Nonlinear Profile Monitoring for Oven-Temperature Data

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Problem: The monitoring of a key input, temperature, in a manufacturing process produces large amounts of data. It is difficult to determine an appropriate control-chart methodology that allows the chart user to determine when there are problems with this step of the manufacturing process. Current approaches for process monitoring involve the output data gathered after the process has been completed. It would be preferable to establish process monitoring on the process inputs. However, this is challenging when there is a large amount of process input data. Current phase I monitoring of the process inputs involve the use of individual control charts on some selected data from the temperature profiles that represent some features determined based on expert judgment. This approach does not use all the data nor does it take into account the potential correlation that exists among the selected data.

Approach: We propose the use of a nonlinear model for modeling the profiles, thereby reducing the profiles to a smaller set of parameter estimates. For this nonlinear model data reduction approach, the parameter estimates and residual variability can then be used in the appropriate monitoring procedure. We show that a control chart based on the classical covariance-matrix estimate fails to detect large significant process changes, but the successive differences covariance matrix performs better. The statistic based on the successive differences is modified to account for the correlation between the profiles. We illustrate both the phase I and phase II analysis for these data.

Results: The proposed data reduction approach and monitoring procedure makes use of all the available data and detects important process shifts where the interpretation of the nonlinear model parameters facilitates the root-cause investigation. This parametric approach can be easily automated using existing statistical software and results in a smaller number of control charts, which is a manageable way to determine the current state of the process. We highlight some issues that are raised by this particular dataset that have not been adequately addressed in the profile-monitoring literature.

Key Words: Common Fixed Design; Multivariate Statistical Process Control; Nonlinear models; Phase I; Principal Components; Temperature Profiles; T^2 Statistic.

1. Problem Statement

This is a situation where we want to monitor the temperature of an oven used in a manufacturing process. Multiple parts are processed simultaneously in each oven run and are then subsequently used as a component assembled into a finished product. The temperature in the oven during a manufacturing run is a key input for this process, which can have an impact on the quality of the component parts. The current approach for process monitoring focuses on monitoring of the final assembled product quality by testing the final assembled product. As a supplement to monitoring the final product quality, it is desirable to monitor the quality of the components. This can be done by monitoring the oven temperature, which allows the control-chart user to more quickly react to potential problems that could occur downstream in the process by preventing low-quality components from continuing on to downstream processing. This can provide potential financial savings and greater protection against potential process upsets.

One key issue that impacts the ability to monitor the process input is the large amount of data generated. In contrast with final assembled product testing, which produces relatively small amounts of data, the temperature can be recorded every few seconds by sensors at multiple locations within the oven. Thus, there is the potential to have hundreds or thousands of temperature measurements for a single oven run. In addition, the number of oven runs can be quite large. We have a historical data set of oven runs that cover several months of manufacturing. Standard control-chart procedures are inadequate to handle the large amount of information produced by this process. Profile monitoring, which was reviewed by Woodall et al. (2004) and Woodall (2007), provides a way to handle the large amount of process input data. A more comprehensive coverage of the topic can be found in a recent book by Noorossana et al. (2011).

One simpler approach of monitoring process inputs previously considered was to select a few key features from the profiles, such as the maximum temperature or the amount of time it takes for the oven to reach a particular temperature. This approach relies on expert understanding and familiarity with the process to determine the key features of interest. Once some features are selected, individual control charts are created for each feature. However, this approach may not capture all unexpected changes that could occur with the process. Nor does it take into account the potential correlation that exists among the features. It is reliant on the expert understanding of the process and does not make full use of the available process input data across all the oven locations.

For confidentiality reasons, we do not share specific engineering or manufacturing details about the product being produced by this process. In addition, we note that the data have been modified in such a way that the key features of the temperature profiles are not impacted. We do not believe that the changes that we have made to the data change the analysis issues associated with the data set.

2. Background and Data Structure

The sensors that are used in the oven allow us to gather a temperature value (in Celsius) roughly every 3 seconds throughout the oven run, which results in approximately 160 data points in a 500-second data-collection period. While the actual oven run can be much longer, the temperature reaches a plateau beyond 500 seconds and the temperature is now stable. It is the initial start-up period that is most crucial to monitor and that is our focus with this dataset. These data points do not necessarily occur at the same time intervals although they tend to be relatively similar to each other. We had a total of 1040 runs for the time period. An initial investigation of the data found six profiles that did not have data recorded for the entire data-collection period, so they were discarded, leaving 1034 runs remaining. We believe that the runs with missing data are due to an issue in the data collection and not due to some underlying root cause where the missing data correspond to product with lower quality. For each run, the temperature is measured at four different locations. In general, we expect the temperature to be different at the different locations within the oven, corresponding to hotter or colder spots. Because of the large size of the total dataset (>160,000 rows), it is not shown here but is available in the supplemental material available with this paper.

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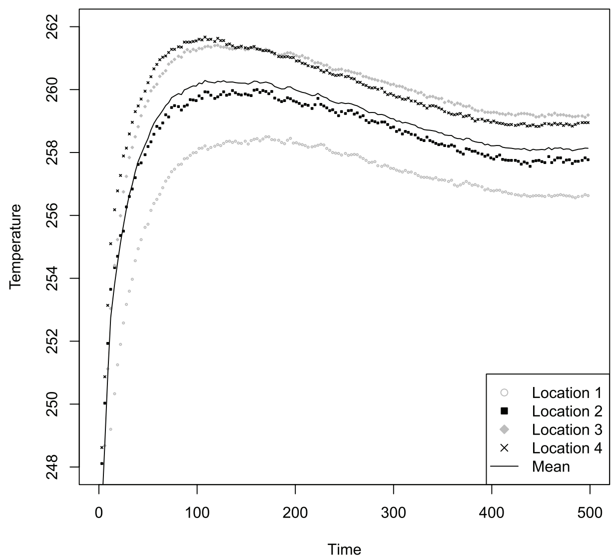

FIGURE 1. Raw Data Plot for First Oven Run Showing the Temperature Profiles for the Four Locations and the Mean Profile as a Solid Line.

During the run, the oven starts at a lower temperature and over time it quickly increases in temperature. After a short time, the temperature decreases slightly and levels off, where it remains stable through the end of the run. This pattern of a rapid increase followed by a gradual decrease and tapering off is consistent with the way the oven is supposed to perform in order to produce good product in the most efficient manner. To illustrate the temperature profile, consider Figure 1, which shows the raw data for the first oven run. The lowest two curves correspond to the temperature recorded at locations 1 and 2, respectively. The line in the middle is the mean of the four locations, and the top two curves correspond to locations 3 and 4, respectively. Notice, also, the noise in the data points for a particular profile where the points bounce up and down around the general pattern of the profile. This noise is inherent in the data-collection system and any monitoring approach must minimize the impact of this noise.

Each of the 1034 runs in the historical dataset yield a similar picture as the one shown in Figure 1. Location 1 is consistently the coldest, while Locations 3 and 4 are consistently the hottest. This particular run is 'in control' as judged from the final assembled product measurements resulting from the downstream quality data. Therefore, a collection of temperature profiles for a run that follows a similar pattern will likely result in good output. It will be of value to determine more quickly when certain oven runs do not follow this pattern, in order to prevent continued processing of parts that will cause problems if assembled into the final product.

The goal in the initial phase I analysis is to determine the appropriate control limits to be be used for phase II of the control-chart scheme, which is real-time monitoring of the process. In general, the phase I analysis determines if there are outlying profiles, step changes, drifts or trends that indicate a nonstable process. If the process is not found to be stable in phase I, then the appropriate subset of the phase I data is used to generate the phase II limits.

We use the historical dataset described here to first illustrate the fitted nonlinear model and phase I analysis in Sections 4 and 5. We will illustrate the phase II analysis in Section 6. Before describing the monitoring of nonlinear model parameters that we use here, we first discuss profile-monitoring approaches that potentially could be used in Section 3. Because of the proliferation of approaches given in the profile-monitoring literature, our intent is not to be comprehensive and illustrate all possible approaches that could be used with these data. We illustrate what we believe to be a reasonable approach and provide the data so that the reader can investigate other approaches with this dataset. We conclude with a discussion of issues highlighted by this dataset.

3. Potential Analysis Approaches

Since the seminal paper on profile monitoring by Woodall et al. (2004), there has been an explosion of literature available on the topic. Before discussing the approach taken for the oven data, we describe some of the methods from the literature that were not used for these data. We need methods for multiple, nonlinear profiles in a phase I application where the points at which the data are collected are not the same for all the profiles.

The situation where all the profiles have data points collected at the same places or points in time is called the "common fixed design" in Zou et al. (2008) and Zhang and Albin (2009). We do not have a common fixed design (CFD) for this dataset and refer to this scenario as an arbitrary design, where the points at which the data are collected are not necessarily the same for all the profiles. In the profile-monitoring literature, the predominant assumption is that the data follow a CFD and the proposed methods are developed under that assumption. The CFD situation is not applicable to this application and so those possible methods are not considered.

One approach we considered was the nonparametric method of Zhang and Albin (2009), which is a phase I approach that can be extended to account for multiple profiles and would otherwise be applicable for the nonlinear profiles we have here. However, the proposed method relies on the CFD assumption. Zhang and Albin (2009) noted that one could use interpolation to fit missing values in a profile to ensure CFD for a dataset that has an arbitrary design. We do not pursue that possibility here because, for these data, it would require a frequent interpolation and not distinguish between observed data and interpolated values. We have approximately 160 points for each profile in a 500-second time period and we would have to interpolate about 340 points for each profile to obtain a data value for each second. We believe that this large amount of interpolation would be inappropriate and make the analysis results more dependent on the interpolated data than on the real data.

An arbitrary design in the profiles also makes it difficult to apply methods that directly use the raw data themselves rather than a model fit of the data. This includes methods based on the fitted principal components of the profile data, which have been discussed in Woodall et al. (2004) and used in the literature; see Ding et al. (2006) for an example. Paynabar et al. (2013) discussed a phase I application for multiple profiles using a variation of the principal-components approach that also requires the assumption of the CFD. In some situations, it may be possible to shift or align the profiles so that they would have the same data points at the same locations within the profile. We do not pursue that path for these data because it is not clear how to align the profiles.

The CFD assumption also precludes many nonparametric methods that directly use the data themselves. This includes the nonparametric regression approach of Zou et al. (2008) and the penalized regression approach of Zou et al. (2014), who do not consider the problem of multiple profiles. We also considered the nonparametric mixed-model approach of Qiu et al. (2010), but that work focused on the phase II application and does not consider multiple profiles. There is potential that such an approach could be modified for a phase I application and could potentially treat the multiple profiles of the oven data as a random effect in the mixed model. However, in this case, the locations within the oven are the ones of interest and are not a random sample of possible locations within the oven.

Noorossana et al. (2010a, 2010b) studied multivariate profiles for a situation where the multiple profiles gathered at the same time point are treated as multivariate responses. This would be applicable for this dataset if the four locations within an oven run are considered as multiple response vectors. However, the work of Noorossana et al. (2010a, 2010b) only dealt with linear profiles; thus, it is not applicable to these nonlinear profiles.

A nonparametric approach that could be applied to these data is the one described in the work of Chang and Yadama (2010), Chang et al. (2012), and Chou et al. (2014). In this approach, the multiple profiles are fit with a nonparametric model and a summary statistic is calculated. The summary statistic is based on the sum of the absolute value of the deviations of the points from the fitted nonparametric model. The summary statistics are then charted as a multivariate exponentially weighted moving average (MEWMA) statistic in lieu of the traditional T^2 control chart. Chou et al. (2014) also proposed a variation of this approach where the profiles are divided into several segments based on expert knowledge of the process. A summary statistic is calculated for each profile by segment combination.

Other possible analysis approaches include the nonlinear mixed model of Jensen et al. (2009) to account for correlation in the profiles. One challenge with a nonlinear mixed-model approach is that the probability of nonconvergence of the estimation procedure increases because of the increased complexity in the iterative estimation procedure. Nor would it reduce the dimensionality of the data more than will be shown with the nonlinear model approach. We also did not pursue the approach of Abdel-Salam et al. (2013), which is a semi-parametric approach that uses a hybrid of parametric and nonparametric approaches.

We illustrate in this case study an approach that we believe is appropriate for these data. This approach is described in the next section as the modeling of the profiles with a nonlinear model for each location and follows the approach described by Williams et al. (2007). We believe the monitoring of nonlinear model parameters is appropriate for the data and the interpretation of the parameters is of value to the process experts.

4. Nonlinear Model for Temperature Profiles

We illustrate the selection of a family of nonlinear models that represent the oven-temperature profiles and for parameters have interpretations as features of the profile. We first seek to find a model that will work well for a single location because the same model may well work for other locations because of their similarity. Some earlier examples of nonlinear profile monitoring can be found in Williams et al. (2007) and Jensen and Birch (2009). The nonlinear models in standard textbooks (e.g., Gallant (1987) or Seber and Wild (2003)) are typically monotonic and are thus not appropriate for this nonmonotonic pattern in the profiles. We were not able to find a nonlinear function from the literature that would work well for this data. As an alternative, we used the idea of linear combinations of linear models from Schabenberger and Birch (2001) to formulate a combination of two different nonlinear functions that will capture the different aspects of the oven curves.

The first component is a mechanistic growth model, which is given by

$$f_1(t;\beta) = \beta_1\left(1-\beta_2 e^{-\beta_3 t}\right), \qquad (1)$$

where β_1 represents the plateau temperature and β_2 and β_3 together represent the rate of increase in the temperature, similar in idea to a slope for a linear function. Figure 2 shows the mechanistic growth model fit to the average temperature from the first run for illustration purposes. This nonlinear model was fit using statistical software with the Gauss-Newton method. The fitted parameter estimates are computed as $\beta_1 = 259.18$, $\beta_2 = .057$, and $\beta_3 = .062$. Notice how this mechanistic model captures the rapid increase in the temperature and then levels off to a plateau.

However, this model does not capture the peak temperature and the subsequent tapering. To capture these additional features of the profile, we propose a second nonlinear model. This second model is the four-parameter logistic function and captures the behavior of the profile where there is a drop in the temperature from the peak. The four-parameter logistic function is given by

$$f_2(t;\gamma) = \gamma_2 + \frac{\gamma_1-\gamma_2}{1+e^{\gamma_3(t-\gamma_4)}}, \qquad (2)$$

where γ_1 represents the upper asymptote, γ_2 represents the lower asymptote, γ_3 represents the rate of increase (or decrease), and γ_4 represents the value of t where the curve is halfway between the upper and lower asymptotes. Figure 3 shows an example of a four-parameter logistic curve with $\gamma_1 = 3$, $\gamma_2 = 0.01$, $\gamma_3 = 0.02$, and $\gamma_4 = 150$.

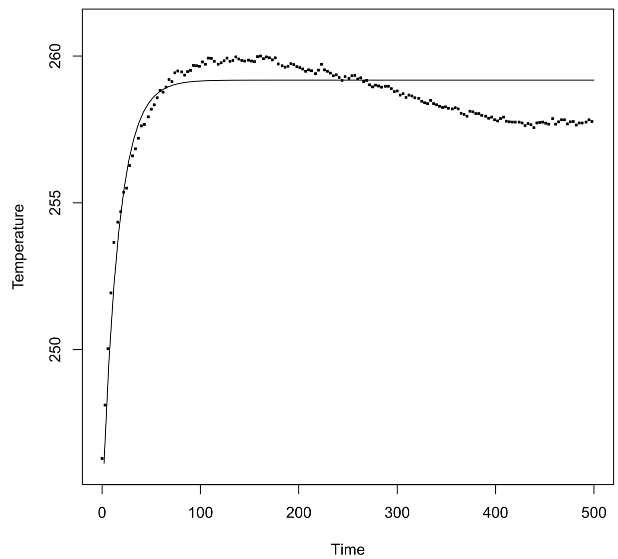

FIGURE 2. Mechanistic Growth Model Fit to the Average Temperatures for the First Oven Run.

We propose combining the two models into a customized nonlinear model that is applicable to the oven-temperature profiles. There is redundancy in the plateau (β_1) in the mechanistic model and the lower asymptote (γ_2) in the four-parameter logistic curve, indicating that six parameters are sufficient.

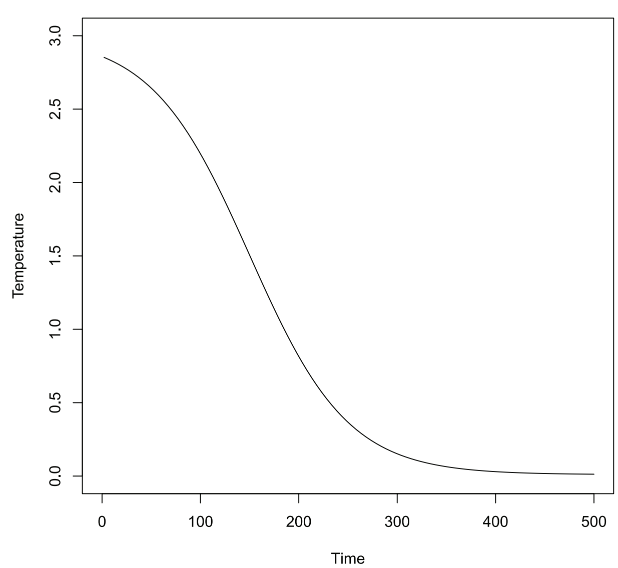

FIGURE 3. Example Four-Parameter Logistic Model.

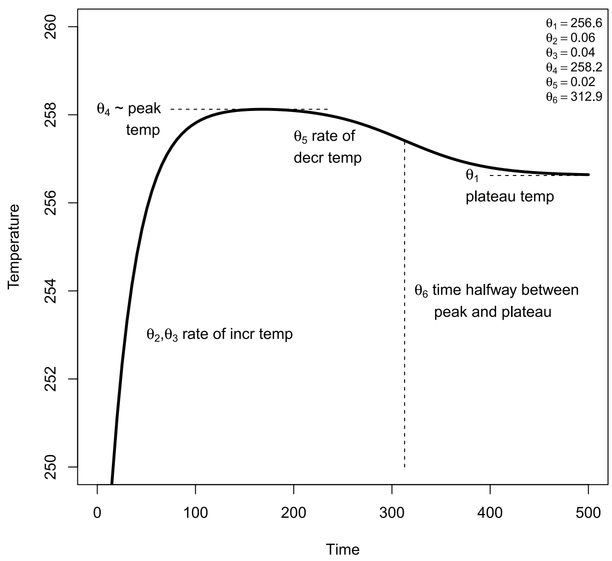

FIGURE 4. Proposed Nonlinear Model Identifying Parameter Interpretations.

The proposed nonlinear model for temperature profiles is

$$h(t;\theta) = \theta_1\left(1 - \theta_2 e^{-\theta_3 t}\right) + \frac{(\theta_4 - \theta_1)}{1 + e^{\theta_5 (t-\theta_6)}}. \qquad (3)$$

This proposed nonlinear model is shown in Figure 4. It is important to note that the parameters still have realistic interpretations in this customized model, as demonstrated in Figure 4. The parameter θ_1 represents the temperature at which the curve levels off (plateau point), θ_2 and θ_3 represent the rate of increase in the temperature up to the peak temperature, θ_4 represents the approximate peak temperature, θ_5 represents the rate of decrease from the peak to the plateau point, and θ_6 represents the time at which the temperature is halfway between the peak and plateau point. Figure 5 shows the overlay of the fitted model from Equation (3) on the average temperature profile for the first oven run and demonstrates that this customized model will capture the important features of the raw data.

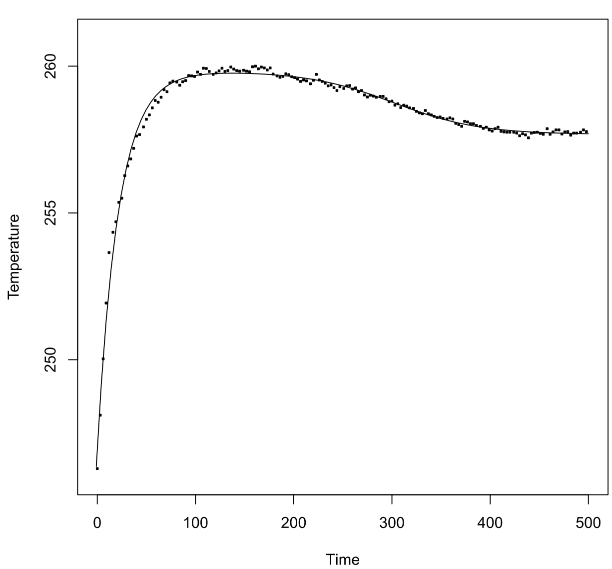

FIGURE 5. Proposed Nonlinear Model Fit to the Average Temperatures for the First Oven Run.

5. Phase I Analysis Using Nonlinear Model Parameters

With a customized nonlinear model in hand, we can now consider how to appropriately reduce the multiple temperature profiles to a manageable set of parameters for monitoring purposes. We consider a separate nonlinear model for each of the four locations, thus giving 24 parameters to monitor for a single oven run. While there are systematic differences in the locations that may allow for further dimensionality reduction, we believe that such reduction could eliminate the ability to detect future special causes where the systematic differences change. This could happen if a hot spot in an oven moved to a different place in the oven because of changes in the airflow within the oven. We will show later, in Figure 11, an example of where the phase II data show changes in the systematic differences in the oven locations.

When fitting nonlinear models, the issue of model convergence becomes crucial because of the iterative methods used to obtain the parameter estimates. In order to increase the probability of convergence, there are several good practices that can be followed. First, use a good selection of starting values. In the situation where there are multiple profiles, a good approach to obtain starting values is to fit the nonlinear model to the average of the profiles combined as a single dataset. This results in a nonlinear model with parameter estimates that mimic an average parameter value for values that would occur from separate nonlinear model fits. These average values serve as good starting values for the individual nonlinear models fit to each run. A second practice is to increase the number of iterations in the software. A final practice is to restrict the range of the parameters that are considered. For example, the parameters θ_1 and θ_4 can be restricted to be positive because it is physically impossible for the peak and plateau temperature to be negative. For this data set, the most problematic location in terms of convergence was location 1, which is the lowest and flattest of the temperature profiles. The other locations did not have convergence issues.

Monitoring of the six parameters for each profile does not account for situations where the model fits poorly or the variability in the individual observations within a profile has increased. Thus, we propose to also monitor the residual variability that remains after fitting the model. This is obtained by computing the mean-square error (MSE) for each fitted profile. The MSE is obtained by first subtracting the actual temperature from the fitted values, i.e. the residual, and then computing the sum of squares of the residuals for all the observations within a run. The sum of squares is then divided by the residual degrees of freedom, which is the number of observations minus the number of parameters in the nonlinear model for each location (six in this case).

As a sum of squared residuals, the MSE is expected to have a skewed distribution. Because the multivariate control charts assume an underlying multivariate normal distribution, the qq-plots indicate log(MSE) better fits the control-chart assumptions. This set of 24 parameter estimates and 4 estimates of log-transformed residual variability represent 28 key features of a single oven run. We have effectively reduced the dimensionality of the problem by summarizing the $\approx 160 \times 4 = 640$ raw points into these 28 estimates. These estimates represent a reasonable reduction in dimensionality of the data set without losing key features of the data. The full set of estimates for all the runs are available as supplemental material. Because of space limitations, we do not illustrate further reduction of the dimensionality of the dataset that could be done because of the similarity in these 28 estimates.

It would be difficult and undesirable to monitor 28 individual charts to determine which oven runs have outlying values for these estimates. Following the parallel to $\overline{X}$- and R-charts, we monitor the process with two multivariate control charts: one chart of the nonlinear profile parameters ($p = 24$) and one chart of the residual variation, log(MSE), from each location ($p = 4$). Let ξ denote the estimates representing the ith profile for the corresponding control chart. In real applications, we never have a known mean vector and variance–covariance matrix so they must be estimated.

Given m profiles in the phase I dataset, the classical approach is to calculate the widely used t statistic given as

$$T^2 = (\mathbf{x}_i - \bar{\mathbf{x}})' \, \mathbf{S}_1^{-1} \, (\mathbf{x}_i - \bar{\mathbf{x}}) \ \text{ for } i = 1, 2, \ldots, m \quad (4)$$

$$\bar{\mathbf{x}} = \frac{1}{m} \sum_{i=1}^{m} \mathbf{x}_i \quad (5)$$

and

$$\mathbf{S}_1 = \frac{1}{m-1} \sum_{i=1}^{m} (\mathbf{x}_i - \bar{\mathbf{x}}) (\mathbf{x}_i - \bar{\mathbf{x}})' . \quad (6)$$

As noted in Mason and Young (2002), under the assumption the $\mathbf{x}_i$ are multivariate normal, the distribution of t is proportional to a beta distribution but the upper control limit (UCL) can be approximated by a χ^2 distribution if $m > p^2 + 3p$. The χ^2 distribution can be used for these data because $m = 1,034$ exceeds $24^2 + 3 \cdot 24 = 648$ and $4^2 + 3 \cdot 4 = 28$. While these t statistics are correlated because we are using the same data to estimate the variance–covariance matrix, we believe the correlation to be small because of the large number of profiles (m). For the oven data, we want to maintain an overall false-alarm rate of $\alpha = 0.05$. To maintain this overall value for α given the large number of profiles in the phase I dataset, instead of the $1 - \alpha$ quantile of the χ^2 distribution with p degrees of freedom, we follow Mahmoud and Woodall (2004) and Williams et al. (2006, 2007) and correct for multiple testing by using the $(1 - \alpha)^{1/m}$ quantile.

For the oven data, this adjustment with $m = 1,034$ gives an $\alpha = 0.05$ UCL of 60.78 for the phase I nonlinear model-parameter estimates chart ($p = 24$) and 25.03 for the phase I residual variation chart ($p = 4$). The top panels of Figure 6 show the control chart for this standard t statistic for the nonlinear parameter estimates ($p = 24$) and residual variation ($p = 4$).

An alternative is to base the t-statistic on the variance–covariance matrix using the successive differences between vectors, denoted by $T^2_{\mathrm{SD},i}$. If $\mathbf{v}_i = \mathbf{x}_{i+1} - \mathbf{x}_i$ is the vector of the ith successive difference, then an unbiased estimator of the variance–covariance matrix is

$$\mathbf{S}_{\mathrm{SD}} = \frac{1}{2(m-1)} \sum_{i=1}^{m-1} \mathbf{v}_i \mathbf{v}_i'. \quad (7)$$

A typical assumption for phase I data is independence, meaning that $\mathbf{x}_i$'s are independent. A diagnostic of independence is the sample autocorrelation

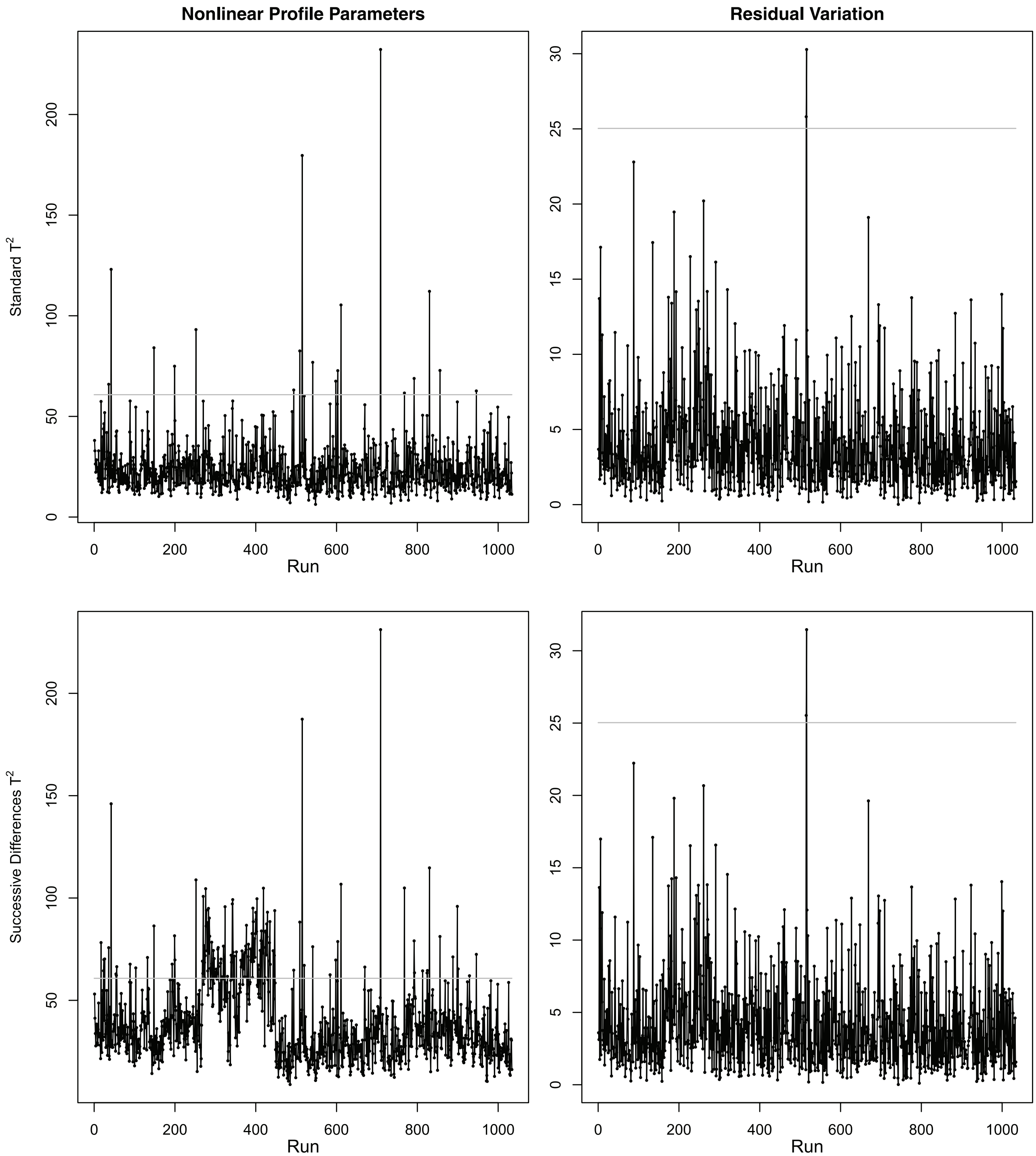

FIGURE 6. Multivariate Control Charts Based on the Nonlinear Profile Parameters (left) and Residual Variation (right). The top panels are the standard t chart while the bottom panels are for $T^2_{\mathrm{SD},i}$ based on the successive differences.

function (ACF), which corresponds to the correlation between the same nonlinear profile parameter and same location at different lags. The ACF for θ_4 (peak) at location 2 is shown in Figure 7 and is typical of the other elements of $\mathbf{x}_i$, where the dotted lines reflect the critical value of the test $H_0 : \rho_\ell = 0$ for a given lag ℓ. We do not show all the possible ACFs for other parameter values and locations. The spikes for

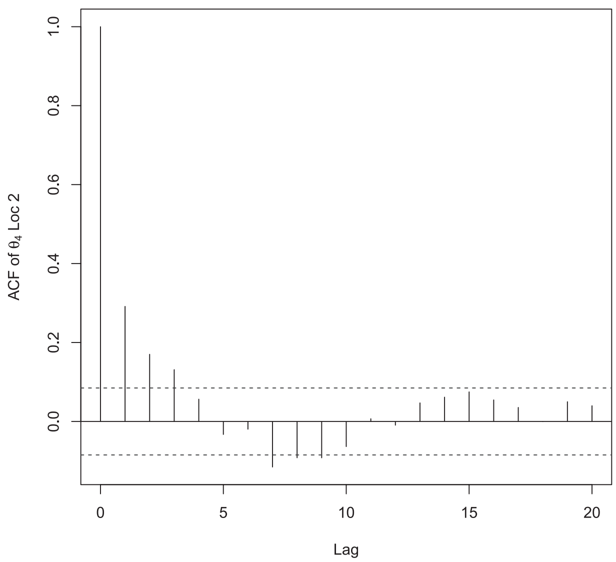

FIGURE 7. Typical ACF for θ_4 and Location 2 Demonstrating Autocorrelation Between Oven Runs and Violation of Typical Phase I Assumption of Independence.

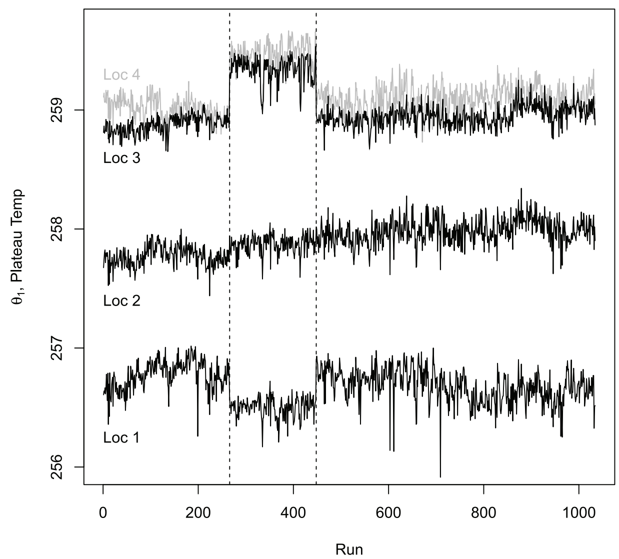

FIGURE 8. Plot of the Estimated Plateau Temperature for All Locations. The runs 266–448 (183 profiles) that were identified as out of control by the successive differences $T^2_{\mathrm{SD},i}$ correspond to higher-than-expected plateau temperatures for locations 3 and 4 and lower-than-expected plateau temperatures for location 1.

lags less than 10 indicate significant short-memory correlation. Because $m = 1,034$ is large, it is hard to argue that these correlations are spurious.

In order to satisfy the assumption of independence between runs in the successive-differences covariance matrix, instead of choosing lag 1, we consider a larger lag. The ACF in Figure 7 suggests that runs that are at least 10 time periods apart are uncorrelated. The other ACF plots not shown also indicate that 10 is an adequate number of time periods to ensure independence. Therefore, we generalize the principal of 'successive differences' to a lag 10 instead of lag 1 by defining $\mathbf{v}_i = \mathbf{x}_{i+10} - \mathbf{x}_i$ in $\mathbf{S}_{\mathrm{SD}}$.

The test statistic, $T^2_{\mathrm{SD},i}$, is computed by replacing $\mathbf{S}_1^{-1}$ with $\mathbf{S}_{\mathrm{SD}}^{-1}$ in Equation (4). Sullivan and Woodall (1996) showed that $T^2_{\mathrm{SD},i}$ is effective in detecting sustained step changes in the process that occur in phase I data. The distribution of this statistic is not known, but was studied in detail by Williams et al. (2006). They provided tables of UCL derived from simulation for $p \leq 10$ and for small values of m. They showed the asymptotic distribution of the statistic follows a χ^2 distribution and suggested the UCL can be approximated by the χ^2 quantiles when $m > p^2 + 3p$, which is the same suggested rule as Mason and Young (2002) for the regular T^2. The bottom panels of Figure 6 show the control chart based on $T^2_{\mathrm{SD},i}$, where the UCL is the same as the upper panel because both are based on the χ^2 approximation.

From Figure 6, we see in the bottom left panel an indication of a process shift in the nonlinear model parameter estimates that begins around run 250 and continues through run 450. We investigated the individual charts for the 24 estimates and found that the shift appears to be in the plateau temperature (θ_1) for some locations, as shown in Figure 8. Figure 8 shows the plateau temperature for locations 3 and 4 are about a half degree higher than the nonshifted runs. There is also a smaller shift in the plateau temperature for location 1.

Given this shift in the plateau temperature for this process, the first step would be to investigate the cause of the shift and determine a potential root cause. Determination of the root cause could then lead to preventive actions that can prevent this shift from occurring in the future. However, this is not possible for this scenario because these are historical data and it is difficult to go back and determine what may have happened at that point in time. We would like to be able to signal shifts of this magnitude in the future. We exclude the profiles corresponding to this time period covering runs runs 266 through 448. This leaves us with $1{,}034 - 183 = 852$ remaining profiles.

We recalculated the successive-differences control charts shown in the bottom panels of Figure 6, where

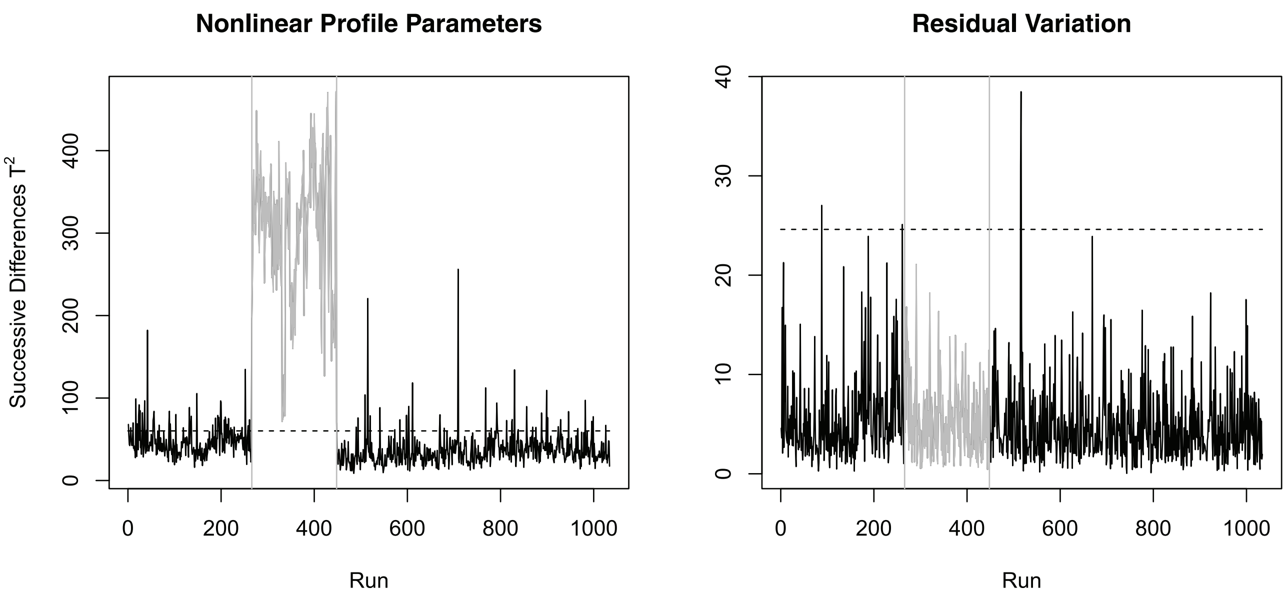

FIGURE 9. Recalculated Successive-Differences T^2 Control Chart Based on the Nonlinear Model Parameter Estimates and MSE after Excluding Shifted Profiles. The left panel monitors nonlinear profile parameters and the right panel monitors residual variation.

$\bar{\mathbf{x}}$ and $\mathbf{S}_{\mathrm{SD}}$ use the $m = 852$ phase I runs that are believed to be in control, and show them in Figure 9. The control limit is again based on the χ^2 approximation (which is still applicable even with slightly smaller m), but the $(1-\alpha)^{1/m}$ quantile yields an UCL of 61.62 for the left panel and 24.61 for the right panel.

In Figure 9, we continue to see a large number of signals for the control chart of the parameter estimates on the left panel. Rather than excluding these points and continuing the process of recalculating the limits, we believe the large number of signals may be an indication that the assumption of multivariate normally distributed data may not be appropriate. Thus, we use the empirical reference approach as discussed in Willemain and Runger (1996). We believe that this approach is underutilized in the statistical process control (SPC) literature and that it has good ability to reduce the likelihood of false alarms. Willemain and Runger (1996) demonstrated the approach for a univariate Shewhart control chart, but we believe that the approach is general enough to apply to any control-chart statistic, like the multivariate statistics that we calculate here. Essentially, we simply assume that the data we have collected are collected under normal operating conditions and represent "good" data rather than relying on a distributional assumption for the data. We believe the remaining profiles to be representative of normal operating conditions. Given the shifts that we saw in the lower left panel of Figure 6, we want to protect against future step shifts so we illustrate the empirical reference approach using the $T^2_{\mathrm{SD},i}$ statistic for the nonlinear parameter estimates. We will continue to use 24.61 as the Phase II limit for the residual variation, as this chart does not have a large number of signals.

We calculate $T^2_{\mathrm{SD},i}$ for the remaining 852 profiles. We want to set the control limits to reduce the likelihood of false alarms. We set that probability to be 0.0027, corresponding to the common three standard deviation limits used for univariate control charts. Thus, we calculate the 99.73^{th} quantile for the order statistics, which results in a value of 168.2525. Notice that this value is more than double the control limit used earlier for the parameter estimates, but that it would still signal the earlier shift shown in Figure 6. This would be the control limit used for phase II. This empirical reference approach requires a large phase I dataset, which we believe will be more common in the future with automated data-collection tools.

6. Phase II Analysis

The application of the control chart in the previous section was a phase I analysis on the historical dataset. Using this historical data, we now have

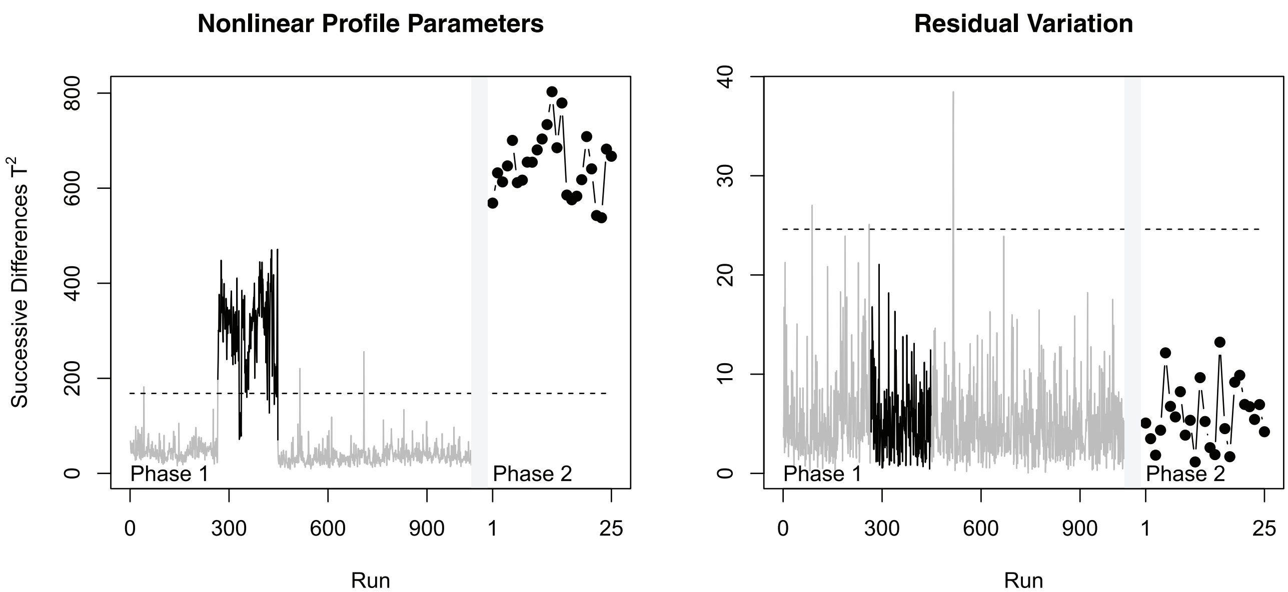

FIGURE 10. Successive-Differences T^2 Control Chart for Phase II. The left panel monitors nonlinear profile parameters and the right panel monitors residual variation. All phase II runs for the nonlinear profile parameters greatly exceed the UCL and reflect an important practical shift in the process.

a customized nonlinear model and control limits to be applied to future production. We illustrate a phase II analysis with these oven profile data. We collected data on an additional 25 runs from the same oven with sensors at the same four locations as phase I. Consistent with the phase I data, the temperature profiles are based on data collected approximately every 3 seconds but not in a CFD. These 25 runs were collected after a known process change had occurred and we want to determine if the proposed method signals the process change. The nonlinear model from phase I was fit to each new profile and the log(MSE) calculated. The raw phase II data and parameter estimates are given in the supplementary material.

When creating the customized parametric nonlinear model, we believed that the proposed model was flexible enough to capture future profile changes. For the phase II runs, the starting values corresponded to the in-control values in the phase I mean vector from Equation (5). Following the recommendation with the phase I runs to increase the number of iterations, all phase II profiles converged but two. The profile from location 3 of phase II run 10 and the profile from location 1 of phase II run 13 required manual adjustment of the starting values for the peak and plateau temperatures in order to obtain convergence. If this had been done in real time, computer software would be required to obtain the nonlinear model parameter estimates. If convergence of the nonlinear model did not occur, then this would be a signal that the process may be out of control. The first step would be to plot the raw data and see if model convergence could be obtained using manual adjustment before computing the test statistics.

The control chart on phase II runs used $T^2_{\mathrm{SD},i}$ with the in-control values $\bar{\mathbf{x}}$ and $\mathbf{S}^{-1}_{\mathrm{SD}}$ from phase I. The control charts for $T^2_{\mathrm{SD},i}$ for both phases I and II are given in Figure 10, where phase II is the far right side of the graphic for each panel. The control chart shows a large shift in the nonlinear profile parameters for phase II runs. Not only do all phase II runs exceed the control limit, the values exceed the collection of phase I runs that were identified and removed. In contrast, the values for the residual variation are still in control, indicating that the proposed nonlinear model fits the profiles well in spite of the shifts in the parameter estimates.

Diagnostic plots by nonlinear profile parameter indicated a large shift in θ_1 for three locations in phase II. As shown in Figure 11, the plateau temperature for location 3 drops over a degree. What was the hottest location in the historical data is now no longer the hottest. There are also large drops in plateau temperature for locations 2 and 4. These drops are likely the result of the process change

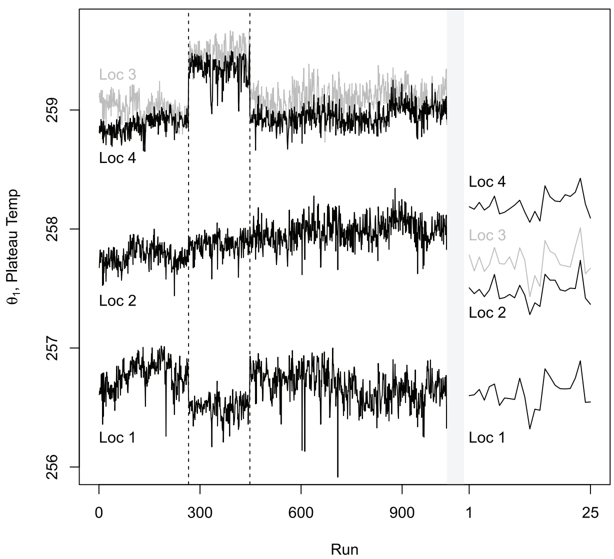

FIGURE 11. Plot of the Estimated Plateau Temperature for Phase II. Notice that location 3 dropped by over a degree from the phase I in-control mean. Large shifts in plateau temperature for phase II are also found for locations 2 and 4.

and we are satisfied that the procedure indicates the known process change. The diagnostic plot is a useful tool to determine the nature of the process shift.

7. Discussion and Conclusions

We have described a parametric technique based on combining two different nonlinear functions for analyzing this oven temperature dataset. The phase I analysis reveals a process shift that we account for prior to performing the phase II analysis. The results of the phase II analysis show that the approach is able to detect a known process change, even in the presence of between-profile correlation. The phase I and phase II data suggest that sudden shifts in the process are possible. These sudden shifts are well detected by the T^2 statistic. If the process monitoring should be sensitive to modest and gradual shifts, then a test statistic based on the multivariate MEWMA could be computed as described in Lowry et al. (1992). The proposed approach was successful in detecting lower quality parts and could be used to prevent them from being used in downstream assembly and reduce overall production costs. The proposed approach is general enough that it can also be used in the future for monitoring of other ovens that have slight differences in the profiles.

We discuss several issues in the profile-monitoring literature that are highlighted by this dataset. First, there is a need to further address the multiple profile situation. The papers of Paynabar et al. (2013), Chou et al. (2014), and Grasso et al. (2014) are a start, but there is a host of unanswered questions to be addressed. We consider the multiple-profile problem to be analogous to the common X-bar/R or X-bar/S charts for univariate data. The multiple-profile problem is a situation where there are more ways that the profiles can be out of control and more sophisticated techniques are needed to account for within-profile variability, the profile-to-profile variability within the same time period or run, and the run-to-run variability across time periods.

Second, we encourage research that focuses on the arbitrary design that can occur in profile monitoring and not simplify matters by assuming the CFD. We believe there is value in not requiring the CFD assumption, because an approach that will work for an arbitrary design will also work for one with a CFD. As a related topic, it would be valuable to do additional study to find ways of converting arbitrary design data, through interpolation or other methods, in order to take advantage of approaches based on the CFD assumption.

Finally, in real applications, the number of available profiles can be far larger than what is addressed in the literature. Some common data examples that have appeared in the literature on profile monitoring typically deal just a few profiles. For example, the widely used particleboard-density data of Walker and Wright (2002) contained 22 profiles, the calibration data of Mahmoud and Woodall (2004) contained 22 profiles, the calibration data of Gupta et al. (2006) contained 10 profiles, the dose-response data in Williams et al. (2007) contained 44 profiles, and the automotive engine data of Amiri et al. (2010) contained 26 profiles. As the real dataset examples contain a smaller number of profiles, so this smaller number of profiles is also used in simulation studies to compare the effectiveness of various approaches for profile monitoring and the broader area of multivariate control-chart methods. This case study illustrates a need to address larger amounts of data and we encourage research in that direction. Zhang and Albin (2009) gave an example of a multiple profile situation where there are 14 locations present in an oven. While the literature has adequately addressed the larger number of observations within a profile, it has not adequately addressed the multiple-profile problem nor large numbers of profiles. With a large number of multiple profiles, it becomes more difficult to appropriately reduce the information contained in the profiles to a smaller dimension in order to apply multivariate methods. In addition, larger numbers of profiles can increase the frequencies of false alarms in the phase I dataset and appropriate adjustments are needed in the control limits to maintain an acceptable false-alarm rate.

Ultimately, it is important to recognize that profile monitoring consists of two key tasks: 1) dimensionality reduction without losing key features of the data and 2) monitoring of the reduced data. For the first task, much of the research in the profile-monitoring literature focuses on the modeling approach of the profiles (parametric and nonparametric) with less emphasis on how to appropriately reduce the data dimension. There has been much work on multivariate SPC methods that have been proposed to handle the second key task. We believe that the first task is crucial in terms of the overall success of the monitoring scheme. There is no single "best" way to reduce the data and still be able to account for every single future process disturbance. Data reduction implies that there will be some risk introduced, in that the user will be susceptible to certain changes in the profiles that would otherwise be detected by looking at the full dataset. However, the user must balance this risk with the ease of monitoring the process. Looking at all the data is cumbersome and may lead to one not bothering to look at the data at all. In our opinion, the negative consequences of not looking at the data are much more severe than the potential negative consequences of only looking at a few key features of the data.

Supplementary Materials

A single zipped file is available online at http://www.asq.org/pub/jqt, containing the following files:

- Raw data used in phase I of temperature for all the ovens runs and the four locations in a text file called "Phase I Oven Temperature Data.txt".
- Raw data used in phase II of temperature for all the ovens runs and the four locations in a text file called "Phase II Oven Temperature Data.txt".
- Fitted nonlinear model parameter estimates and computed log(MSE) values from phase I raw data in a text file called "Phase I Parametric model estimates.txt".
- Fitted nonlinear model parameter estimates and computed log(MSE) values from phase II raw data in a text file called "Phase II Parametric model estimates.txt".

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