SIMCA-online

Application Note

Control Advisor

22 November 2019

Control Advisor is available since SIMCA-online 13.3 extending real-time multivariate monitoring capabilities to include a **Forecast** mode for predictive monitoring and an **Advised future** mode for process optimization with model predictive control (MPC).

Control Advisor includes powerful predictive capabilities utilizing a combination of imputation and regression methods to forecast future trajectories of batch processes. Predictions of final batch qualities and yields are made available early in the batch evolution and process deviations may be detected *before* they happen, allowing for proactive corrective action. The Advised future provides suggested process adjustments that may be implemented manually or automatically providing closed loop control.

Prediction method

In many cases the future trajectory and final conditions of a batch can be inferred from operation up to the current maturity. For example, in cell culture processes, high or low cell performance is detectable at very early stages. Utilizing the correlation structure captured in the multivariate batch level model (BLM), imputation methods estimate the future evolution using operation data up to the current time.

Integrated into Control Advisor is the patent pending Imputation by Regression (IBR) algorithm. IBR combines the single component projection imputation method with partial least squares (PLS) regression to provide high resolution, computationally efficient, predictions. In benchmark studies the predictive ability of IBR performs as well or better than traditional methods such as iterative imputation (II) or projection to model plan (PMP) and the computational efficiency of IBR permits real-time optimization of large, complex systems.

Data Types

Control Advisor has two types of variables:

- **Manipulated** variables are process parameters that are assignable and used for steering the process. Manipulated variables are typically setpoints for PID or base level controls.
- **Dependent** variables include process measurements and raw materials. Dependent variables are not controlled to influence the process.

Manipulated variables are handled differently from dependent for modeling and predictions. Future values of manipulated variables are target setpoints or recipe values which are known, whereas future values of dependent variables must be predicted.

Limitations

Calibrating models with forecasting ability require that;

- later stages of a batch process depend on early stages, and
- the generation of a dataset contains sufficient information to map the time-varying correlation.

Process experiments are often required to generate a dataset for predictive modeling. These requirements are slightly different depending on the Control Advisor mode:

- **Forecast:** Future trajectories must be correlated to operation up to the current time.
- **Advised future:** Future trajectories must be correlated to operation up to the current time and future adjustments in manipulated variables.

Forecasting requires only correlation between past and future operation whereas optimization requires a causal relationship between the process and manipulated variables.

Forecast

At each execution of SIMCA-online all predictions of future process trajectories are updated as new data is collected from the process and the predictions are displayed in the batch evolution control charts and batch level plots.

Batch evolution control charts include predictions of the measured values in the process up to the current time and predicted values to batch completion, including the ability to track future trajectories of univariate process parameters as shown in Figure 1. Diagnostic tools, such as contributions, are available for all predicted values allowing identification and diagnosis of future deviations. Batch level plots for final conditions, for instance yield or batch level scores, are updated and displayed at each execution.

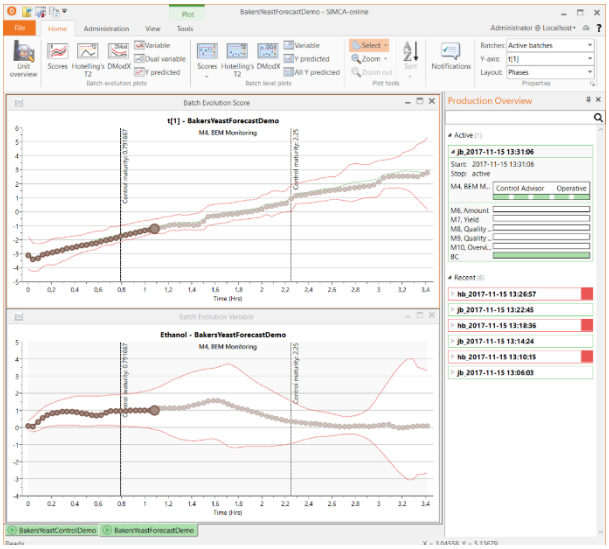

Figure 2, Batch evolution score (top) and univariate (bottom) control charts for Control Advisor in Forecast mode.

Advised future

The Advised future mode of Control Advisor provides recommendations for process adjustments to accomplish many types of objectives, such as;

- optimize final batch yield,
- control final batch qualities,
- minimize operational costs or energy consumption,
- steer the process down a desired path, such as, to maintain the process within SPC limits or to follow a desired cell performance trajectory for biological systems

Model Predictive Control (MPC)

Advised future is built on MPC technology leveraging Umetrics' multivariate batch modeling experience

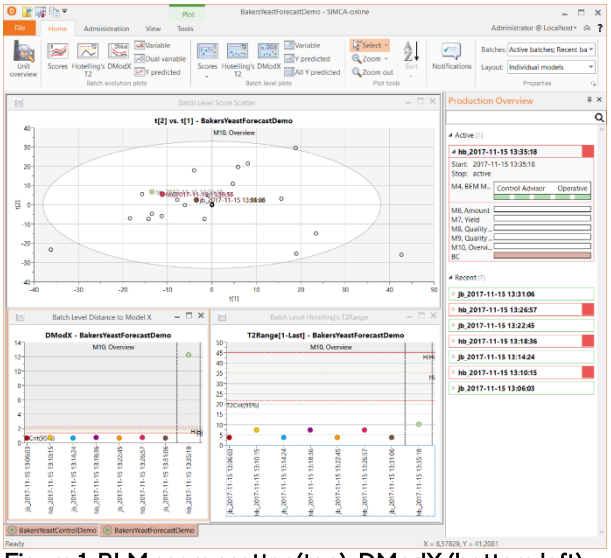

Figure 1, BLM score scatter (top), DModX (bottom left) and Hotelling's T2 (bottom right) plots showing a completed batch (blue) and the forecast of a batch still in production (pink).

and powerful predictive methods to provide a unique batch control solution. The goal of the controller can be described as finding the optimal process adjustments that;

- minimize the deviation in BLM Y from their specifications
- maintain important process variables on desired BEM trajectories
- maintain the process within BEM and BLM multivariate SPC limits
- utilize minimum changes in the manipulated variables from their normal setpoints

A simplified mathematical description of the control objective has the following form.

$$J = \sum \theta_{Y,i}\left(\hat{y}_i - y_{i,SP}\right)^2 + \theta_{T2,BLM}{T2_{BLM}}^2 + \theta_{DModX,BLM}{DModX_{BLM}}^2 +$$
$$\sum \theta_{T2,BEM}{T2_{BEM}}^2 + \sum \theta_{D,BEM}{DModX_{BEM}}^2 +$$
$$\sum \theta_{Xd,j}\left(\hat{x}_{d,j} - x_{d,j,SP}\right)^2 + \sum \theta_{Xmv,k}\left(\hat{x}_{mv,k} - x_{mv,k,SP}\right)^2$$

In this formula θ are penalty weights, SP refers to a setpoint or target, i is the ith BLM y, j is the jth dependent variable (xd) and k is the kth manipulated variable (xmv). For simplicity, scaling details and terms such as individual scores are not shown. The complete equation and definitions can be found in the help or in the user guide. The inclusion of multivariate SPC (Hotelling T2, scores and DModX) terms and control of batch processes, both BEM and BLM, is unique and unavailable in traditional MPC technologies.

Using the multi-objective function shown, optimization of many goals may be achieved simultaneously. Terms are easily removed to focus on a single or any relevant combination of objectives.

Closed loop control

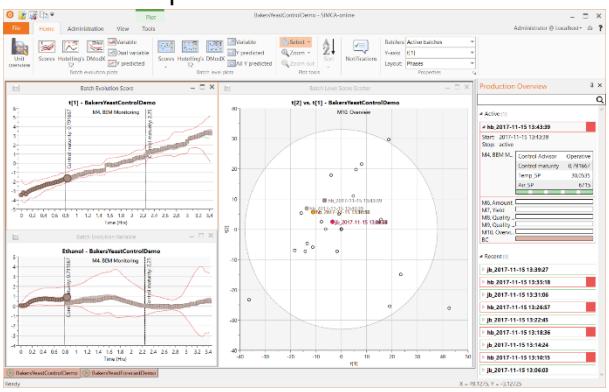

Figure 3, Batch control charts in Advised future mode showing predictions of future process performance for a) following the normal process settings (the Forecast mode) and b) implementing the Advised future settings.

In the Advised future mode control charts in SIMCA-online display predicted future trajectories assuming the optimal settings for the manipulated variables are implemented and include predictions if the manipulated variables are left at their normal setpoints. This can be described as displaying predictions for the open and closed process performance. The Advised future may be used simply as a tool to display recommendations to operations that may be implemented manually if they choose or configured to be written directly to the automation layer using the write back functionality of SIMCA-online for automatic closed loop control.