag{14}$$

where $y(n)_k^T$ refers to the vector of available measurements at sample time point n of the k^{th} batch. The dimension of such a lifted vector is typically very high and may cause difficulties in applying the subspace identification algorithm. To address this problem, we first recognize that variations in the elements of $\mathscr{Y}_k$ tend to be strongly correlated since the variations are likely due to a few dominant disturbances, which affect the measurements altogether. Hence, we can use the principal component analysis (PCA) to compress the lifted on-line measurement vector to a much lower dimension. Let $\underline{\mathscr{Y}}$ represent the score vector from applying PCA to data for $\mathscr{Y}$. The quality measurement vector q can then be appended to this reduced vector. The resulting data containing the compressed online data and quality data are then differenced with respect to the batch index in order to minimize the effect of nonstationary batch-to-batch drifts potentially contained in the process data. Let us denote the differenced score vector by

$$\Delta\underline{\mathscr{Y}}_k = \underline{\mathscr{Y}}_k - \underline{\mathscr{Y}}_{k-1} \tag{15}$$

Then, by applying the subspace algorithm to the differenced data, a state space model of the following form can be identified

$$\underline{\mathscr{X}}_{k+1} = A\underline{\mathscr{X}}_k + K\underline{\mathscr{E}}_k \tag{16}$$

$$\begin{bmatrix} \Delta\underline{\mathscr{Y}}_k \\ \Delta q_k \end{bmatrix} = \begin{bmatrix} C_{\mathscr{Y}} \\ C_q \end{bmatrix} \underline{\mathscr{X}} + \underline{\mathscr{E}}_k \tag{17}$$

Here, the output matrix is split into $C_{\mathscr{Y}}$ and C_q to correspond to the reduced process measurement vector and the full quality vector. This model can allow for predictions at all time points during the batch by rewriting the model in a time-based output equation as demonstrated below. This requires us to create the following augmented form of the original model

$$\underline{\mathscr{Z}}_k = [\mathscr{X}_k \quad \underline{\mathscr{Y}}_k \quad q_k \quad q_{k-1} \quad \mathscr{E}_k]^T$$

To illustrate the handling of delayed measurements, we have also assumed that the quality variables are delayed by one batch, and appended the quality measurements from the previous batch to the state vector. The augmented model form is obtained as

$$\underline{\mathscr{Z}}_{k+1} = \underbrace{\begin{bmatrix} A & 0 & 0 & 0 & K \\ C_{\mathscr{Y}}A & I & 0 & 0 & C_{\mathscr{Y}}K \\ C_qA & 0 & I & 0 & C_qK \\ 0 & 0 & I & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}}_{\Phi} \underline{\mathscr{Z}}_k + \underbrace{\begin{bmatrix} 0 & \\ [I_{n_{\mathscr{Y}}} & 0] \\ [0 & I_{n_q}] \\ 0 & \\ I & \end{bmatrix}}_{\Gamma_\varepsilon} \mathscr{E}_{k+1} \tag{18}$$

$I_{n_{\mathscr{Y}}}$ and I_{n_q} are used here to indicate the identity matrices of dimensions of the reduced on-line and full off-line measurements, respectively. The model can be used in real time by creating the following time varying output equation

$$\hat{y}_k(t) = H(t)\Theta\underbrace{(\mathscr{C}\underline{\mathscr{Z}}_k(t|t))}_{\underline{\hat{\mathscr{Y}}}_k(t)} + \varepsilon_k(t) \tag{19}$$

where the residual white noise term ε is added because we have thrown some information away through PCA. We define $\mathscr{C} = [0 \quad I_{n_{\mathscr{Y}}} \quad 0 \quad 0 \quad 0]$ such that the current reduced space vector $\underline{\mathscr{Y}}_k$ is seleeted from $\underline{\mathscr{Z}}_k$. Also, Θ is the matrix containing the PCA loading vectors and expands the reduced vector to the full measurement space. $H(t)$ is a time-varying matrix that picks out those measurements that become available at the t^{th} sample time. This is used together with the batch-to-batch update equation above to form a periodically time-varying system with period M, which in turn can be used to construct a Kalman filter and update the state vector based on incoming on-line measurements $y_k(t)$

$$\underline{\mathscr{Z}}_k(t|t) = \underline{\mathscr{Z}}_k(t-1|t-1) + \mathscr{K}(t)[H(t)\Theta\mathscr{C}\underline{\mathscr{Z}}_k(t-1|t-1) - y_k(t)],\ t \in 1, \ldots, M$$

$$\underline{\mathscr{Z}}_{k+1}(0|0) = \Phi\underline{\mathscr{Z}}_k(M|M) \tag{20}$$

When off-line measurements are available, $H(t)$ should be chosen to include the delayed quality variables from the state equation. This model form thus allows end product quality predictions throughout the batch based on current incoming measurements and previous batch measurements.

Multiple reactor case

The application of the subspace identification method to the multiple parallel reactor configuration that we showed earlier is rather straightforward. The state-space model for the multiple reactor case is created by simply including all of the measurements from the three reactors together in the same output equation. However, the size of the model output that would result from this procedure would be too high for a direct application of the subspace method. Again, to reduce the size of the output equation, one can perform PCA on measurements from the individual reactors, to reduce the dimension of the output vector to a more suitable one. Let $\underline{\mathcal{Y}}^i$ represent the reduced online measurement vector and Θ^i the loading vectors from each autoclave (i = 1, 2, or 3). The lifted vector is formed from the combined reduced on-line measurement sets from each reactor

$$\underline{\mathcal{Y}}_k = [\underline{\mathcal{Y}}_k^{1^T} \quad \underline{\mathcal{Y}}_k^{2^T} \quad \underline{\mathcal{Y}}_k^{3^T}]^T \tag{21}$$

The quality measurements from each reactor are also collected as

$$Q_k = [q_k^{1^T} \quad q_k^{2^T} \quad q_k^{3^T}]^T \tag{22}$$

The state-space model can then be identified based on the differenced form of the reduced data

$$\underline{\mathcal{X}}_{k+1} = A\underline{\mathcal{X}}_k + K\underline{\mathcal{E}}_k \tag{23}$$

$$\begin{bmatrix} \Delta\underline{\mathcal{Y}}_k \\ \Delta Q_k \end{bmatrix} = \begin{bmatrix} C_{\mathcal{Y}} \\ C_Q \end{bmatrix} \underline{\mathcal{X}}_k + \mathcal{E}_k \tag{24}$$

The real-time use of the above model presents some challenges since the actual production of each autoclave is staggered. This requires that the model make a transition to the next set of batches once autoclave 1 has finished, and that the remaining measurements from autoclaves 2 and 3 be treated as delayed variables with respect to the model. This can be done by appending the complete reduced measurements from the previous batch index onto the state vector to allow for correction based on incoming measurements. The augmented model is defined as

$$\begin{bmatrix} \underline{\mathcal{X}}_{k+1} \\ \underline{\mathcal{Y}}_{k+1} \\ Q_{k+1} \\ \underline{\mathcal{Y}}_k \\ Q_k \\ \mathcal{E}_{k+1} \end{bmatrix} = \underbrace{\begin{bmatrix} A & 0 & 0 & 0 & 0 & K \\ C_{\mathcal{Y}}A & I & 0 & 0 & 0 & C_{\mathcal{Y}}K \\ C_QA & 0 & I & 0 & 0 & C_QK \\ 0 & I & 0 & 0 & 0 & 0 \\ 0 & 0 & I & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}}_{\Phi} \begin{bmatrix} \underline{\mathcal{X}}_k \\ \underline{\mathcal{Y}}_k \\ Q_k \\ \underline{\mathcal{Y}}_{k-1} \\ Q_{k-1} \\ \mathcal{E}_k \end{bmatrix} + \underbrace{\begin{bmatrix} 0 \\ [I_{n_{\mathcal{Y}}} \quad 0] \\ [0 \quad I_{n_Q}] \\ 0 \\ 0 \\ 0 \\ I \end{bmatrix}}_{\Gamma_\varepsilon} \mathcal{E}_{k+1} \tag{25}$$

To use this model for real-time prediction, we first define the time-varying output equations for the three autoclaves

$$y^1(t)_k = H^1(t)\Theta^1\mathcal{C}^1\underline{\mathcal{Y}}_k \tag{26}$$

$$y^2(t)_k = H^2(t)\Theta^2\mathcal{C}^2\underline{\mathcal{Y}}_k \tag{27}$$

$$y^3(t)_k = H^3(t)\Theta^3\mathcal{C}^3\underline{\mathcal{Y}}_k \tag{28}$$

Here, $\mathcal{C}^i$ is used to extract the reduced measurement sets, $\underline{\mathcal{Y}}^i$ (either $\underline{\mathcal{Y}}_k^i$ or $\underline{\mathcal{Y}}_{k-1}^i$ depending on whether the k^{th} batch has already started for the i^{th} autoclave), from each autoclave, Θ^i projects the reduced vector back to the full batch dimension for each autoclave, and $H^i(t)$ is used to select the vector of current measurements for sample time t from $\mathcal{Y}^i$. This model can be used to formulate the Kalman filter, which can be used for real-time prediction based on all incoming measurements from the three reactors.

Batch-to-Batch Control Formulation

For the nylon example, the amount of excess of monomer (HMD) is a potential input, which can be adjusted only at the start of the batch. The other potential input is the pressure setting in the reactor for the later stage of reaction. The directionality of these input moves typically requires that they be moved together. Therefore, the control approach for this study will be restricted to batch-to-batch control. Two control formulations will be considered. In one approach, the control adjustment for each autoclave will be calculated independently of the conditions of the other running autoclaves. In the other approach, the conditions of the other autoclaves are taken into account in the control calculation by using a multireactor prediction model and also by including the prediction of the blended quality in the objective function.

Modeling the blender

The product blender serves two functions. The first function is to disperse variations that occur through time during casting of a particular autoclave into the volume of the blender. The blender also acts to disperse variations across the different autoclaves to obtain a more uniform product. The blender will be modeled as a first-order low-pass filter. The future state of the blended quality can be represented as a function of the current state of the blender and the properties of the polymer that is added to the blender

$$\bar{q}_{k,i}^b = (1 - \alpha)q_k^i + \alpha\bar{q}_{k,i-1}^b \tag{29}$$

Note that this model is identical to the exponential moving average filter. The model parameter α is set according to the average residence time of the blender, that is, $\alpha = e^{-t_B/\tau}$ where t_B is a 1/3 of the batch length and $\tau = V/F$ where V is the volume of the blender and F is the average blender charge rate per time. The quality of the product of the current autoclave i to be charged to the blender is designated as q^i. The quality of the blended product output after the charge of the i^{th} batch in the k^{th} cycle is denoted by $\bar{q}_{k,i}^b$. Note that, for the three batch blender $\bar{q}_{k,0}^b = \bar{q}_{k-1,3}^b$. This blender model allows for control decisions to be made for each autoclave based on the predicted impact on the final blended product quality. In terms of reducing the final product variability, the blender is effective at

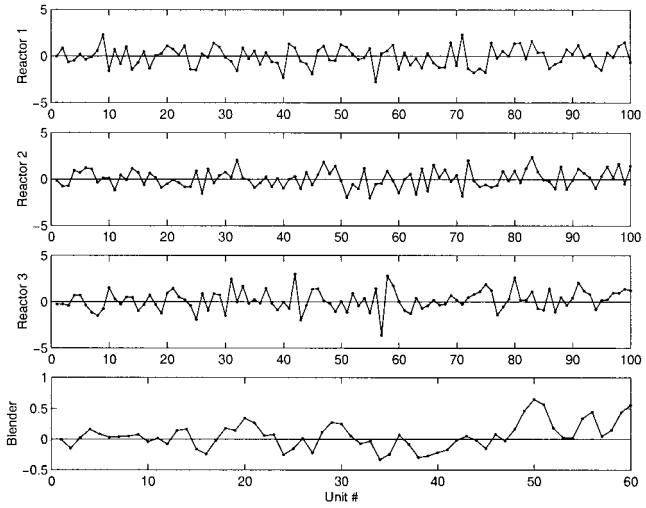

Figure 6. Blended product quality when no correlation exists through the parallel autoclaves.

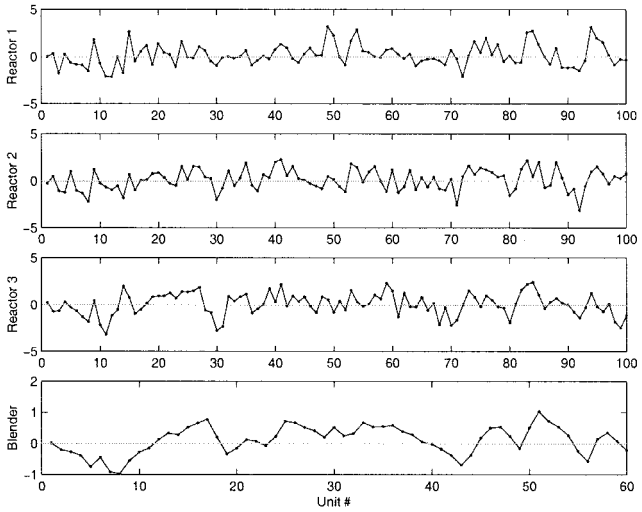

Figure 7. Blended product quality with a moderate level of correlation across the parallel autoclaves.

reducing high frequency variations, but has difficulty in blending away sustained drifts or other low frequency disturbances.

To illustrate the effect of disturbances of different frequencies, we model the changes in the feed concentrations of adipic acid and HMD from the evaporator as

$$d_{j+1} = \phi d_j + \varepsilon_{j+1} \tag{30}$$

where ε is a zero-mean, normally distributed random variable and ϕ is a parameter used to adjust the level of correlation in the successive charges and, hence, the level of correlation across the parallel autoclaves. For example, $\phi = 0$ is used to simulate the case where there is no correlation in the feed to the parallel reactors. The resulting product quality fluctuations for the outputs of the three autoclaves and the blended product for a 100 batch realization of this model is shown in Figure 6. It is assumed that the final product is shipped in volume of 5 batches and, therefore, its quality displayed in the figure is the average of every 5 outputs of the blender equation. Figure 7 shows the same for an intermediate level of correlation in the feeds across the autoclaves with $\phi = 0.4$. In Figure 8, a stronger degree of correlation, $\phi = 0.9$, was used to show the predicted impact on product blending when strong correlations exist across the autoclaves. The results match our intuition that the blender effectively reduces high frequency variations, but are less effective in reducing slow variations in the product quality. This can be seen by the more sustained drifts in the blended output in the strongly correlated cases. These drifts in the product containers could lead to downstream processing problems. Hence, from the control perspective, it is desired to minimize correlations across the autoclave bank in order to complement the product blender.

Traditional independent batch-to-batch control approach

One common control approach is to control each reactor independently in the plant-wide configuration. First, we define the quality control error for batch k as

$$e_k = q_k - q^r \tag{31}$$

where q^r is the desired or reference quality vector. A common assumption in formulating a batch-to-batch control law is that any errors that occur in the current batch will repeat in the next batch. Let us assume the effect of control adjustments on the product quality is described as

$$\Delta q_k = D\Delta U_k \tag{32}$$

We can then express the predicted quality deviation for the next batch as

$$e_{k+1|k} = e_k - D\Delta U_{k+1} \tag{33}$$

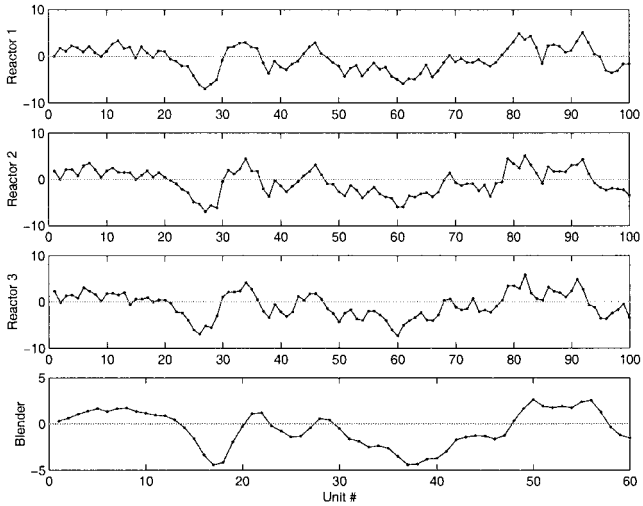

Figure 8. Blended product quality with a strong level of correlation across the parallel autoclaves.

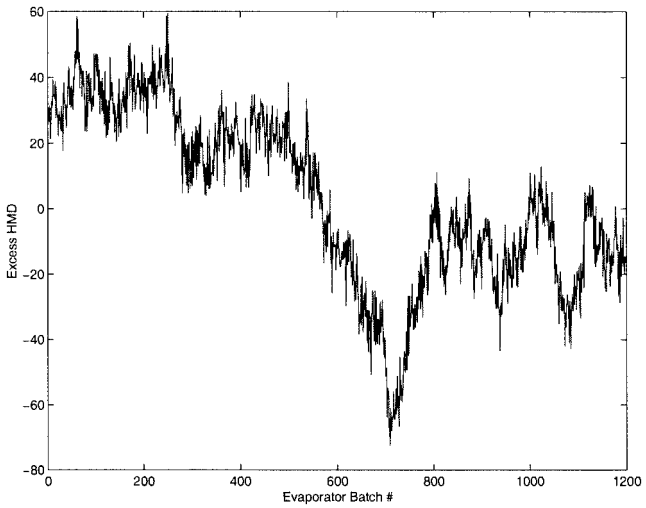

Figure 9. Excess diamine disturbances in salt charge from the evaporator.

which states that quality errors will repeat in the next run unless control action ΔU is prescribed. Using a standard quadratic criterion of

$$\min_{\Delta U_{k+1}} e_{k+1|k}^T Q e_{k+1|k} + \Delta U_{k+1}^T R \Delta U_{k+1} \tag{34}$$

one can calculate the desired input change ΔU_{k+1} based on predictions of e_{k+1} at the end of each batch k and Eq. 33

$$\Delta U_{k+1} = (D^T Q D^T + R)^{-1} D^T Q e_{k+1} \tag{35}$$

Q and R are weighting parameters that can be used to filter the high frequency variations or noise and make the control adjustment less aggressive. For the nylon example considered here, these calculations are made independently for each autoclave. This means that quality predictions for autoclaves 2 and 3 are not considered in calculating control input moves for autoclave 1.

Plant-wide control approach

As pointed out in the discussion around the product blender, the ability to generate a uniform product quality can be improved by reducing correlations that exist across the parallel reactors. This can be done by directly considering the conditions of the other two autoclaves in determining the control adjustment for the current autoclave to be charged from the evaporator. Note that the output of the current autoclave in question will be cast into the blender only after the other two autoclaves in the parallel batch configuration are cast. One possible way of accomplishing this is to control the blended product output, which is predicted based on the outputs of the multireactor predictor discussed in the previous section. This way, one can minimize correlations across the autoclaves, as well as reducing variations that might occur within any individual reactor.

In forming the control law for this scenario, we should consider the predicted blender output prior to the casting of the current autoclave in question. As an example, consider that batch $k-1$ of autoclave 1 has just been completed and it is desired to calculate control input moves for batch k. The parallel batch configuration implies that batch $k-1$ of autoclaves 2 and 3 will charge, in succession, into the product blender prior to batch k of autoclave 1. Thus, by recursion of the blender model, the predicted blender output after casting batch $k-1$ of autoclave 3 is

$$\bar{q}_{k,0}^b = \alpha^3 \bar{q}_{k-1,0}^b + (\alpha^2 - \alpha^3) q_{k-1}^1 + (\alpha^1 - \alpha^2) q_{k-1}^2 + (1-\alpha) q_{k-1}^3 \tag{36}$$

where 0 in the subscript $(k, 0)$ implies that none of the batches for the k^{th} cycle have yet been considered. Similar prediction equations can be developed for the other autoclaves

$$\bar{q}_{k,1}^b = \alpha^3 \bar{q}_{k-1,1}^b + (\alpha^2 - \alpha^3) q_{k-1}^2 + (\alpha^1 - \alpha^2) q_{k-1}^3 + (1-\alpha) q_k^1 \tag{37}$$

$$\bar{q}_{k,2}^b = \alpha^3 \bar{q}_{k-1,2}^b + (\alpha^2 - \alpha^3) q_{k-1}^3 + (\alpha^1 - \alpha^2) q_k^1 + (1-\alpha) q_k^2 \tag{38}$$

These prediction equations can be used to formulate the future control error for the product blender as a function of the calculated input move for the autoclave in question, which enters through q_k^i

$$e_{k,i}^b = \alpha \bar{q}_{k,i-1}^b + (1-\alpha) q_k^i - q^r \tag{39}$$

where $q_k^i = \hat{q}_k^i + D\Delta U_k^i$. Note that $\hat{q}_k^i$ is a quality predictions provided by the multireactor predictor based either on the moving window PLS or the subspace identification. This control error for the blender can be combined with the control error for the individual reactor, which is developed in the same manner as in the previous section. In this case, we use e^i to denote the predicted control error $(q_k^i - q^r)$ for each individual

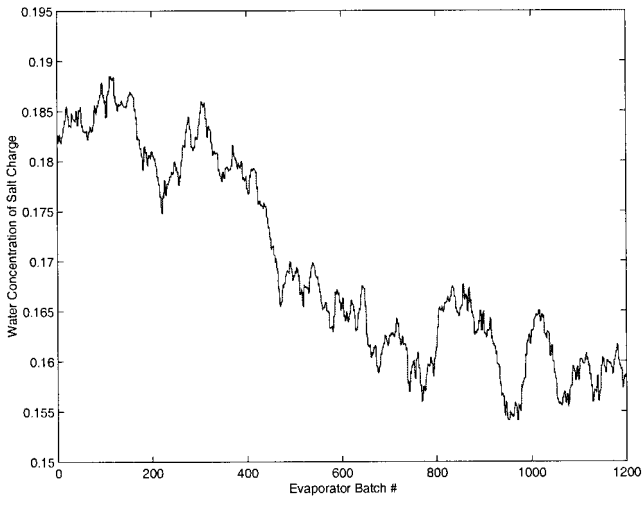

Figure 10. Initial water concentration disturbances in salt charge from the evaporator.

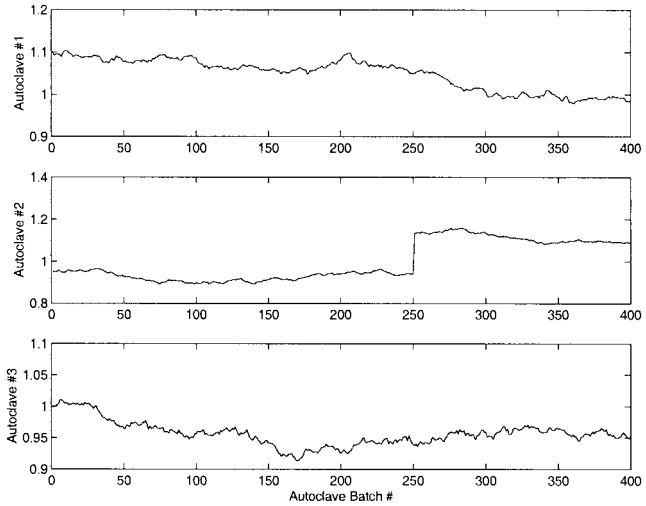

Figure 11. Heat-transfer parameter multiplier for the three autoclaves to simulate reactor fouling.

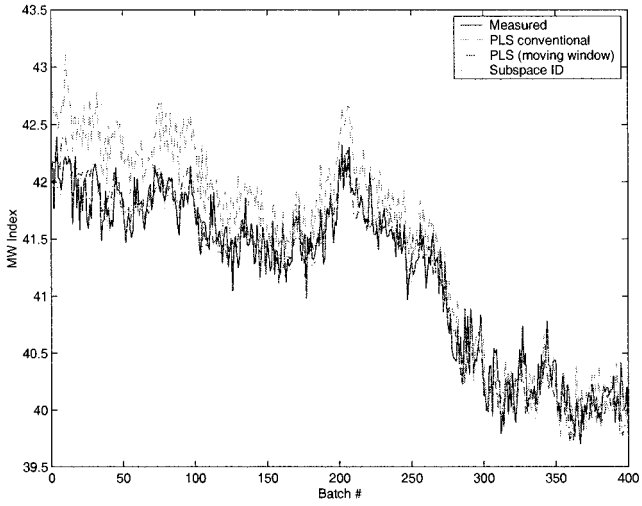

Figure 13. Average molecular weight predictions from the three modeling methods with open-loop data from autoclave 1.

reactor (1, 2, and 3). The error vector, which is to be minimized by the control calculation is

$$e_{k,i} = \begin{bmatrix} e_k^i \\ e_{k,i}^b \end{bmatrix} \tag{40}$$

The desired input moves can then be calculated by using the same quadratic form of Eq. 34. Here, the performance weight Q can be used to weigh the importance of controlling product quality at the autoclave level vs. that at the blender level.

Results for the Nylon Plant Example

To demonstrate the performance of the proposed plant-wide modeling and control strategies, we use a fundamental model of the nylon autoclave (Russell et al., 1998a, 2000) to simulate the autoclaves. For this study, both correlated and independent batch-to-batch changes are considered for various model parameters. The evaporator disturbance, for example, was simulated by changing the initial conditions for excess mass of HMD and the overall water concentration of the charged salt as integrated white noises. Figures 9 and 10 show the diamine and water disturbances, respectively, that were used to simulate the salt variations in the control study. The 1,200 points shown represent the charges from the evaporator and correspond to 400 batches for each of the three autoclaves.

In addition to the correlated changes brought about by the evaporator, independent changes were introduced to the heat-transfer equations and catalyst variations for each reactor. The heat-transfer variations for each reactor are shown in Figure 11 and were designed to simulate a gradual fouling of the reactor, thus hindering the rate of heat input to the reactor. An abrupt change in the heat-transfer properties of autoclave 2 was also

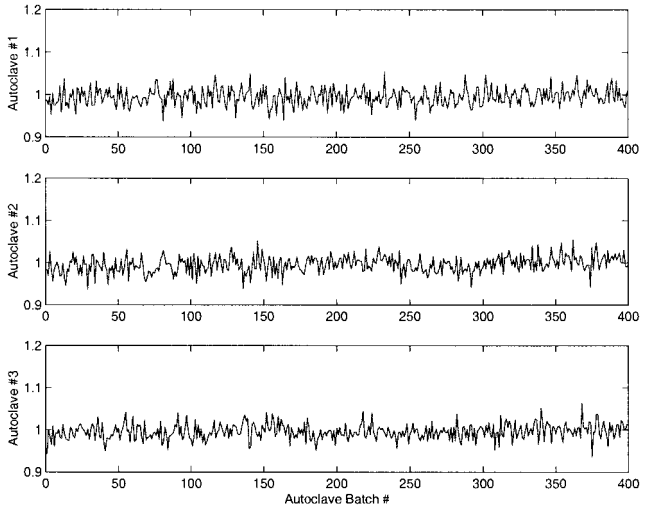

Figure 12. Polymerization reaction rate pre-multiplier to simulate kinetic variations for the three different autoclaves.

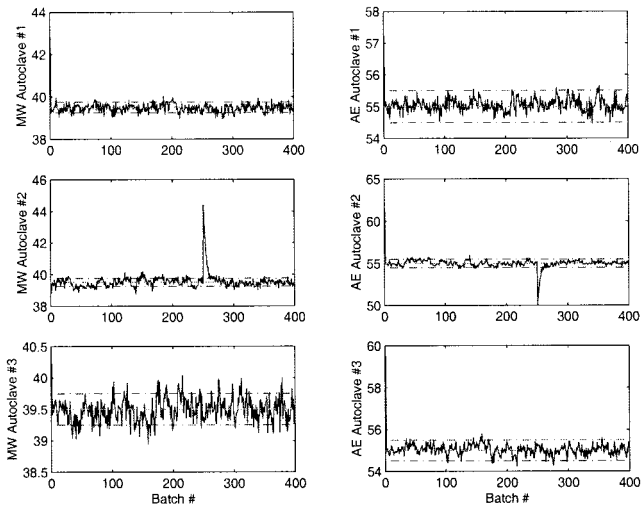

Figure 14. Results of independent batch control using the independent PLS modeling approach for each reactor.

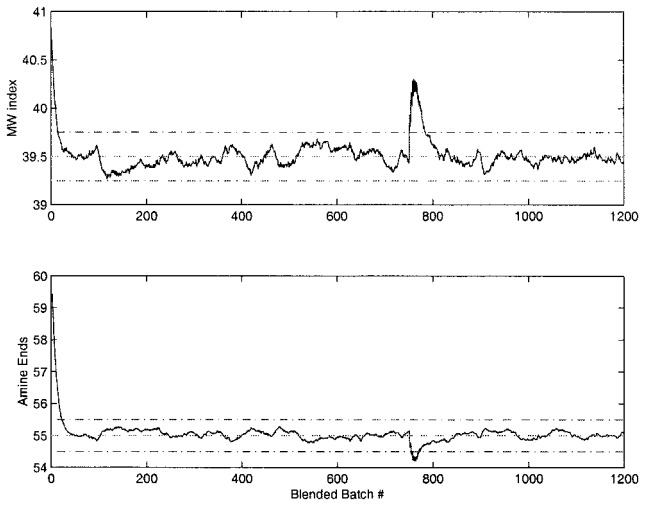

Figure 15. Blended product quality resulting from the independent batch control approach based on independent PLS models.

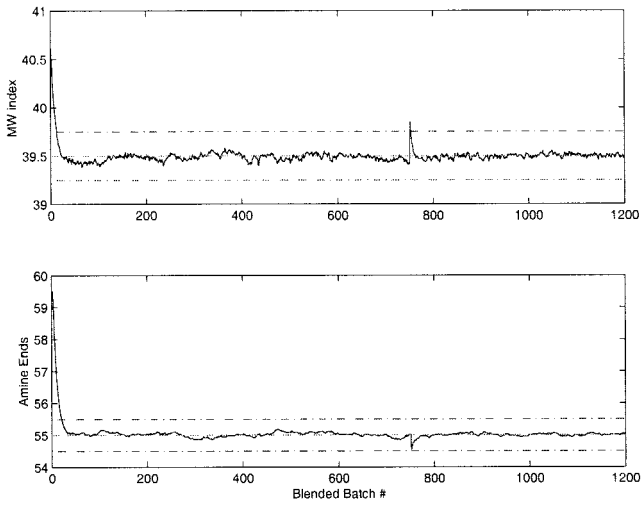

Figure 17. Blended product quality resulting from the plant-wide control formulation with the moving window PLS model.

included to introduce a disturbance that was exclusive to one reactor. Catalyst variations were also considered for each reactor and were introduced as a pre-multiplier to the polymerization reaction rate constant. These autoclave-independent type variations are shown for each autoclave in Figure 12.

Prediction models of the various forms were developed based on 200 batch history of the three autoclaves using new, but statistically similar disturbances in initial diamine, initial water concentration, heat-transfer coefficients, and a catalyst factor. Then, the control study was performed with the disturbances shown in Figures 9–12. The open-loop quality predictions in the presence of these disturbances are displayed in Figure 13 for the average molecular weight of autoclave 1. The mean squared error (MSE) for the conventional PLS model predictions was 0.1333, the MSE for the moving window approach was 0.0355, and the MSE for the subspace identification approach was 0.0114. These results indicate the benefit of including information from the parallel reactors in the plant-wide configuration. Note that the subspace identification framework brings further benefit by including two-batch delayed quality information from the autoclaves.

While many combinations are possible for the model and control approaches, the independent batch-to-batch control approach was coupled only with the predictions from the three independent PLS models around each autoclave. The plant-wide control approach was applied with both the multireactor moving window PLS model and the multireactor subspace ID model. The results from applying the three different control strategies are shown in Figures 14–19. Equal weighting between molecular weight and amine ends was applied for all formulations. For the plant-wide

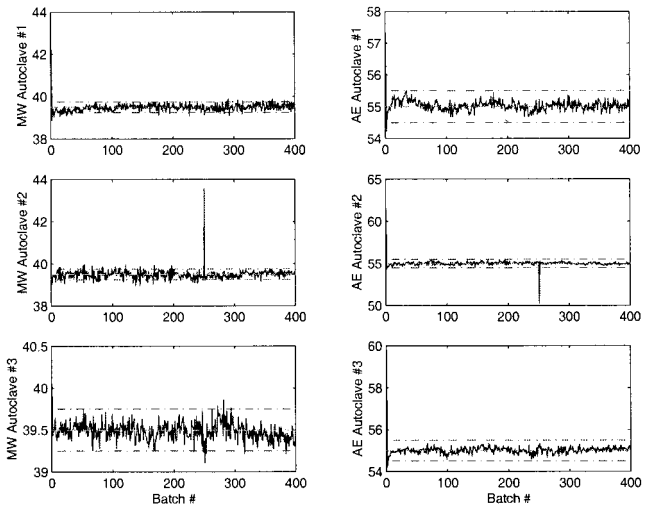

Figure 16. Control results for each autoclave from the plant-wide control formulation with the moving window PLS model.

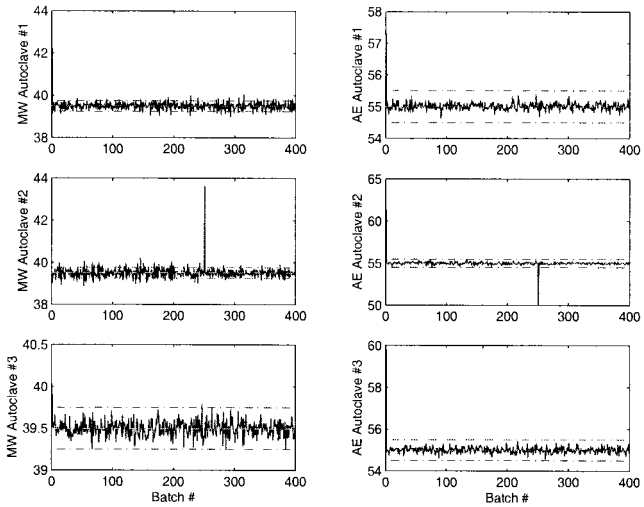

Figure 18. Control results for each autoclave from the plant-wide control formulation with the model from the subspace identification framework.

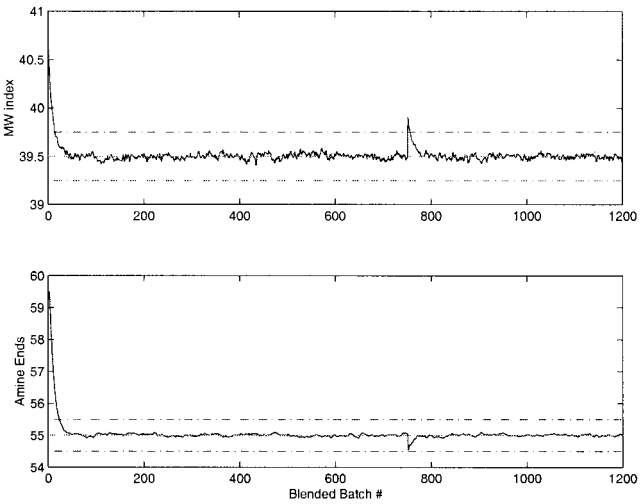

Figure 19. Blended product quality resulting from the plant-wide control formulation with the model from the subspace identification framework.

formulations, equal weighting was used between the autoclave level and blender level control errors.

To quantify the performance of the control approaches, the variances of the average molecular weight and amine ends were calculated for the blended outputs for each approach. These values are summarized in Table 1. Notice that all the control formulations offer significant improvements over the open-loop scenario. However, there is greater than 70% improvement in the average molecular weight control for the two plant-wide control schemes over the independent batch control approach. A smaller improvement (around 10%) was attained for the control of the amine ends concentration.

Another indicator for the controller's effectiveness is the covariance of the quality variables across the bank of autoclaves. This gives an indication of the ability of the controller to compensate for the correlation that exists among the reactors. Note that, if all the reactors are operating in a more or less independent manner, the product blender should be able to blend out the errors. The covariance matrix was estimated for the quality variables across the three autoclaves using the 400 batches in the control study in the following form

$$\begin{bmatrix} E\{e_k^{1^T} e_k^1\} & E\{e_k^{2^T} e_k^1\} & E\{e_k^{3^T} e_k^1\} \\ E\{e_k^{1^T} e_k^2\} & E\{e_k^{2^T} e_k^2\} & E\{e_k^{3^T} e_k^2\} \\ E\{e_k^{1^T} e_k^3\} & E\{e_k^{2^T} e_k^3\} & E\{e_k^{3^T} e_k^3\} \end{bmatrix} \tag{41}$$

where e^i represents the control error in the quality variables for the i^{th} autoclave. Table 2 shows the estimated covariance matrix for the average molecular weight across the three autoclaves for the open-loop and various control cases. Notice that the proposed plant-wide control approaches result in off-diagonal elements of significantly smaller magnitudes, indicating less correlated errors across the different reactors, as well as reduced variances for the individual reactors. This ability to compensate for the correlation in the product quality for the different reactors allows the blender to operate effectively, as shown in Table 1.

Table 1. Total Variance for Blended Output

Method	Blended MW Variance	Blended AE Variance
Open Loop	0.3998	0.4712
Conventional PLS	0.022	0.1342
Plant-Wide PLS	0.0058	0.1101
Subspace ID	0.0063	0.1200

Table 2. Estimated Covariance of Average Molecular Weight across the Autoclave Bank

Method	Molecular Weight Covariance
Open-Loop	$\begin{bmatrix} 0.509 & -1.295 & -0.022 \\ -1.295 & 5.119 & 0.188 \\ -0.022 & 0.188 & 0.285 \end{bmatrix}$
Conventional PLS	$\begin{bmatrix} 0.066 & -0.004 & 0.003 \\ -0.004 & 0.211 & 0.001 \\ 0.003 & 0.001 & 0.038 \end{bmatrix}$
Plant-Wide PLS	$\begin{bmatrix} 0.046 & -0.001 & 0.002 \\ -0.001 & 0.075 & -0.004 \\ 0.002 & -0.004 & 0.013 \end{bmatrix}$
Subspace	$\begin{bmatrix} 0.051 & 0.000 & 0.005 \\ 0.000 & 0.088 & -0.001 \\ 0.005 & -0.001 & 0.010 \end{bmatrix}$

Summary

In this article, a plant-wide batch control problem was considered for production of nylon 6,6. The advantage of modeling correlation among the operating units in parallel was investigated. Models that can account for the correlation lead to better quality uniformity by allowing for both improved quality predictions and control decisions. It was shown that the statistical modeling techniques of PLS and subspace identification can be adapted to build models for the proposed plant-wide control approach. The resulting models allow for information to be shared among the reactors operated in parallel for improved quality prediction performance. The subspace identification also offers a further benefit of being able to capture any correlation along the batch index. This ability enables a direct inclusion of previous batch information, such as delayed quality measurements, into the estimator design for improved prediction performance. While the plant-wide approach was developed with application to the nylon 6,6 plant in mind, it is expected that other batch plants with parallel reactor configurations sharing common feed/utility sources would benefit from a similar approach.

Acknowledgment

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