

# SARTORIUS

## Simplifying Progress

## SIMCA® 18 – What's New?

Release April 3, 2023



# SIMCA® 18 Overview

- Umetrics® Suite SIMCA® delivers a complete data analysis experience, from data import and organization to data driven decision making supported by multivariate models
- SIMCA® 18 introduces Adaptive Process Mode modelling to address challenges of continuous culture processes and other combinations of dynamic and steady state processes
- Continued improvements to spectroscopy data analysis by providing support for calibration transfer
- With the latest user experience improvements, there has never been a better time to get started with SIMCA®
  - Better possibilities to use Python scripts to solve complicated tasks and enhance existing functionality
  - Scripts\* for creating and testing forecast models bundled with installation package
  - Scripts\* for scalable model maintenance bundled with installation package
  - Sample code for creation of custom functions
  - Data import to get it right first time and modelling options when adding batch data

\*Example scripts, we encourage the user to customize scripts to suit their particular use case

# SIMCA® 18 Highlights

- Adaptive Process Mode
  - Combine dynamic and steady state process data
  - PLS | OPLS® models for dynamic phases
  - PCA for steady state phase in batch project
  - Combine dynamic and steady state phases at the batch level
- Calibration Transfer
  - Guided workflow for transfer of multivariate calibration models with spectroscopic data
  - Methods for transfer
    - Piecewise Direct Standardization
    - Offset correction
    - Custom via Python plugin
  - Support for subset selection (Kennard-Stone)
- Python Scripting
  - Generate Control Advisor data and models for SIMCA®-online
  - Test created Forecast models
  - Scalable model maintenance – for single and multiple projects
- Other Improvements
  - Import of batch data and added options post import
    - Reorder phases
  - Database import of large datasets
    - Improved and faster auto-formatting rules
    - Better performance and quicker checks for missing values
  - Generate variables from qualitative data
  - SIMCA® 17 and 16 compatibility

# Learning What's New in SIMCA® 18

- In the following slides you will get an overview of the changes and additions made in SIMCA® 18
- For more details on how to use the features, watch the what's new videos that you can reach from the start page of SIMCA® 18
- Also check out more videos on SIMCA® and other Umetrics® suite products by looking up Sartorius Data Analytics on YouTube

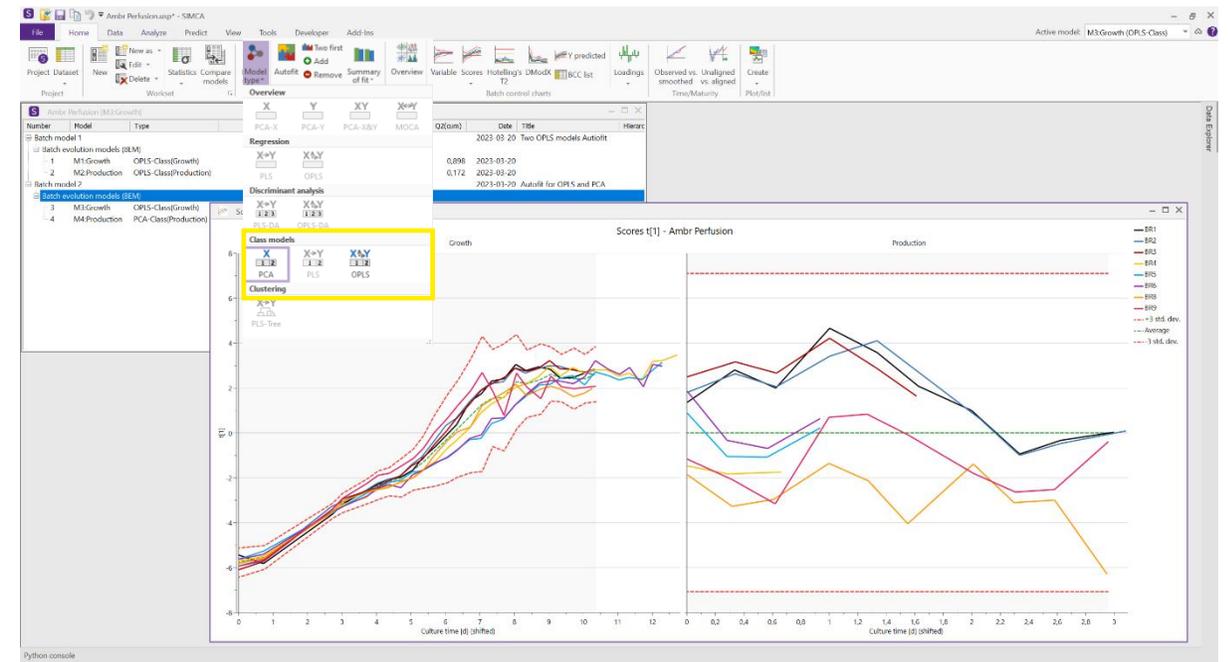
# SIMCA® 18 What's New

- Adaptive Process Mode
  - What
    - Combine OPLS® and PCA models in Batch projects
  - Why
    - Combine dynamic and steady state process data in one project
      - Create batch level models for steady-state phases
      - Combine dynamic and steady state phases at the batch level
      - One configuration in SIMCA®-online
  - How
    - Use PCA for true steady state phase modelling



# Added Flexibility for Batch Process Modelling

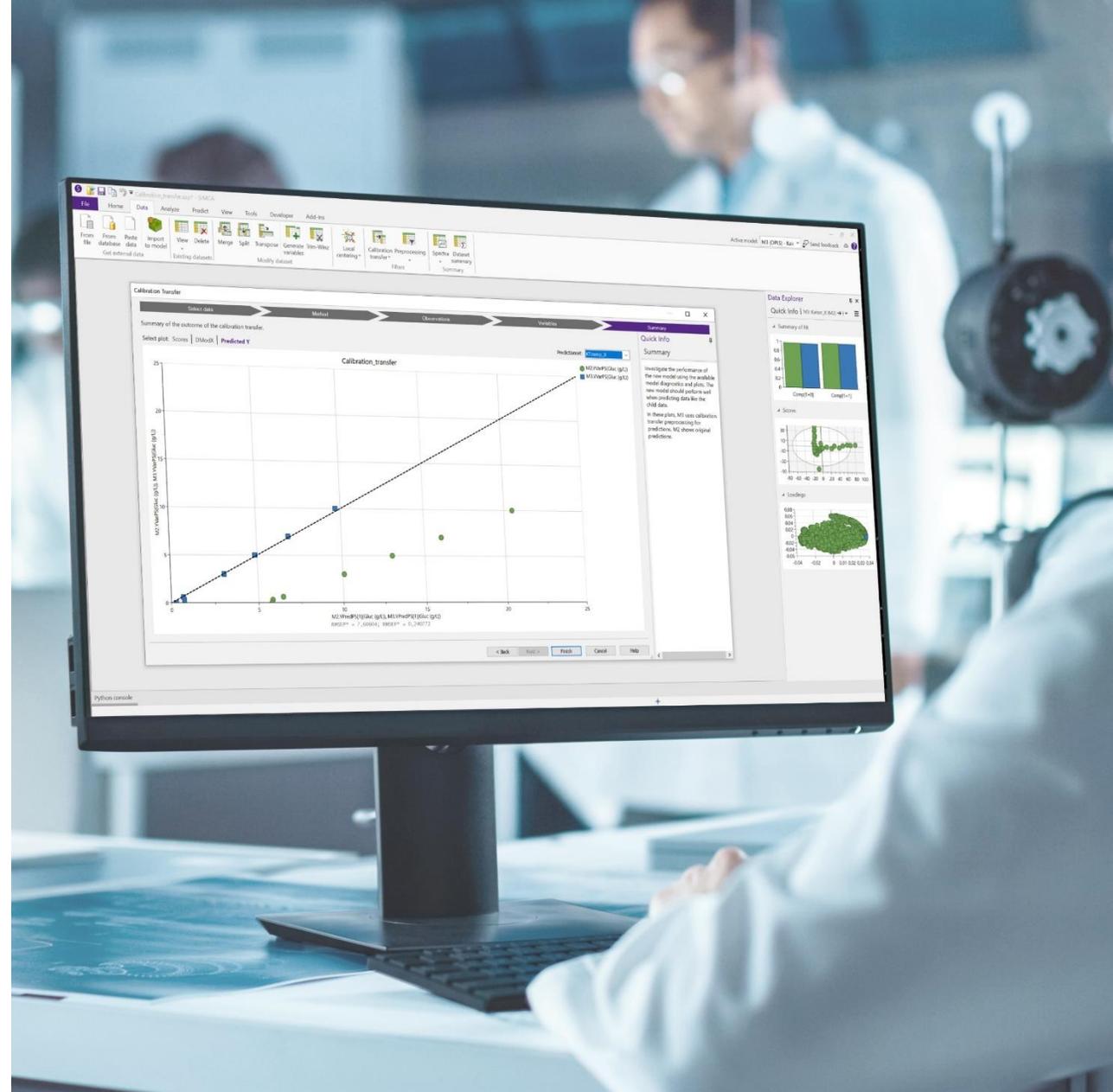
- Benefits
  - Improved modelling of steady-state phase in batch projects
  - Create one project for entire process
  - Combine dynamic and steady state phases in single project configuration
  - Predictions of Critical Quality Attributes possible for all phases
- Applies to
  - All processes with a steady | non-varying | continuous phase
  - Biopharma examples: chemostat, perfusion
  - Other: sterilization
- Changes
  - Possible to change model type from OPLS® to PCA for phase model in batch projects



# SIMCA® 18 What's New

## Calibration Transfer

- What
  - Added guided workflow for calculating Calibration Transfer weights to set up a model for new multivariate calibration solution
- Why
  - Use existing calibration | soft sensor model in a new setting without need for measuring all samples
  - Updating models after service or maintenance has been performed
  - Replacing/adding instrument to inventory
- How
  - Calibration transfer weights are calculated using Piecewise Direct Standardization (PDS). Weights are used for preprocessing new spectra.
  - Suggest new samples to analyze to enable calibration transfer



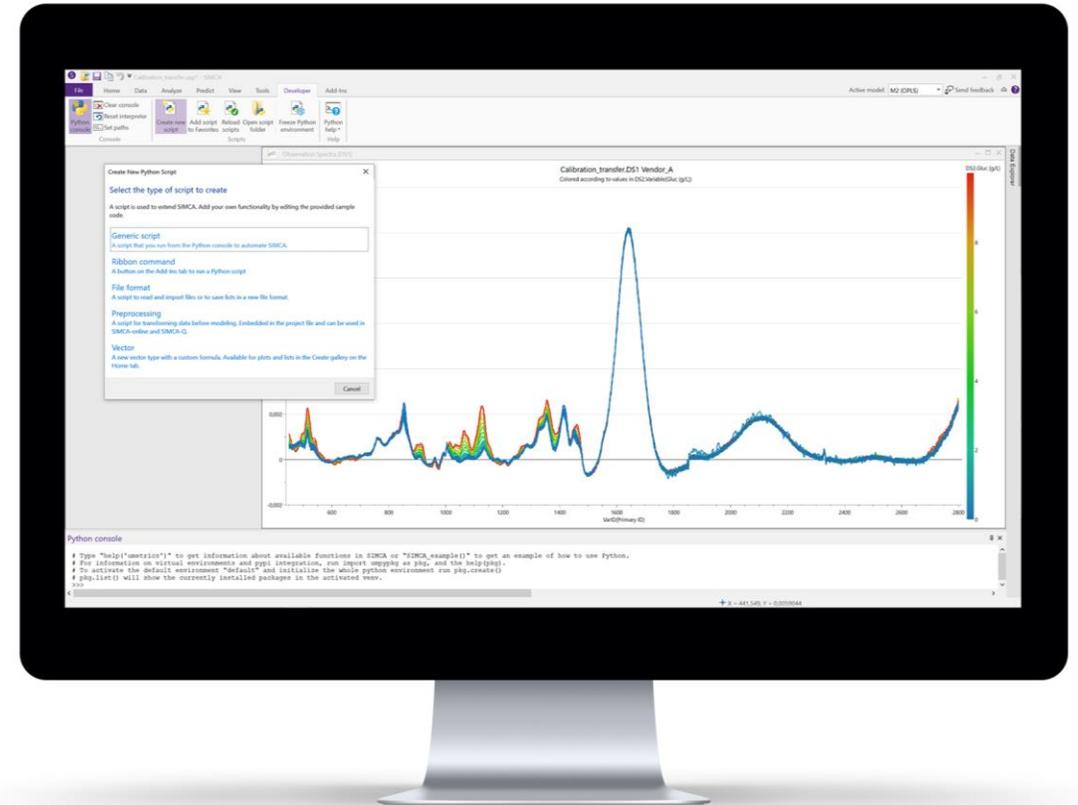
# Calibration Transfer – Guided Workflow

- Select data
  - Parent dataset – original dataset that calibration model was built on
    - Use raw data or preprocessed data (in case it exists)
  - Child dataset – spectra from new setup
- Method
  - Select method to calculate calibration transfer weights
- Observations
  - Match observations in the calibration model (parent) to representative new observations (child)
- Variables
  - Exclude | include variables to be used in new setup and align if necessary
- Summary
  - Model statistics
  - Decision basis for accepting model in new setup



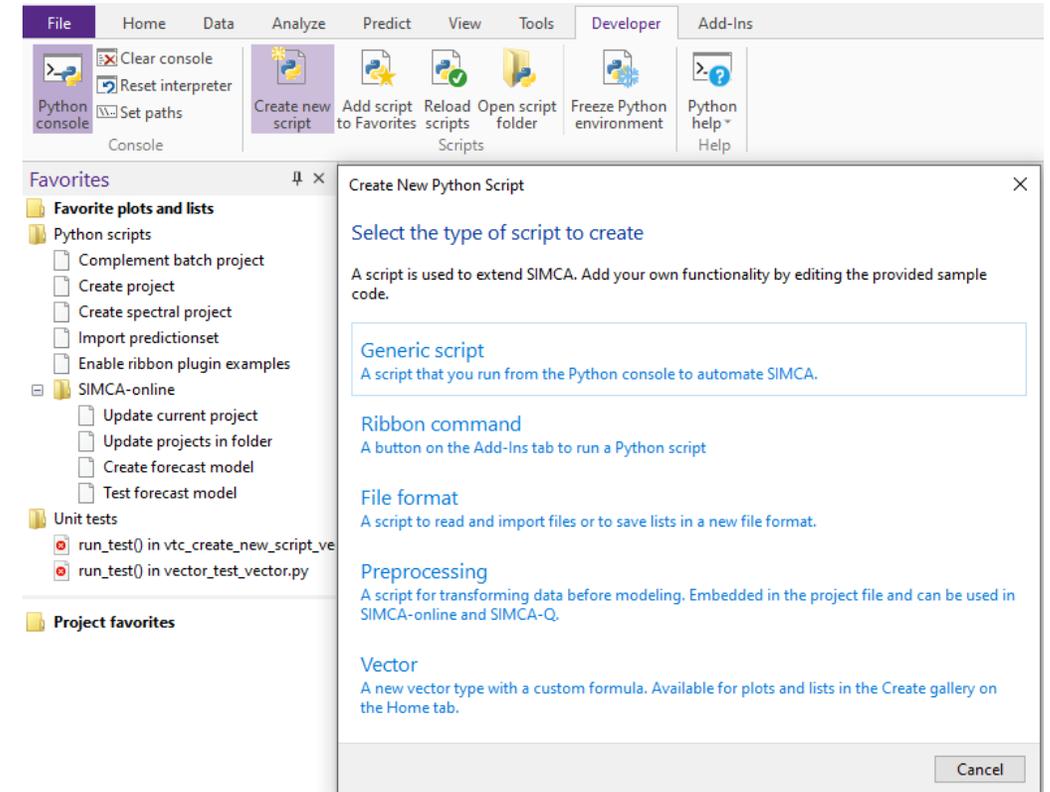
# SIMCA® 18 What's New

- Python Scripting
  - Create New Script
    - Added content
  - User experience
    - Unit test automatically created
- Bundled scripts
  - Generate Control Advisor data and models
  - Test created Forecast models
  - Scalable model maintenance – for single and multiple projects



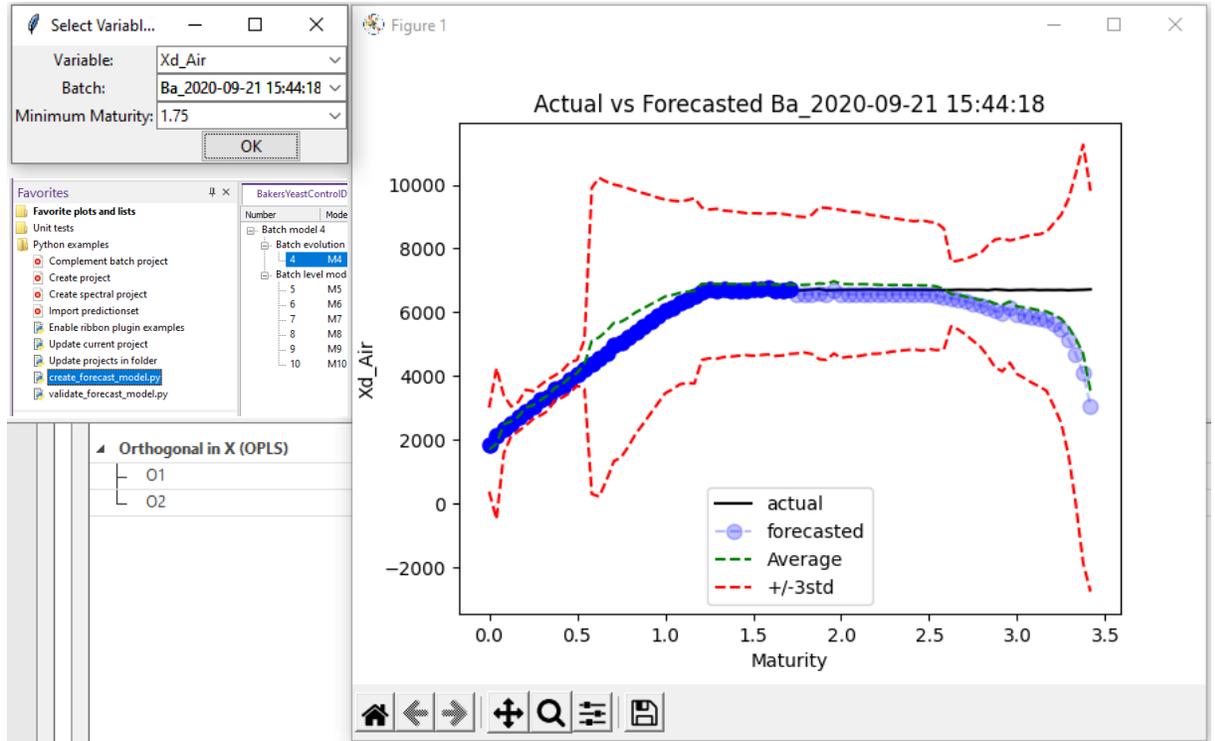
# Create New Python Script and Other Improvements

- Get it right from the start
  - Better dialog texts explaining the different options
  - Improved Python sample scripts
  - Python Help overhaul in included SIMCA® Scripting Guide
- New
  - Create 'Vector' for use in plots and lists in SIMCA®
  - Automatically created unit tests and a shortcut in Favorites to run the test during the development of the Python script
  - Reload scripts button for changes to take effect in SIMCA®
  - Python console – tab to display functions and help
- Sharing Python Scripts
  - Bundled example scripts
  - External file share with additional example scripts



# Bundled Scripts – Control Advisor Model Generator

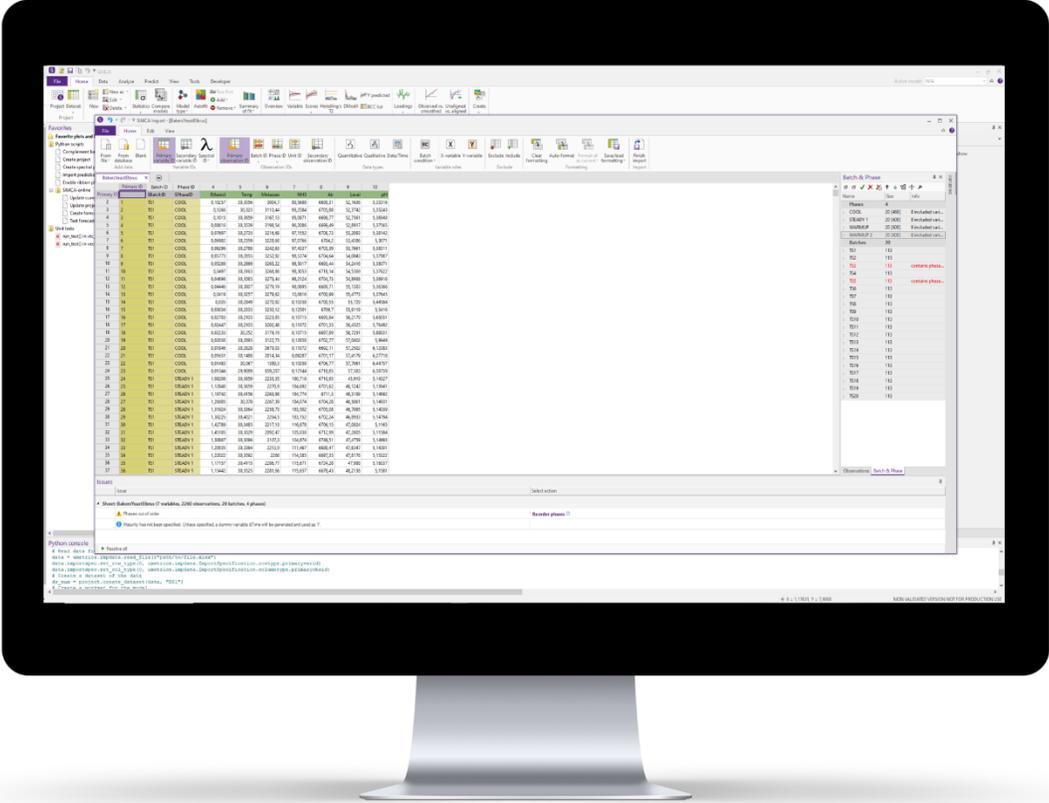
- Generate Control Advisor data and models
  - Create forecast model Python script\*, for creating datasets and models for SIMCA®-online
- Test created Forecast models
  - Verify that the created Control Advisor models give expected results that are in line with intended use before deploying in SIMCA®-online
- Scalable SIMCA®-online model maintenance
  - For single projects, open file with added data and run script to update project
  - For multiple projects, loops through all project files in a specified folder
  - $Q^2$  model diagnostics before and after update



\*All bundled scripts are provided as is and customers are encouraged to modify

# SIMCA® 18 What's New

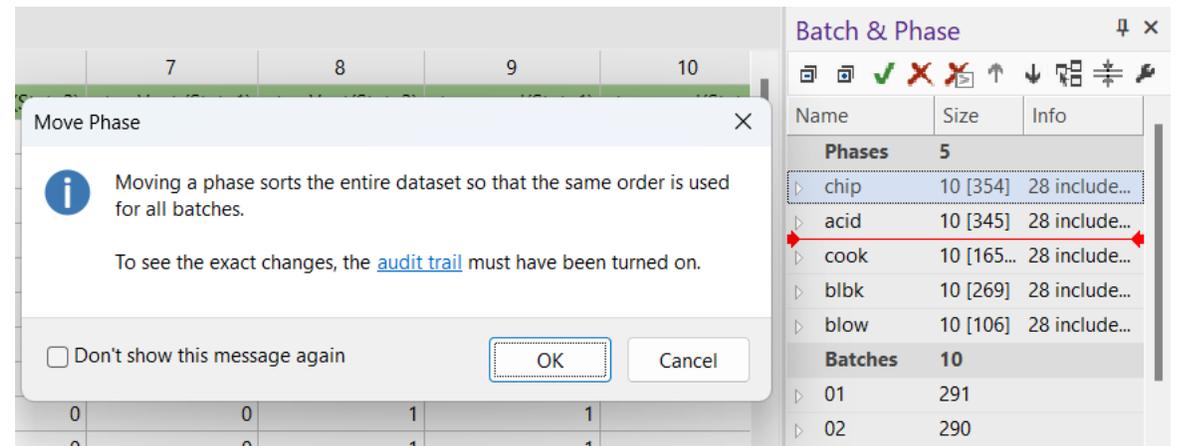
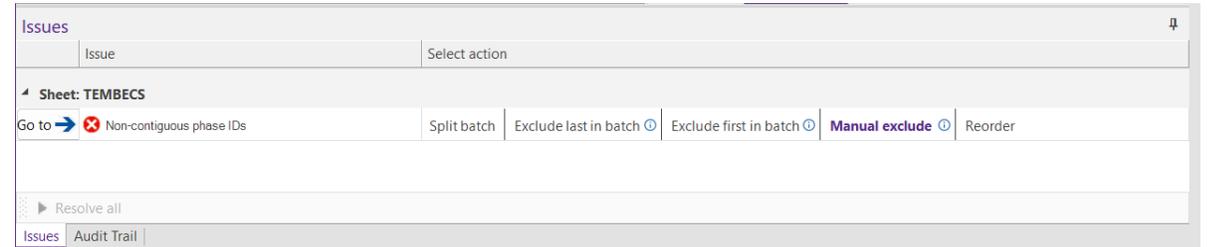
- Other improvements
  - Import performance
  - Improvements to resolving issues during import of batch and phase data
  - Ability to reorder phases in multiphase model
  - Generated variables from qualitative
  - Correlation matrix updates
  - Orthogonal component visualization
  - Enable use of secondary BatchID in batch level



# Import of Batch and Phase Data

## Problem Statement

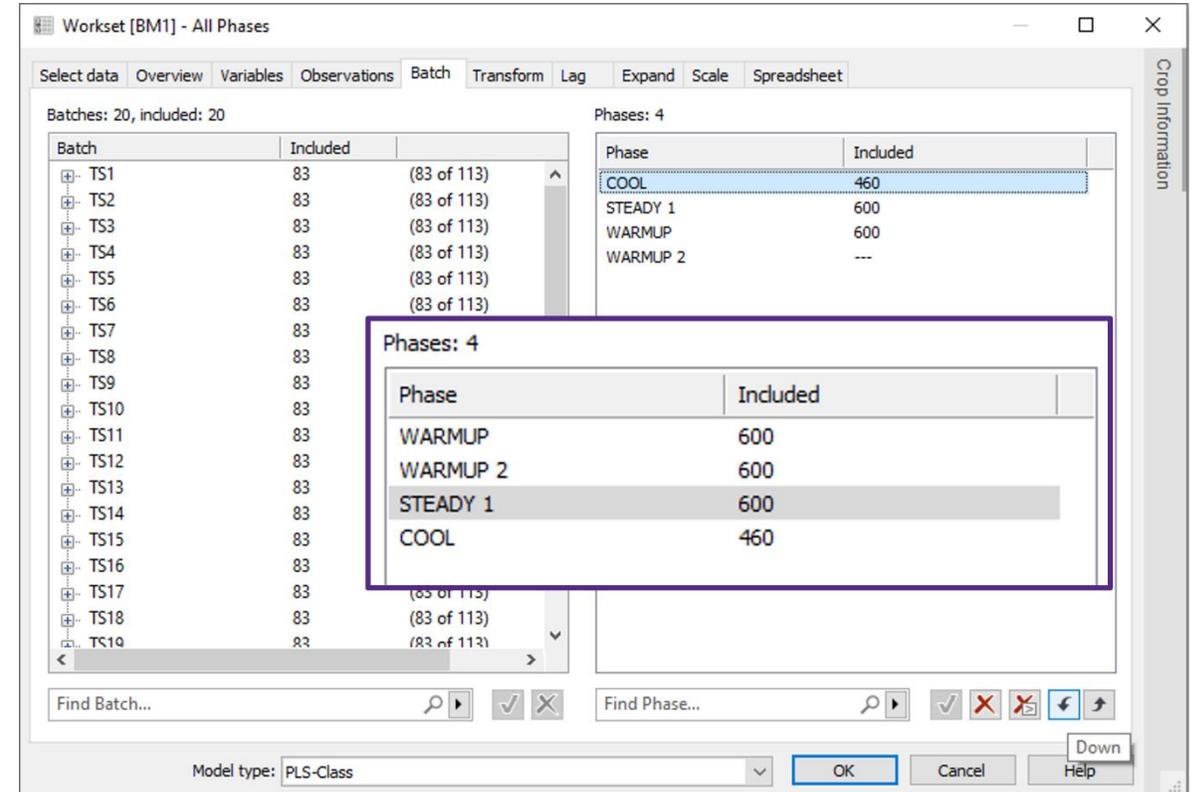
- During import of data into SIMCA® the order of the phases is not correct
- New | Change
  - Improved visibility of possible solutions to solve identified issues
  - Updating Batch & Phase ordering
    - Drag and drop
    - Ease of use when many updates need to be made



# Ability to Reorder Phases

## Problem Statement

- During import of data into SIMCA® the order of the phases was not correct, or all data was not available
  - The order of the phases needs to be corrected without importing the project another time
  - Additional phase data needs to be added
- New | Change
  - It is possible to reorder phases in the workset dialog
  - The order of the models is reflected in plots and will be shown in the same way in SIMCA®-online
  - Will be compatible with SIMCA®-online 18 when released



# Generated Variables From Qualitative Variables

## Problem Statement

- For SIMCA® projects with qualitative | categorical variables it should be possible to include qualitative in generated variables.
- New/Change
  - Possible to create generated variables from qualitative | categorical variables
  - Example
    - If(v9==1,v2,v4)
    - Where v9 is the variable index of the qualitative
    - '1' is the index of the setting, i.e. the first of the possible qualitative settings, 'Opening' in the example
    - 'v2' is the variable value to use when 'v9==1' is true
    - 'v4' is the variable value to use when 'v9==1' is false

The screenshot shows the 'Generate Variables' dialog in SIMCA software. The main window displays a table of BEM data with columns: 1 (Primary ID), 2 (SBatchID), 3 (Ethanol), 4 (Temp), 5 (Molasses), 6 (NH3), 7 (Air), 8 (Level), 9 (pH), 10 (\$Time), 11 (Valve\_01). Below the table, the expression 'If (v9==1, v2, v4) ^v1' is entered. The 'Generate Variables' window is open, showing the generated variables table with columns 1 through 19. The expression 'If(Valve\_01==1, Temp, NH3)^Ethanol' is visible in the 'Generated variables' section. To the right, a 'Statistics' panel shows Mean: 69,3643 and Standard deviation: 80,1522. Below the statistics, there is a 'Frequency histogram' and a 'Line plot'.

# Correlation Matrix Update

## Problem Statement

- Correlation Matrix in SIMCA® should use color scheme common to other Umetrics® Suite products
- New | Change
  - Color range
  - Red - perfectly negative correlation
  - White - no correlation
  - Blue - perfectly positive correlation
  - Number format possible to edit/set

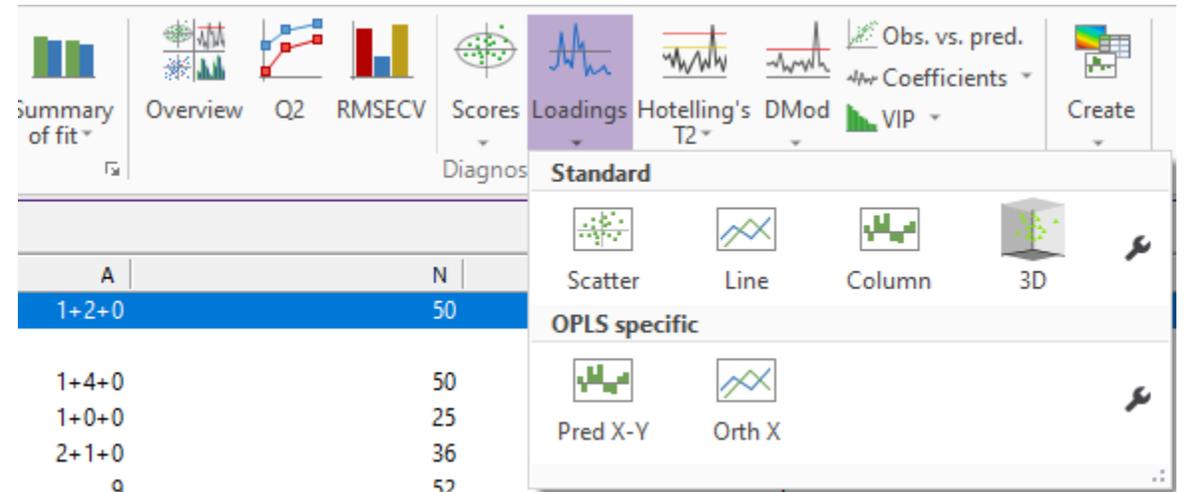
The screenshot displays the 'Correlation Matrix [M4]' window in SIMCA software. The matrix is a 11x11 table with columns labeled 1 through 11 and rows labeled with variables: Ethanol, Temp, Molasses, NH3, Air, Level, pH, Temp\_SP, Air\_SP, and Time (Hrs). The diagonal elements are all 1.0. The off-diagonal elements are color-coded: red for negative correlations, blue for positive correlations, and white for zero correlation. A 'Properties' dialog box is open in the foreground, showing the 'Number format' section. The 'Type' dropdown is set to 'Default', and the 'Precision' dropdown is set to '3'. The 'Options' section has the 'Color by absolute values' checkbox checked.

	1	2	3	4	5	6	7	8	9	10	11
1											
2 Ethanol		1	-0.365	-0.0666	0.431	-0.0805	-0.404	-0.224	-0.453	-0.118	-0.363
3 Temp		-0.365	1	-0.00337	-0.6	0.346	0.748	0.455	0.897	-0.135	0.734
4 Molasses		-0.0666	-0.00337	1	0.484	0.669	0.311	-0.0961	0.0929	0.0979	0.334
5 NH3		0.431	-0.6	0.484	1	0.248	-0.462	-0.28	-0.622	0.275	-0.402
6 Air		-0.0805	0.346	0.669	0.248	1	0.63	0.429	0.375	0.0367	0.729
7 Level		-0.404	0.748	0.311	-0.462	0.63	1	0.59	0.781	-0.238	0.965
8 pH		-0.224	0.455	-0.0961	-0.28	0.429	0.59	1	0.448	-0.103	0.626
9 Temp_SP		-0.453	0.897	0.0929	-0.622	0.375	0.781	0.448	1	-0.103	0.767
10 Air_SP		-0.118	-0.135	0.0979	0.275	0.0367	-0.238	-0.103	-0.103	1	-0.231
11 Time (Hrs)		-0.363	0.734	0.334	-0.402	0.729	0.965	0.626	0.767	-0.231	1

# Orthogonal Component Visualization

## Problem Statement

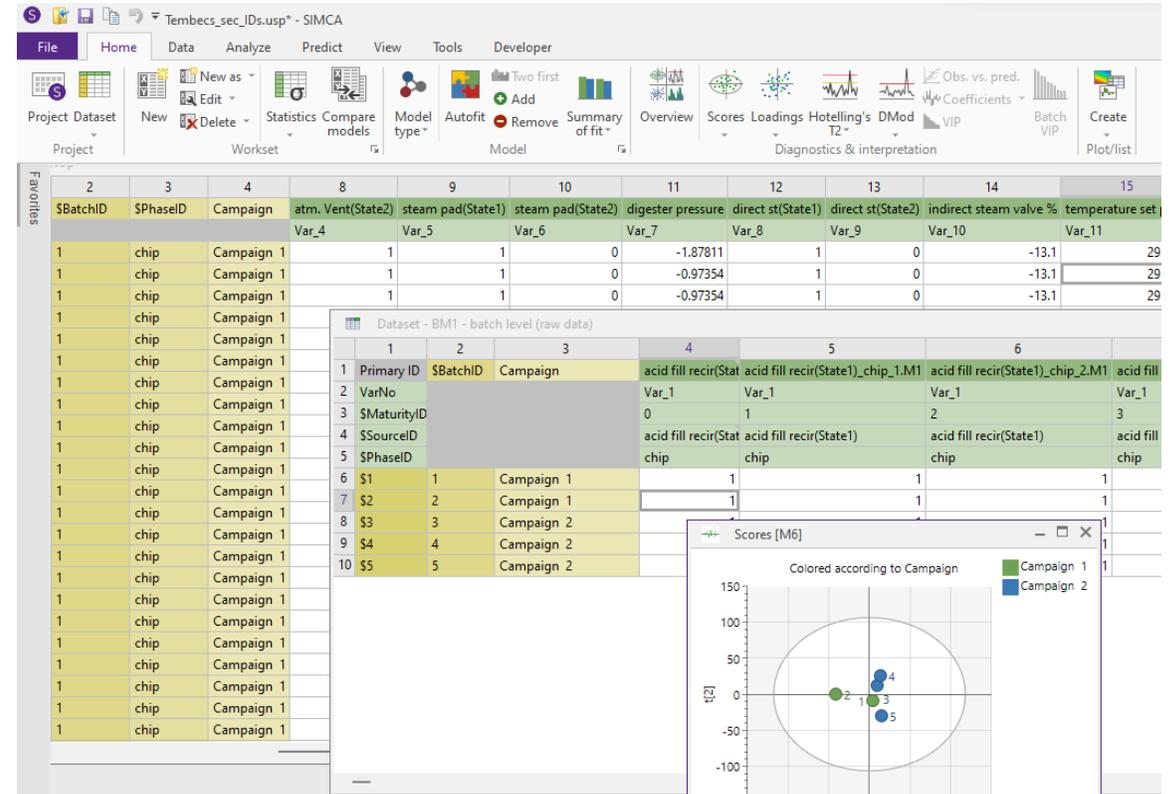
- Not straightforward to visualize orthogonal component of trademark method OPLS®
- New | Change
  - Default line plot for Spectroscopy projects
  - Makes model interpretation straightforward



# Secondary Batch ID for Batch Level Models

## Problem Statement

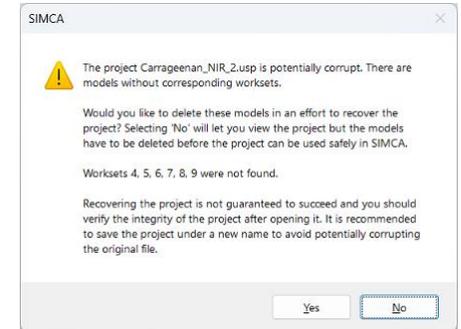
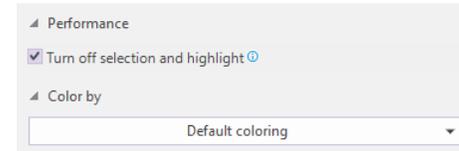
- Not possible to show secondary Batch ID at batch level in batch projects with multiple phases
- New | Change
  - Secondary Batch ID available in all batch projects



# Improved Stability and Project Recovery

## Stability and Recovery

- New option for 3D plots, 'Turn off selection and highlight', to improve performance for large datasets
- Open a project that needs to be recovered
  - Now possible to open possibly corrupt project with option to remove the datasets | models that makes SIMCA unstable
- All customer reported stability issues have been fixed
- Minor improvements
  - Number of variables shown in project window
  - And many more...



Number	Model	Type	A	N × K
1	M1	PCA-X&Y	2	110 × 29
2	M2	PLS	2	110 × 29
3	M3	PCA-X	0	110 × 27
Class model 1				
4	M4	PCA-Class(1)	2	55 × 27
5	M5	PCA-Class(2)	2	55 × 27

# SIMCA® Compatibility

- SIMCA® 18 saves project USP files in a backward compatible file format when the project doesn't contain functionality that requires a newer version
- SIMCA® 18 is saves in format for
  - **16** if a project doesn't use 17 or 18 specific functionality
  - **17** if the project uses 17 functionality but not 18 functionality
  - **18** if a project uses 18 functionality
- This make most projects compatible with previous releases of SIMCA®, SIMCA®-online and SIMCA®-Q
- Features in SIMCA® 18 **not compatible** with SIMCA® 17/16
  - Adaptive Process Mode modelling
  - Calibration transfer
  - Reorder phases
- Filters in SIMCA® 17 **not compatible** with SIMCA® 16
  - Smoothing
    - Savitzky-Golay Quartic, Quintic
    - EWMA
    - Moving window
    - AsLS smoothing
  - Baseline correction
    - Offset
    - Linear
    - AsLS correction
  - Normalization
    - Peak height
    - Peak area
  - Other
    - Derivatives 1st Quartic, Quintic
    - Derivatives 2nd Quartic, Quintic
    - Derivatives 3rd Quartic, Quintic
    - Derivatives 4th Quintic

# Thank You for Your Interest in SIMCA<sup>®</sup> 18

Don't forget to check out the instructional videos in [Sartorius Data Analytics YouTube channel](#)

**SARTORIUS**