SIMCA®

Application Note

Improve Process Performance

10 June 2020

Introduction

A basic assumption in chemical manufacturing is that if process parameters are controlled tightly, results will be identical. However, this assumption is flawed because raw materials differ from lot to lot and process variables will deviate slightly resulting in variations in quality of the process and yield. The objective of this analysis was to apply multivariate batch modeling in SIMCA to identify the normal process evolution of high performing batches, sometimes referred to as the “Golden Batch”, and to investigate how the low yield batches differed from this.

The obtained model helps to build process knowledge and can be applied as a real-time process monitoring tool allowing identification and interpretation of deviations during the process execution. Based on the analysis, actions can be taken to counteract the deviating behavior. This technology is referred to as Batch Statistical Process Control (BSPC).

Application to a chemical process

The example data is from a medium sized (1000 l) chemical reactor in which several process steps, or phases, are executed. Here the phases designated *Addition A, Addition B, Heating and Cooling* are modeled. Data from a total of 25 batches were collected and of these, 9 batches were regarded as high yield batches. For each of these 25 batches a total of 7 parameters were measured: *Reactor Temp, Mantel Temp, Pressure, Weight, Stirring Speed, CoolerTemp, NDA (Non-Disclosed Attribute).* Data were collected each minute and the process ran for around 10 hours.

Building the Batch Evolution Model in SIMCA

The first step towards BSPC is to build a batch evolution model (BEM) for all batches in SIMCA. This model (not shown) is used to find and handle obvious errors in the data and to decide which parameters should be used in each separate phase. As in all data analysis it is crucial that the data is relevant to the question, correct and reliable.

Secondly, a model is built on only the high yield batches creating the normal process evolution model. In addition to being high yield batches it is important to ensure that there are no errors in the data before finalizing the model. This model now represents a normal variation in a well behaving process. Figure 1 shows a typical multivariate chart where the x-axis represents elapsed process time and the y-axis a multivariate summary parameter combining information from all 7 original parameters. The plot is divided into segments representing the four phases. The red dotted lines are the 3 standard deviations giving the boundaries of the models and the colored lines represent the individual batches.

Identifying causes for low performing batches in SIMCA

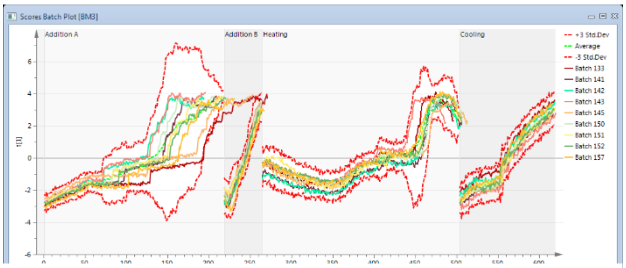

Figure 1: Multivariate batch control chart showing the model boundaries within each phase of the process and the evolution of the high performing batches.

By projecting the 16 low yield batches into the model based on the high yield batches it is easy to analyze the process deviations, as shown in figure 2. In the “*Addition A”* phase 6 batches deviated. In the “*Addition B”* phase only one of the low yield batches were inside the model boundaries. Also, in the “*Heating”* and “*Cooling”* phases a few batches deviate. In summary the models identified deviations in all the 16 low performing batches. The next step is to interpret the source of these deviations.

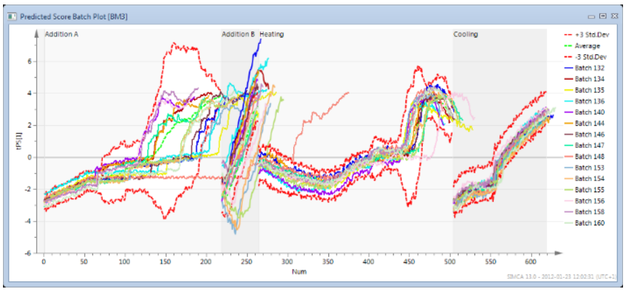

Figure 2: The low performing batches are projected onto the models built on the high performing batches. Each line represents a low yield batch and the red dotted lines represent the boundaries for a batch to be high performing.

Using the drill down tools to build process knowledge

Zooming in on the "*Addition B*" phase shows that all batches but one are outside the model boundaries. The drill-down functionality in SIMCA clearly reveals which variables are behind this deviation. A click on the deviating batch activates the contribution tool and illustrates which parameter(s) that differ from the high yield batches and how they differ. In the example below, figure 3 a and b, the NDA (Non-Disclosed Attribute) was found to be considerably higher for the low yield batches compared to the high performing batches.

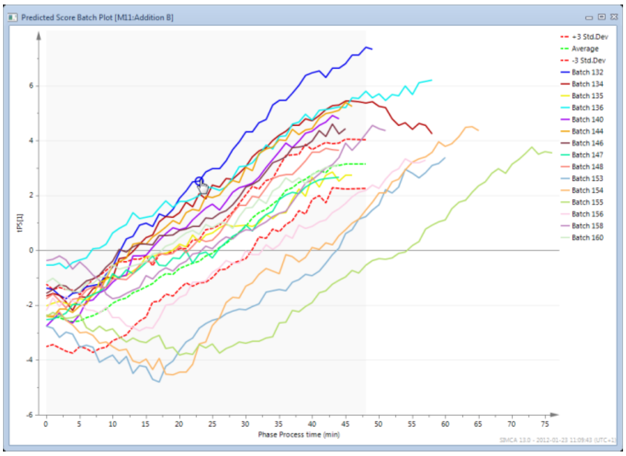

Figure 3: Zoom in on figure 2 on phase Addition B.

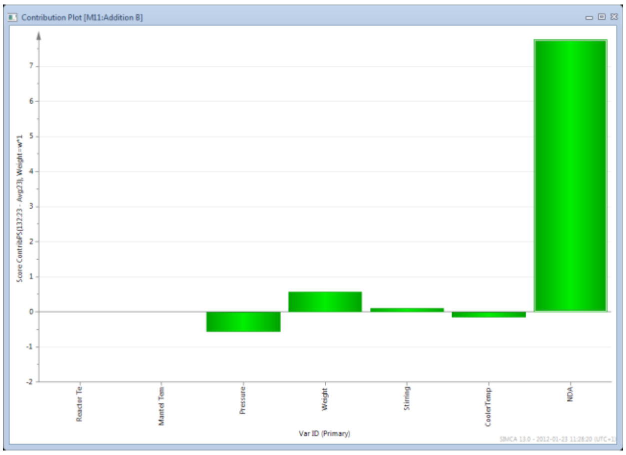

Figure 4: Contribution plot showing parameters contributing to the deviation of the blue batch at the time marked in figure 3.

By clicking on the contribution bar for NDA a raw data control chart is produced showing exactly how the deviating batch differs from the high yield batches relative to the levels of NDA, figure 4. As seen from these graphs there is a large difference in NDA trajectories for high and low yield batches.

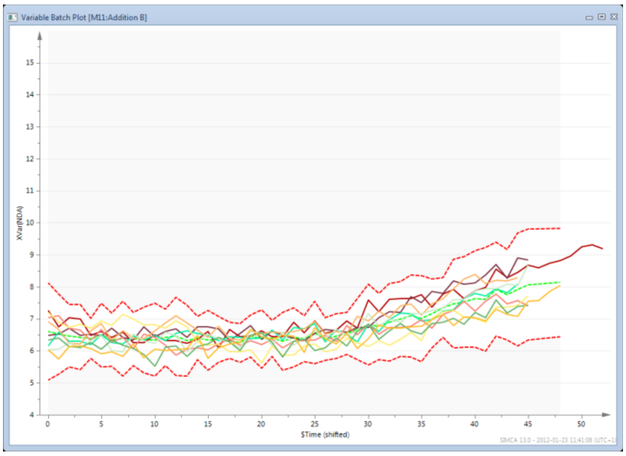

Figure 5: Batch control chart for NDA raw data showing the NDA levels for the high yield batches throughout the phase evolution.

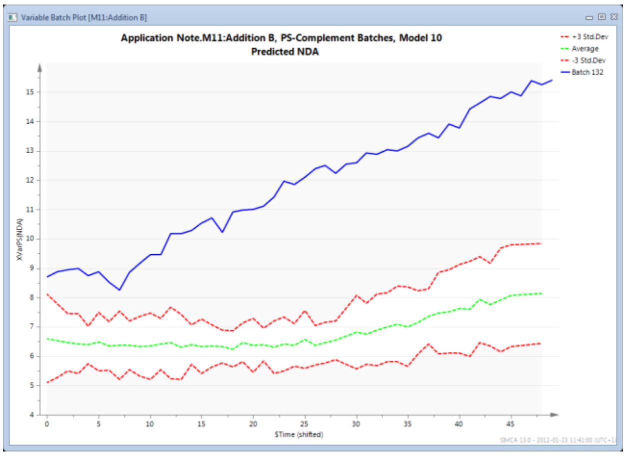

Figure 6: Batch control chart for NDA shoving the 3 standard deviation limits from the high yield batches and the actual value for the investigated deviating batch.

Occasionally the deviation is strictly univariate, but it is often the case that many variables deviate simultaneously. The second example below, figure 5, clearly shows such an example where most parameters are too low. This second example also clearly demonstrates that there are many ways for the process to deviate but regardless of reason it will influence productivity.

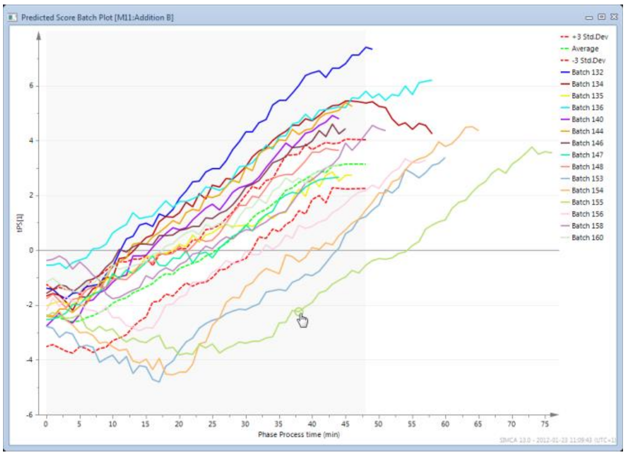

Figure 7: The indicated point was analyzed resulting in.

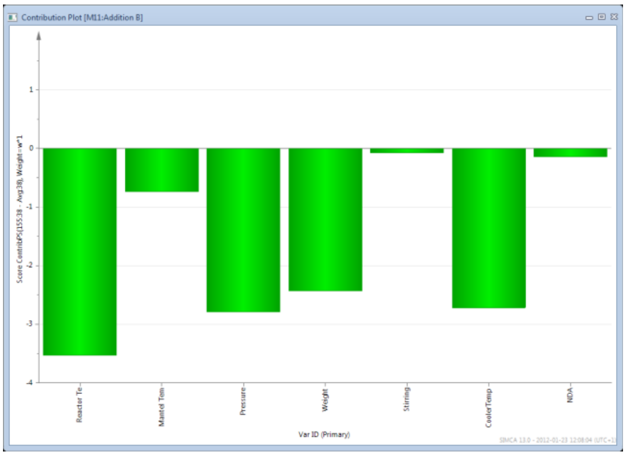

Figure 8: Contribution plot shoving a multivariate case of process deviation.

By repeating the same approach for all batches, a complete analysis of all deviations can be made.

Apply the model to monitor and control the process in SIMCA-online

There is significant value in understanding process variation. The information presented above can be used to prevent deviating performance and poor quality. Umetrics' SIMCA family includes real-time solutions that utilizes existing data for real time prediction of critical parameters or early fault detection.

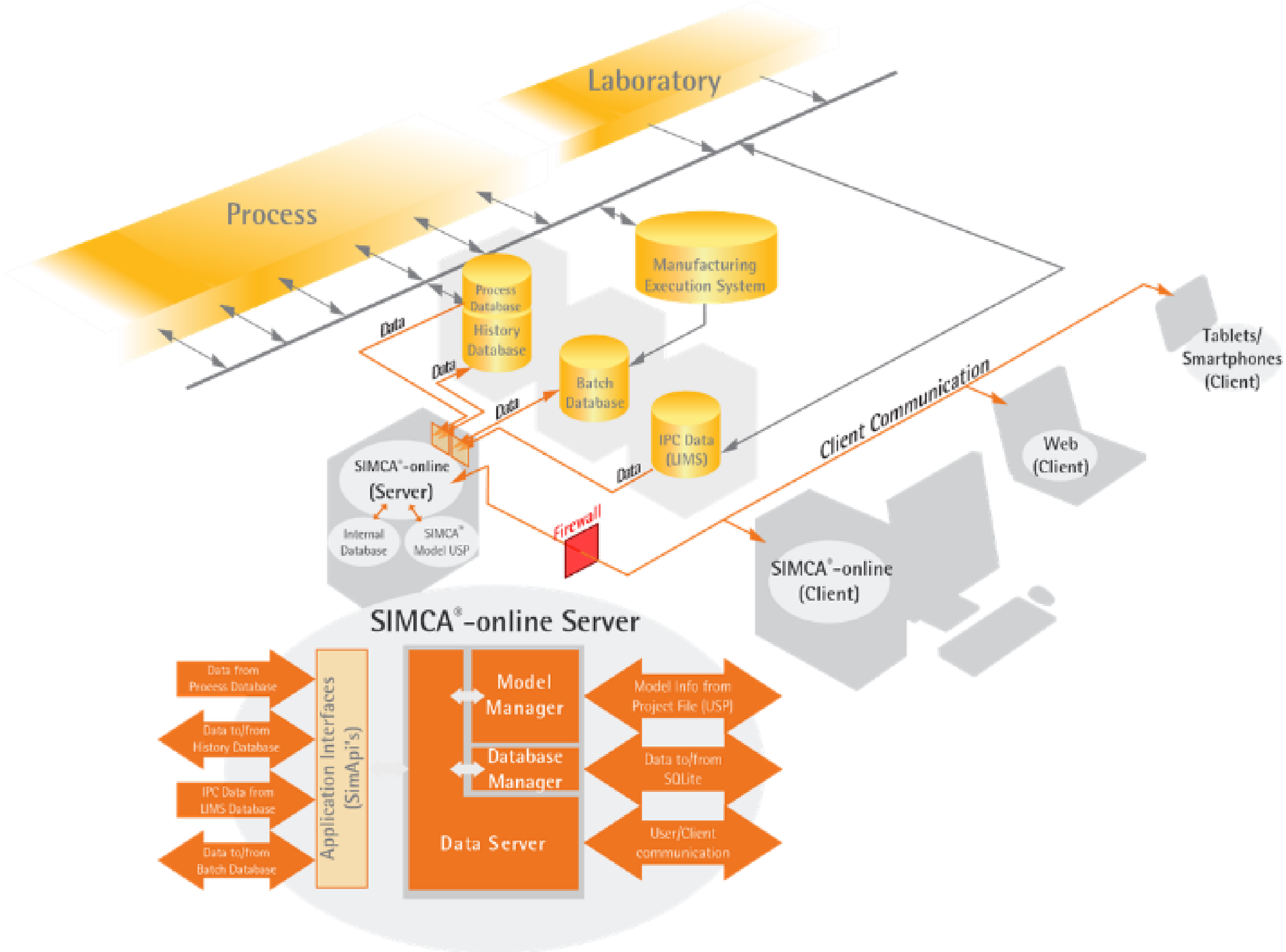

Figure 9: The SIMCA-online system reads data from the process databases and makes it available for analysis in real-time.

1. Real-time monitoring

Map the dynamic nature of batch processes characterizing the design space and identifying process boundaries. Real-time monitoring assures consistent manufacturing, provides early fault detection, and offers the ability to drill down and identify possible root cause parameters.

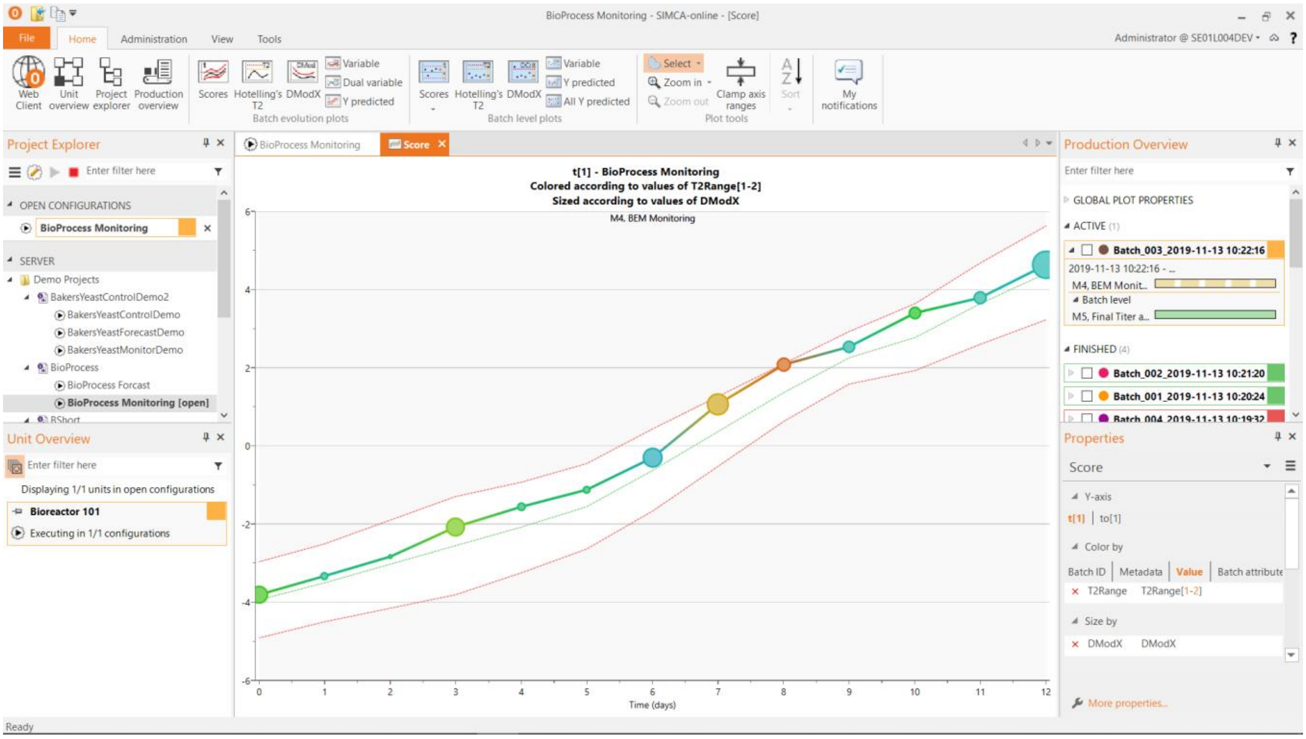

Figure 10: In the SIMCA-online client, data from the running processes are displayed in relation to the good process behavior (red lines). Any deviation from the known good process behavior is seen as an abnormal event and should be analyzed and diagnosed.

2. Final quality prediction

Predict the quality of your batch before it has finished. The benefits of quality prediction using multivariate batch modeling techniques include improved productivity, higher quality, and greater process knowledge.

3. Forecasting and open/closed loop control

The ultimate step in process analysis, closed loop process control offers the ability to make automatic adjustments to batches as they evolve based on intelligence gathered during previous batches. Turn problem batches into acceptable ones.