Statistical Process Control in the Presence of Multiple Batch Effects

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Abstract
Ensuring the quality of outgoing products is a critical component of most manufacturing processes; however, it is not always cost effective to test or inspect every unit produced. For example, in the production of forged metal parts for aerospace manufacturing, it is crucial to ensure that each part meets specific strength and other property requirements, but testing each part is very expensive. For this reason, it is often beneficial to implement statistical process control (SPC) in order to demonstrate the consistency of a process and reduce the cost associated with testing each part or product produced. In order to implement SPC, a process must first demonstrate its stability and then be qualified by demonstrating that it meets a specific, predefined requirement, often stated in terms of process capability index (C_{pk}), with a predetermined level of confidence. This qualification procedure is well documented for processes without batch effects, and methods are available to handle a single batch effect. However, the process for producing metal parts often consists of multiple levels of process batching, such as batches of raw material and batches of forged parts. Ignoring or improperly accounting for all batch effects can lead to incorrectly qualifying a process that does not meet the specified requirement. No previous methods have been published to verify requirements in the presence of complicated batching structures with more than one batch effect. Additionally, once a manufacturer's process has been qualified but before reduced sampling can be implemented, control charts must be developed to track changes in the process over time. Proper control charting strategies in the presence of multiple batch effects are not straightforward and have not been previously documented. We will describe a method for verifying C_{pk} requirements and building control charts under nearly all practical batching structures. This development fills an important technology gap in Statistical Process Control for aerospace and other industries, reducing the likelihood of escapes and false alarms by correctly characterizing process variation.
Key Words: statistical process control, SPC, batch effects, manufacturing, aerospace, process capability, control charts

1. Introduction

SPC implementation can greatly reduce testing costs for metal parts suppliers by reducing the number of units that need to be tested in each lot of materials that is delivered. Through adequate qualification and thorough monitoring of processes, the risk of escape can be well controlled even though the number of tested parts is small. In order for the benefits of SPC to be realized and the risks to be properly managed, qualification and monitoring must be carefully conducted by properly accounting for all relevant aspects of a process. Batch effects are an important aspect of processes that are often overlooked. These batch effects occur when parts within a group are more similar to each other than they are to parts in other groups. Batch effects are often generated from processing of parts in heat treat lots and can also result from the use of different lots of raw materials, among other things. If batch effects are not properly accounted for, estimates of process variation may be incorrect. Incorrect variance estimates may result in qualification of inadequate parts and incorrect control charting if SPC is implemented. If qualification of a supplier producing inadequate parts occurs, the risk of escapes is increased. Additionally, incorrect control charting may lead to high false alarm rates and thereby increased testing and process monitoring costs. Therefore, it is crucial to properly account for batch effects for both qualification and control charting. Existing methods (Scholz and Vangel 1998) are available for accounting for a single batch effect in the qualification of a process. However, more than one batch effect is common in typical production processes, though the extension of the existing methods to more complex batching structures is non-trivial. As an example of a more complex batching structure, raw materials may come in batches with substantial between batch variation; and parts may be produced in heat treat lot batches.

2. Background

SPC is widely used throughout industry to monitor production processes through the use of statistical sampling and charting. The benefits of SPC include controlling the fallout rate of accepted material, early problem detection, and continuous process improvement. The steps in the SPC process are depicted in Figure 1. A successful approach ensures first-time quality by correctly rejecting processes that produce parts that do not meet specified requirements, saves time and cost by correctly accepting processes that yield products which can meet requirements, and protects buyers from risk of escapes while driving continuous improvement through process monitoring.

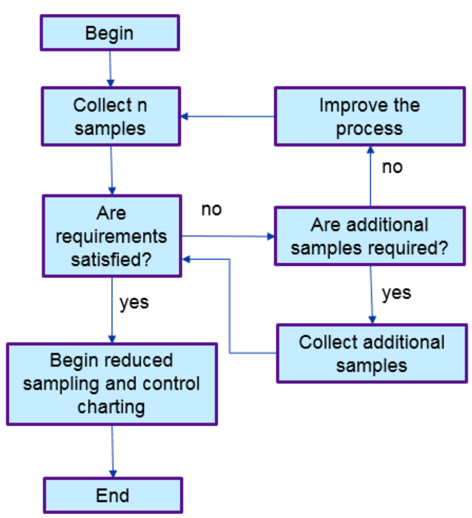

Figure 1: Flow chart for SPC implementation

Before reduced sampling begins, the production process is required to demonstrate capability, typically stated in terms of C_{pk}. C_{pk} is a process capability index which provides a measure of the quality of the process distribution with respect to specification limits. High C_{pk} indicates low fallout rates. For example C_{pk} of 1 means that 99.7% of a distribution will fall within a two-sided specification under normality. C_{pk} is defined as the minimum of C_{pu} and C_{pl}, which are defined below for processes without batch effects (Joglekar 2003):

$$C_{pk} = \min\left(C_{pu}, C_{pl}\right) \ where \ C_{pu} = \frac{USL - \hat{\mu}}{3\hat{\sigma}} \ and \ C_{pl} = \frac{\hat{\mu} - LSL}{3\hat{\sigma}},$$

$LSL = lower\ specification\ limit\ \ and\ USL = upper\ specification\ limit,;\ \hat{\mu}$ represents the sample mean, $\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x_i$; and $\hat{\sigma}$ represents the sample standard deviation, $\hat{\sigma} = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \hat{\mu})^2$.

To ensure the process meets capability requirements, sampling error must be taken into account and thus, the requirement is modified to incorporate a confidence level. This requirement modification is dependent on sample size. For example, if the requirement states that the process must produce a C_{pk} of 1.0 with 90% confidence, then the process must provide a C_{pk} of 1.30 with only 20 samples and a C_{pk} of 1.15 with 60 samples. This modified C_{pk} requirement is referred to as C_{pk}*. The C_{pk}* value decreases (i.e., the requirement is relaxed) as sample size increases or confidence level decreases. The formula to calculate C_{pk}* is ${C_{pk}}^* = \frac{1}{3\sqrt{n}} t_{n-1, C_0\sqrt{n}, 1-\alpha}$, where n is the sample size, α is the Type I error rate associated with the confidence level of interest, C_0 is the C_{pk} requirement value, and $t_{n-1, C_0\sqrt{n}, 1-\alpha}$ is the $(1-\alpha)$ quantile of a non-central t-distribution with $n-1$ degrees of freedom and non-centrality parameter $C_0\sqrt{n}$.

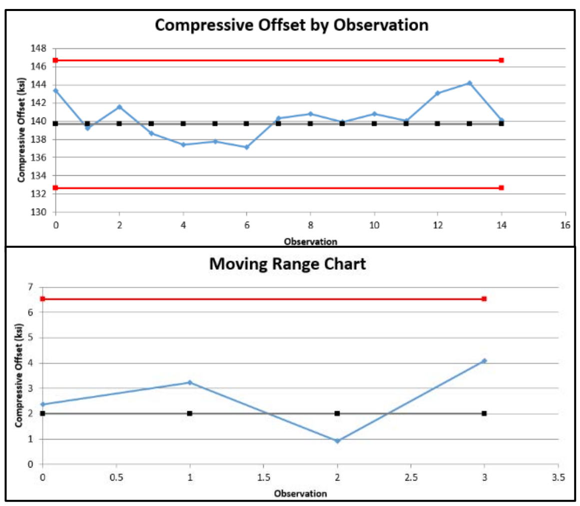

Figure 2: Example of individual and moving range control chart

Once a process meets the C_{pk}* requirement for the appropriate sample size, reduced sampling and control charting begin. Reduced sampling and control charting enables stakeholders to monitor the process without the cost associated with 100% inspection. Sampling plans typically account for the inherent sources of variation in the process. Control charts must monitor both trends in central tendency and trends in variation. Traditional control charts include a pairing of individual and moving range charts (see Figure 2 for an example) or a pairing of x-bar (mean) and range charts. Individual and moving range charts require a sampling plan such that 1 sample is collected per lot. In this case, the central tendency of the process distribution is monitored through plotting the individual observations over time on the individual chart, and the variation is monitored through the moving range (the difference in two consecutive observations). If more than 1 sample is required per lot, then x-bar and range charts may be used to monitor the process. In this case, x-bar charts monitor the average of each set of observations per lot over time and the range charts monitor variation by plotting the range of observations per lot over time.

Computing C_{pk}*, developing sampling plans, and building control charts become very complex when batching exists in the production process. Batching introduces new sources of variation, and the components of SPC must monitor all sources of variation. Batching exists when a correlation structure is present in the production process. Commonly, observations within the same batch will be more similar than observations from different batches. For example, parts created from the same batch of raw metal, or mill heat, tend to be more similar than parts created from two different mill heats. When multiple batching variables exist, the correlation structure is much more complex. For the forged metal parts example, imagine that raw metal from a given mill heat is used to create forged metal part, which are then heat treated in batches known as heat treat lots. In this example scenario, the expectation is that observations from the same heat treat lot are more similar than observations from different heat treat lots. Moreover, observations from the same mill heat are more similar than observations from different mill heats. Furthermore, observations from the same mill heat and the same heat treat lot are more similar than any other combination of mill heat / heat treat lot. Clearly, the number of batching variables may increase as production processes become more and more complex. As the number of batching variables increases, the number of batching combinations which must be monitored can increase dramatically. Furthermore, different types of batching exist and these different types of batching require different handling to appropriately account for variation sources in the production process.

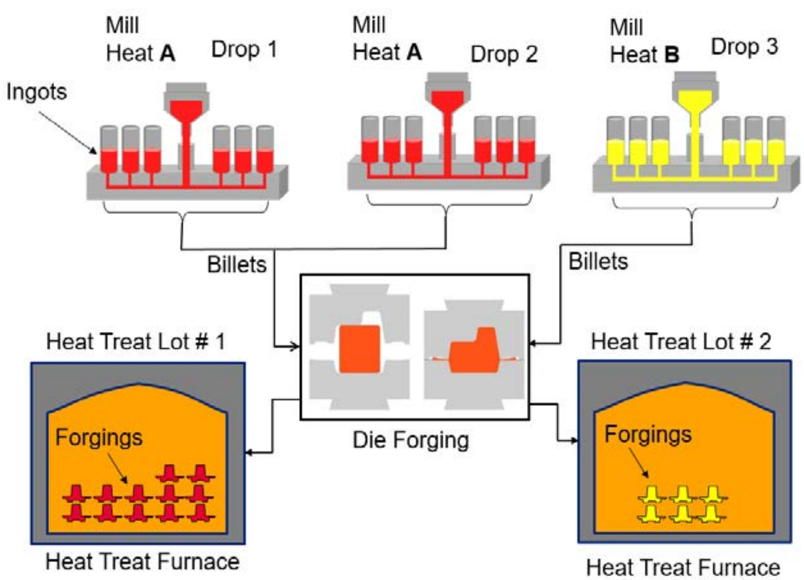

Figure 3: Example of nested batch effects

Types of batching structure include both nested and crossed effects. Nested batch effects include groupings which only appear within a particular level of a different grouping. In

Figure 3, which illustrates nested batch effects, all of the parts in heat treat lots are made from material from mill heat A, and all of the parts in heat treat lot 2 are made from material from mill heat B. We assume that there are additional heat treat lots containing material from mill heat A as well as additional heat treat lots containing material from mill heat B so that the two batching variables are distinguishable from each other. For this case, heat treat lots never contain material from multiple mill heats. Thus, heat treat lot is nested within mill heat. Crossed batch effects, on the other hand, include observations from a single group appearing across multiple groups of a different batching variable. In Figure 4, material from mill heat A is used in both heat treat lot 1 and 2, thus mill heat is crossed with heat treat lot. Different types of batching must be characterized appropriately in the computation of C_{pk}* and the sampling / control charting plan. Methods currently exist to control for one batching variable, but the handling of multiple batching variables has remained elusive. In this manuscript, we describe a method for handling multiple batch effects in the context of SPC and provide details for properly estimating C_{pk}* and constructing control charts.

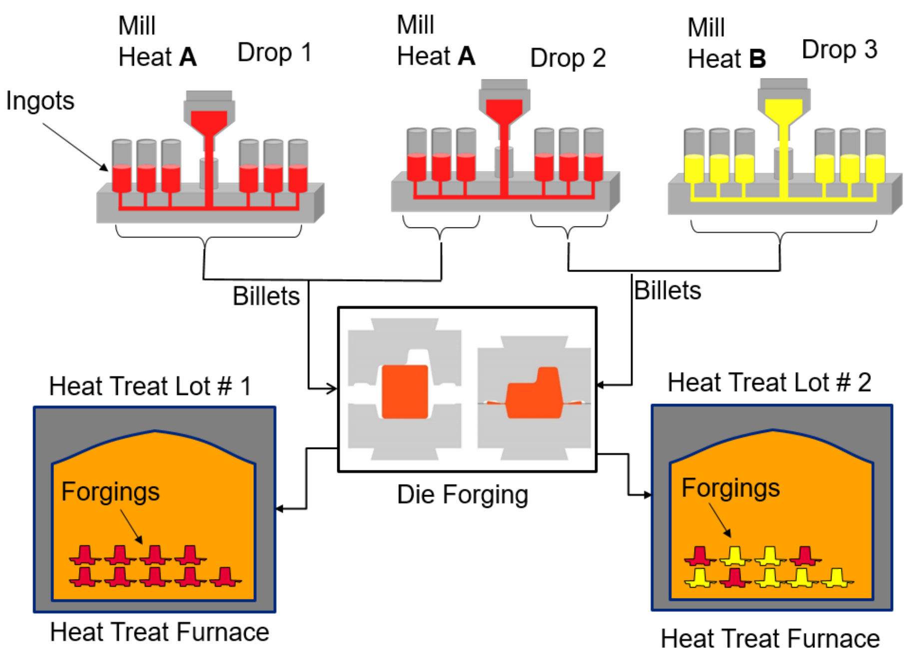

Figure 4: Example of crossed batch effects

3. Methods and Results

3.1 Assessing C_{pk} Requirements in the Presence of Multiple Batch Effects

The methods for calculating C_{pk} and C_{pk}* described above are based upon the assumption of independent samples from a normal distribution. When batch effects are present, samples within a batch are correlated and are therefore no longer independent. If the variance or standard deviation of these samples is estimated without accounting for this lack of independence, the produced estimate will be incorrect. Since samples within a batch are typically positively correlated (samples within a batch are more similar to each other than to samples from other batches), the variance of the process will often be underestimated if traditional methods that do not account for batching are used. Underestimation of process variation can lead to overestimation of C_{pk} and underestimation of C_{pk}*, which means that an inadequate process could be qualified.

To calculate the proper variance components to use in C_{pk} calculation, we use a linear mixed model. The model for the case with two crossed batch effects (one for mill heat of raw metal and one for heat treat lot of forged parts) is $y_{ijk} = a + h_j + m_k + e_i$, where i is the observation, j is the heat treat lot, and k is the mill heat. In this model, y is the outcome, a is the model intercept, $h \sim N(0, \sigma_{HL}^2)$ is the heat treat lot effect, $m \sim N(0, \sigma_{MH}^2)$ is the mill heat effect, and $e \sim N(0, \sigma_e^2)$ is the error term (representing within batch variation). To calculate the estimated C_{pk} using this model, the appropriate formula to use is

$$C_{pk} = min(C_{pu}, C_{pl}) \ where \ C_{pu} = \frac{USL - \hat{\mu}}{3\hat{\sigma}} \ and \ C_{pl} = \frac{\hat{\mu} - LSL}{3\hat{\sigma}},$$

$\hat{\mu} = \hat{a}$, and $\hat{\sigma} = \sqrt{\widehat{\sigma_{HL}^2} + \widehat{\sigma_{MH}^2} + \widehat{\sigma_e^2}}$

For the more general case of any number of batch effects (B), the model becomes $y_i = a + (\sum_{j=1}^{B} b_{ij}) + e_i$. For this model, the estimated standard deviation used to calculate C_{pk} becomes $\hat{\sigma} = \sqrt{(\sum_{i=1}^{B} \widehat{\sigma_i^2}) + \widehat{\sigma_e^2}}$.

To determine the appropriate value of C_{pk}* to use, it is first necessary to determine the effective sample size (Scholz and Vangel 1998). The effective sample size (n^*) represents the estimated number of independent contributions after accounting for correlation structure. This quantity is derived by matching the variance of the estimate of the mean for the batched data and the variance estimate for the mean of a hypothetical independent sample of size n^* from the same distribution (see Scholz and Vangel 1998 for details). Extending the method of Scholz and Vangel, for two crossed batch effects effective sample size is given by $n^* = 1/\left[\frac{\widehat{\sigma_h^2}+\widehat{\sigma_m^2}}{\widehat{\sigma_h^2}+\widehat{\sigma_m^2}+\widehat{\sigma_e^2}} \sum_{i=1}^{H} \sum_{j=1}^{M} \left[\frac{n_{ij}}{n}\right]^2 + \frac{1}{n} \frac{\widehat{\sigma_e^2}}{\widehat{\sigma_h^2}+\widehat{\sigma_m^2}+\widehat{\sigma_e^2}}\right]$, where n is the total sample size and n_{ij} is the sample size in heat treat lot i and mill heat j, H is the total number of heat treat lots, and M is the total number of mill heats. This can be extended to any number of crossed or nested batch effects using the formula $n^* = \left(\frac{\sum_{i=1}^{B} \widehat{\sigma_i^2}}{(\sum_{i=1}^{B} \widehat{\sigma_i^2}) + \widehat{\sigma_e^2}} \sum_{j \in J} \left(\frac{n_j}{n}\right)^2 + \frac{1}{n} \frac{\widehat{\sigma_e^2}}{\sum_{i=1}^{B} \widehat{\sigma_i^2} + \widehat{\sigma_e^2}}\right)^{-1}$, where J represents the set of all possible combinations of batching variables.

After calculating the effective sample size, the C_{pk}* value, which incorporates the appropriate confidence level into our requirement, can be calculated using the formula ${C_{pk}}^* = \sqrt{\frac{n-1}{n}} \frac{1}{3\sqrt{n^*-1}} t_{n^*-1, C_0\sqrt{n^*}, 1-\alpha}$, where $t_{n^*-1, C_0\sqrt{n^*}, 1-\alpha}$ is the $(1-\alpha)$ quantile of a non-central t-distribution with $n^* - 1$ degrees of freedom and non-centrality parameter $C_0\sqrt{n^*}$.

3.2 Control Charting in the Presence of Multiple Batch Effects

Prior to building control charts, one must develop a sampling plan. Sampling plans for processes with multiple batch effects must consist of samples from every combination of batches. For the example of mill heats and heat treat lots, one or more samples must be obtained from every combination of mill heat and heat treat lot that occurs. The specific sampling plan with vary from process to process and must be tailored to the process. The choice of how many samples to obtain from each combination of batch effects should be based on many factors, including the mean and variance components of the process and the acceptable risk of escape.

As described above, control charts for processes with multiple batch effects must be able to monitor the central tendency as well as all sources of process variation, meaning every variance term in the linear mixed model described above. Although an x-bar chart in the presence of batch effects is similar in appearance to an analogous chart for a process without batch effects, the calculation of the control limits differs. Furthermore, a single range chart or moving range chart can monitor process variation without batch effects, whereas multiple charts are necessary to monitor the multiple variance components that exist in processes with multiple batch effects. For processes with batch effects, range charts are used to monitor within batch variation and moving range charts are used to monitor between batch variation. Note that sampling plans requiring only a single sample per batch combination cannot include a range chart because calculating the range requires at least two observations. Therefore, within batch variation cannot be explicitly monitored. However, the within batch variation term is also present in the control limits for moving range chart, so within batch variation can be indirectly monitored through moving range charts.

3.2.1 X-bar and Individual Charts

For sampling plans with two or more samples per batch combination, an x-bar chart is often used to monitor the central tendency of the process over time. For each combination of batch effects (i.e. every combination of heat treat lot and mill heat that occurs in production), the selected number of samples will be tested and the mean value of the test results from these samples will be plotted on the x-bar chart. In order to construct the proper control limits of the x-bar chart, the proper variance need to be used. The appropriate formulas for constructing these control limits are described below.

$$Center\ Line\ (CL) = \hat{\mu}\ (see\ equations\ for\ C_{pk} calculations\ above)$$
$$Upper\ Control\ Limit\ (UCL) = \hat{\mu} + 3s,$$
$$Lower\ Control\ Limit\ (LCL) = \hat{\mu} - 3s,$$
$$where\ s = \sqrt{\widehat{\sigma_h^2} + \widehat{\sigma_m^2} + \frac{\widehat{\sigma_e^2}}{n_{samp}}},$$

and n_{samp} is the number of samples obtained from each batch combination.

These equations describe the formula for our example with two batch effects. This can be extended to any number of batch effects by updating the formula for the standard deviation to $s = \sqrt{\left(\sum_{i=1}^{B} \widehat{\sigma_i^2}\right) + \frac{\widehat{\sigma_e^2}}{n_{samp}}}$.

For sampling plans that collect a single sample from each batch combination, an individual chart is used in place of an x-bar chart. The construction of an individual chart is the same as the construction of an x-bar chart except that a single measurement value is plotted for each batch combination rather than a mean of two or more values. The formulas to calculate the center line and control limits are the same as for the x-bar chart.

3.2.2 Range Charts

For processes with batch effects, range charts are typically used to monitor within batch variation. For our example with two batch effects, this within batch variation represents the variance of observations within the same heat treat lot and within the same mill heat. The range is calculated as the difference between the maximum of the samples collected from each batch combination and the minimum of the samples, i.e.,

$$Range = \max(x_i) - \min(x_i),$$

where x_i is the set of samples collected from a given batch combination. The center line and control limits for the range chart can be calculated using the variance components of the linear mixed model using the formulas below.

$$Center\ Line\ (CL) = d_2\sqrt{\widehat{\sigma_e^2}},$$

$$Upper\ Control\ Limit\ (UCL) = d_2\sqrt{\widehat{\sigma_e^2}} + (D_4 - 1)d_2\sqrt{\widehat{\sigma_e^2}},$$

$$Lower\ Control\ Limit\ (LCL) = d_2\sqrt{\widehat{\sigma_e^2}} + (D_3 - 1)d_2\sqrt{\widehat{\sigma_e^2}}$$

In these equations, d_2, D_3, and D_4represent commonly used constants for control charting, available from many sources, including Appendix G of *Statistical Methods for Six Sigma* (Joglekar 2003). Note that these constants vary depending on the number of samples collected from each batch combination. In the case in which we are collecting only a single observation from every batch combination, within batch variation can be monitored indirectly through moving range charts, described in the next section.

3.2.3 Moving Range Charts

The moving range is defined as the absolute value of the difference between two observations from subsequent batch combinations (for sampling plans that measure only one sample per batch combination) or the absolute value of the difference between the means of two sets of observations from subsequent batch combinations (for sampling plans that measure two or more samples per batch combination), i.e.

$$MR = |x_i - x_{i-1}|\ for\ 1\ sample\ plans$$
$$MR = |\overline{x_\iota} - \overline{x_{\iota-1}}|\ for\ \geq 2\ sample\ plans$$

Moving range charts are used to monitor between batch variation. In the case of multiple batching variables, there is more than one between batch variation component. For example, with crossed batch effects for heat treat lot and mill heat, there is a between batch variation component for both heat treat lot and mill heat. This means that there are three possibilities for samples from different batch combinations: samples are from the same heat treat lot but different mill heats, samples are from different heat treat lots but the same mill heat, or samples are from different heat treat lots and different mill heats. Note that for nested batch effects, one of these combinations will not occur. For example, if heat treat lot was nested within mill heat, samples could be from different heat treat lots but the same mill heat or they could be from different heat treat lots and different mill heats, but samples from the same heat treat lot but different mill heats would not be present.

For processes with multiple batch effects, more than one moving range chart must be constructed. The number of moving range charts will be equal to the number of possible combinations of batching variables, for crossed batch effects this number will be 2^b-1 where b is the number of batching variables. For nested batch effects, the number of possible combinations of batch effects will be equal to the number of batching variables. Formulas are provided below for producing the three moving range charts for the example case with two crossed batch effects.

Case 1: Different heat treat lot, same mill heat

$$Center\ Line\ (CL) = d_2 \sqrt{\widehat{\sigma_h^2} + \frac{\widehat{\sigma_e^2}}{n_{samp}}},$$

$$Upper\ Control\ Limit\ (UCL) = d_2 \sqrt{\widehat{\sigma_h^2} + \frac{\widehat{\sigma_e^2}}{n_{samp}}} + (D_4 - 1)d_2 \sqrt{\widehat{\sigma_h^2} + \frac{\widehat{\sigma_e^2}}{n_{samp}}},$$

$$Lower\ Control\ Limit\ (LCL) = d_2 \sqrt{\widehat{\sigma_h^2} + \frac{\widehat{\sigma_e^2}}{n_{samp}}} + (D_3 - 1)d_2 \sqrt{\widehat{\sigma_h^2} + \frac{\widehat{\sigma_e^2}}{n_{samp}}}$$

Case 2: Same heat treat lot, Different mill heat

$$Center\ Line\ (CL) = d_2 \sqrt{\widehat{\sigma_m^2} + \frac{\widehat{\sigma_e^2}}{n_{samp}}},$$

$$Upper\ Control\ Limit\ (UCL) = d_2 \sqrt{\widehat{\sigma_m^2} + \frac{\widehat{\sigma_e^2}}{n_{samp}}} + (D_4 - 1)d_2 \sqrt{\widehat{\sigma_m^2} + \frac{\widehat{\sigma_e^2}}{n_{samp}}},$$

$$Lower\ Control\ Limit\ (LCL) = d_2 \sqrt{\widehat{\sigma_m^2} + \frac{\widehat{\sigma_e^2}}{n_{samp}}} + (D_3 - 1)d_2 \sqrt{\widehat{\sigma_m^2} + \frac{\widehat{\sigma_e^2}}{n_{samp}}}$$

Case 3: Different heat treat lot, different mill heat

$$Center\ Line\ (CL) = d_2 \sqrt{\widehat{\sigma_h^2} + \widehat{\sigma_m^2} + \frac{\widehat{\sigma_e^2}}{n_{samp}}},$$

$$Upper\ Control\ Limit\ (UCL) = d_2 \sqrt{\widehat{\sigma_h^2} + \widehat{\sigma_m^2} + \frac{\widehat{\sigma_e^2}}{n_{samp}}} + (D_4 - 1)d_2 \sqrt{\widehat{\sigma_h^2} + \widehat{\sigma_m^2} + \frac{\widehat{\sigma_e^2}}{n_{samp}}},$$

$$Lower\ Control\ Limit\ (LCL) = d_2 \sqrt{\widehat{\sigma_h^2} + \widehat{\sigma_m^2} + \frac{\widehat{\sigma_e^2}}{n_{samp}}} + (D_3 - 1)d_2 \sqrt{\widehat{\sigma_h^2} + \widehat{\sigma_m^2} + \frac{\widehat{\sigma_e^2}}{n_{samp}}}$$

Note that the formulas for each case include the variance terms for batch effect variables that are different, but not for batch effect variables that are the same for the case of interest. This pattern can be used to easily extend these formulas to produce MR charts for any number of batching variables.

4. Conclusion

Statistical Process Control has a dual role in minimizing testing cost while ensuring the quality of end products. A key component of a sound SPC plan is understanding sources of variation in process characteristics. Batching effects are nearly ubiquitous sources of variation in industrial processes that often go overlooked. Appropriately accounting for batch effects ensures proper estimates of variance, mitigating the risk of escapes due to overestimating process capability as well as controlling the false alarm rate in process monitoring. In this manuscript, we have detailed a method for accounting for multiple complex batch effects which allows computation of accurate process capability indices and appropriate control chart planning.

*The research described in this manuscript is patent pending (16/184293).

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