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Simplifying Progress

Umetrics® Ecosystem SIMCA® News

2025-05-23

SIMCA® 18.1

SIMCA® 18.1

Alarm Configuration Aligned With SIMCA®-online

- Completely synchronized functionality

Sartorius Extensions Tab

- Enables rapid prototyping by Sartorius Application Engineering
- Extension distribution through my.sartorius.com

New Calibration Transfer Method

- Added method for transfer slope and bias in Y variables

User Experience Improvements

- Adaptive Process Mode models managed in Workset dialog
- Calibration and Filter wizards now supports changing select and zoom tools in plots
- Improved Python debugging

Smaller Updates

- SIMCA®-online Control Advisor model scripts updated
- Python upgraded to 3.13

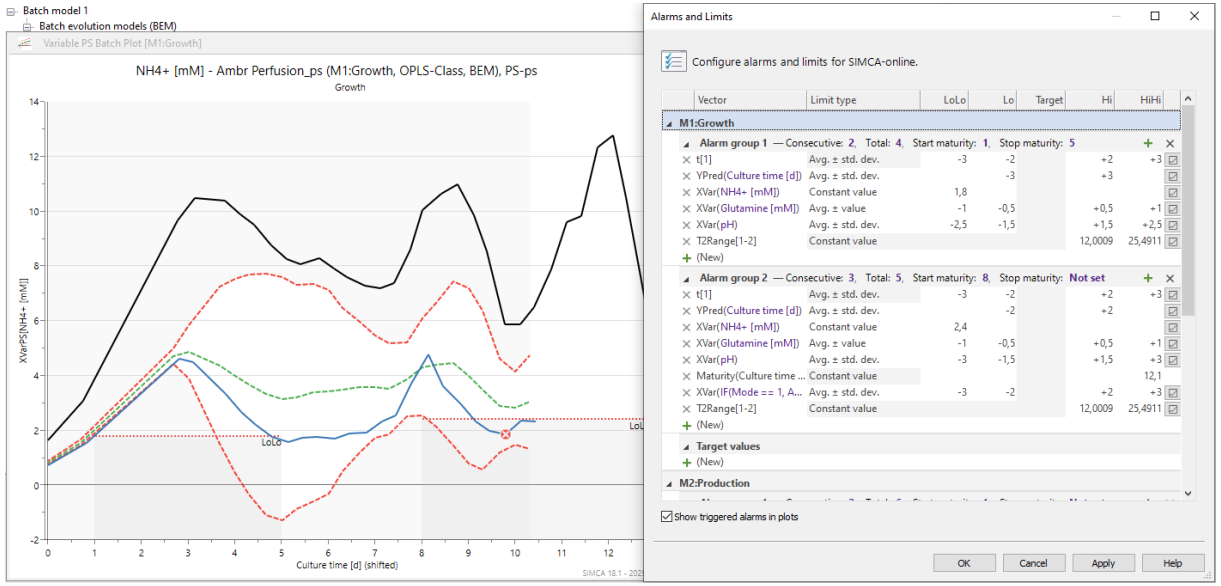
Alarm Configuration Aligned With SIMCA®-online

Benefits

- Set and test highly specific alarms already in SIMCA®
- Edit existing alarms at the same time project is updated

Changes

- Added multiple alarm groups that each have triggers, region and vectors
- Option to add Start and/or Stop Maturity for Alarms triggers that defines region where alarms are evaluated
- Outside the region an alarm is not evaluated and cannot be triggered



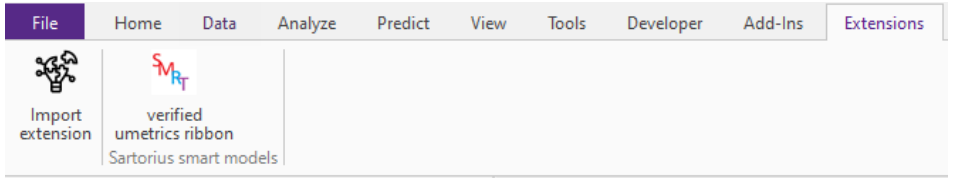
Sartorius Extensions Tab

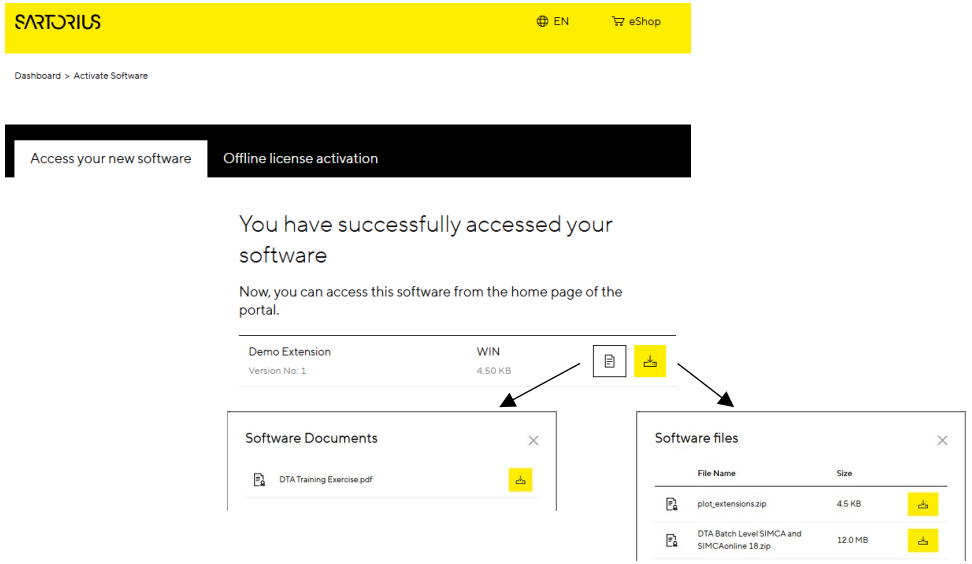
Benefits

- Professionally integrate application specific and general functionality to extend SIMCA®
- Rapidly add usefulness to SIMCA®

Changes

- Added tab in SIMCA® with machine learning extensions
- Only Sartorius extensions eligible for new tab
- Functionality validated as part of development process





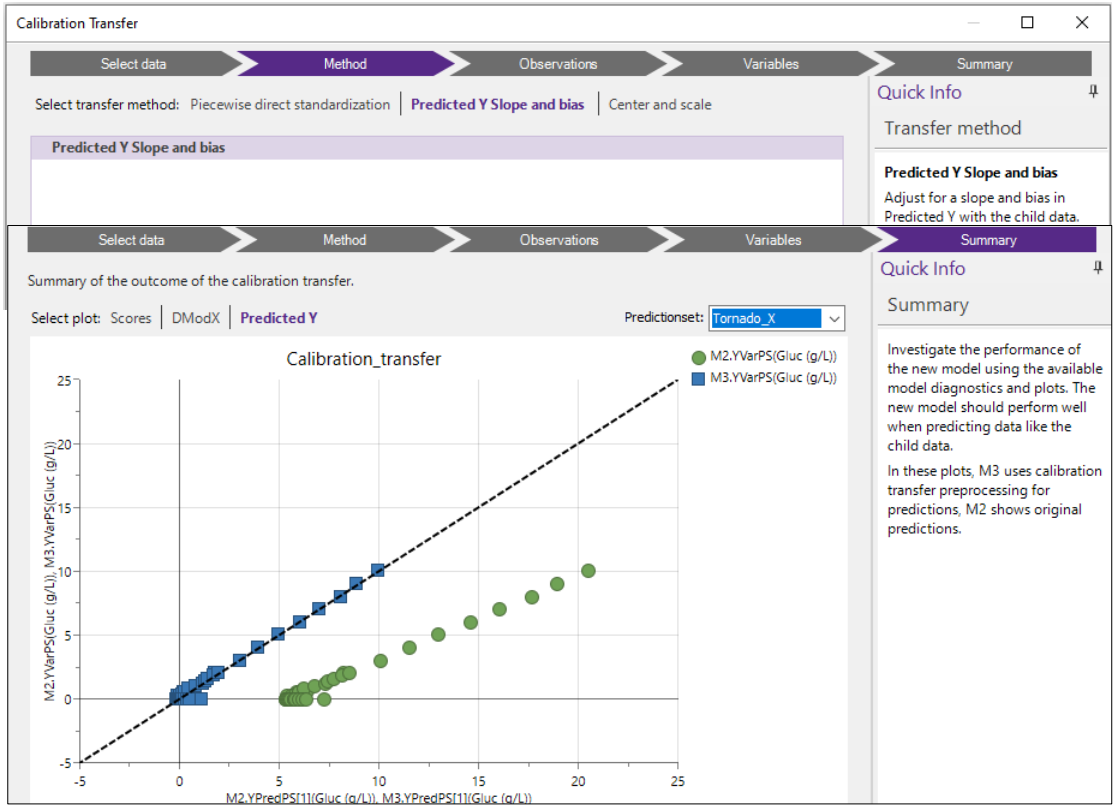
New Calibration Transfer Method

Benefits

- Now able to perform slope and bias calibration transfer to adjust predicted Y data
- Performed in compliance with USP 1039, following common practice within spectroscopy community

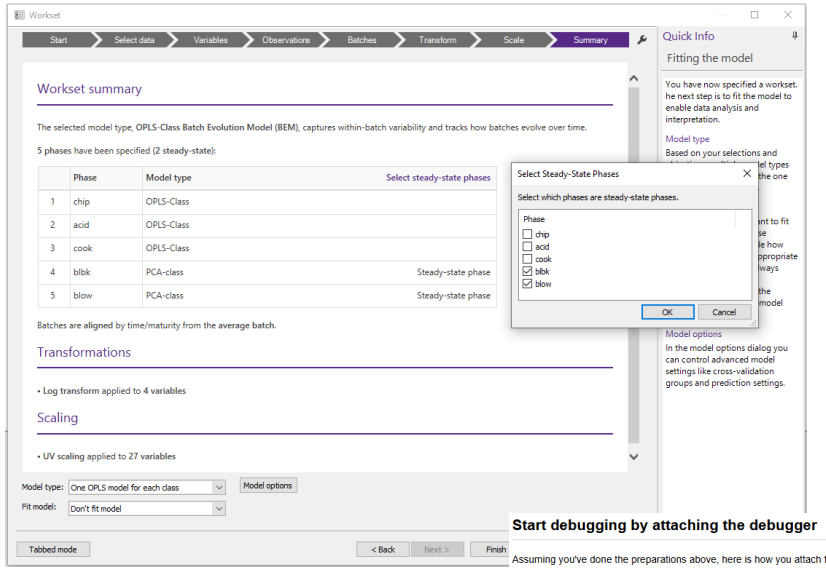
Changes

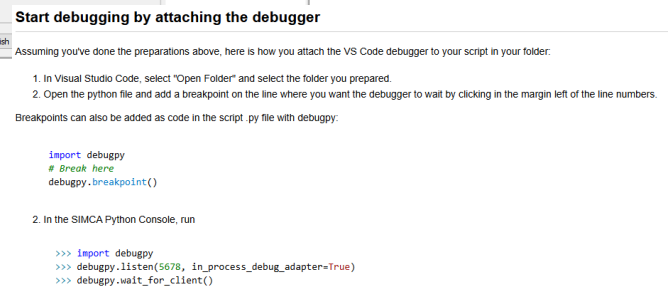
- Added method for slope and bias adjustment for predicted Y



User Experience Improvements

- Adaptive Process Mode models managed in Workset wizard
- Workset wizard summary page updated to show more relevant information
- Calibration and Filter wizards now supports changing select and zoom tools in plots
- Improved Python debug in SIMCA®





Start debugging by attaching the debugger

Assuming you've done the preparations above, here is how you attach the VS Code debugger to your script in your folder:

1. In Visual Studio Code, select "Open Folder" and select the folder you prepared.
2. Open the python file and add a breakpoint on the line where you want the debugger to wait by clicking in the margin left of the line numbers.

Breakpoints can also be added as code in the script .py file with debugpy:

```
import debugpy
# Break here
debugpy.breakpoint()
```

2. In the SIMCA Python Console, run

```
>>> import debugpy
>>> debugpy.listen(5678, in_process_debug_adapter=True)
>>> debugpy.wait_for_client()
```

SIMCA® 18

SIMCA® 18 Overview

- 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® Ecosystem 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

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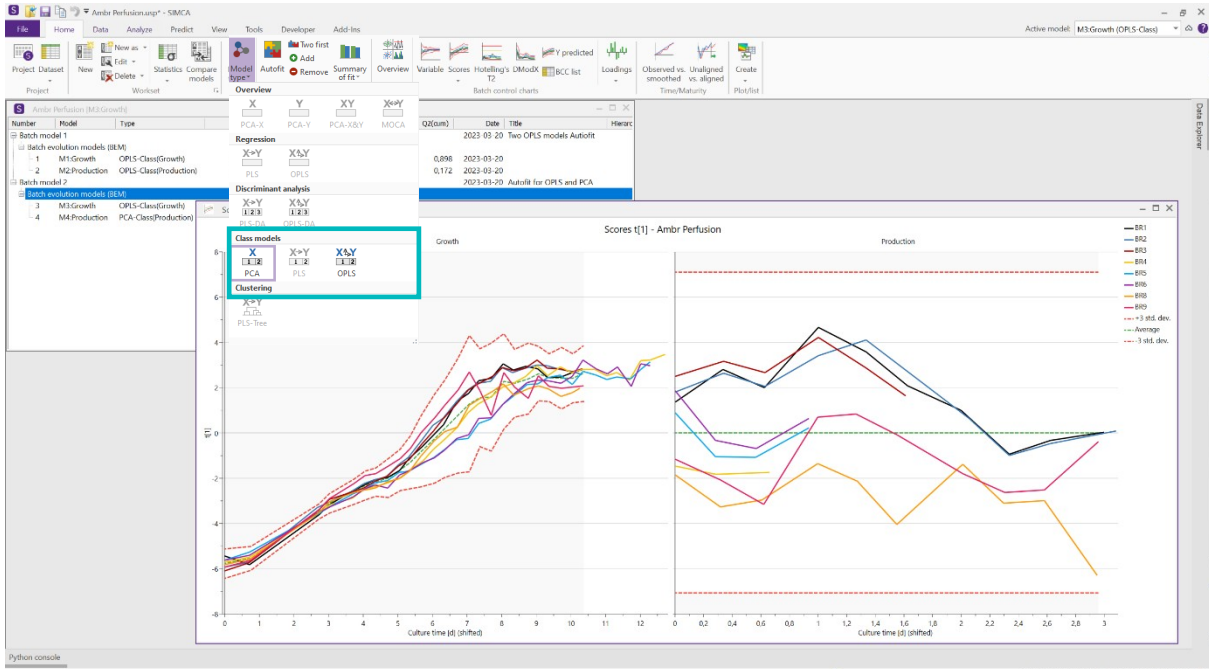
Added Flexibility for Batch Process Modelling

- 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: perfusion, chemostat, turbidostat
  - Other: Steam-in-Place, Clean-in-Place
- Changes
  - Possible to change model type from OPLS® to PCA for phase model in batch projects



*Results from 2020 at Sartorius, Göttingen, experiments run by Steffi Scholze, data Johannes Lemke

The run has 8 batches and 14 parameters measured 2-3 times a day

Continuous Culture Processes in Biopharma

Ambr 250 HT Perfusion experiment*

- OPLS®
  - Low explained variation, little variation over time
  - Glutamine/Glutamate/Ca/Osmolality decrease
- PCA
  - Osmolality/Glutamine/Glutamate/Gluc/NH4/K/Ca positively correlated
  - Small/non-significant negative correlation with
    - Total cell concentration/Viable cell concentration/Viability
  - Good batches consume more nutrients, found in lower part of control chart

*Results from 2020 at Sartorius, Göttingen, experiments run by Steffi Scholze, data Johannes Lemke

The run has 8 batches and 14 parameters measured 2-3 times a day

SIMCA® 18 What's New

Calibration Transfer

What

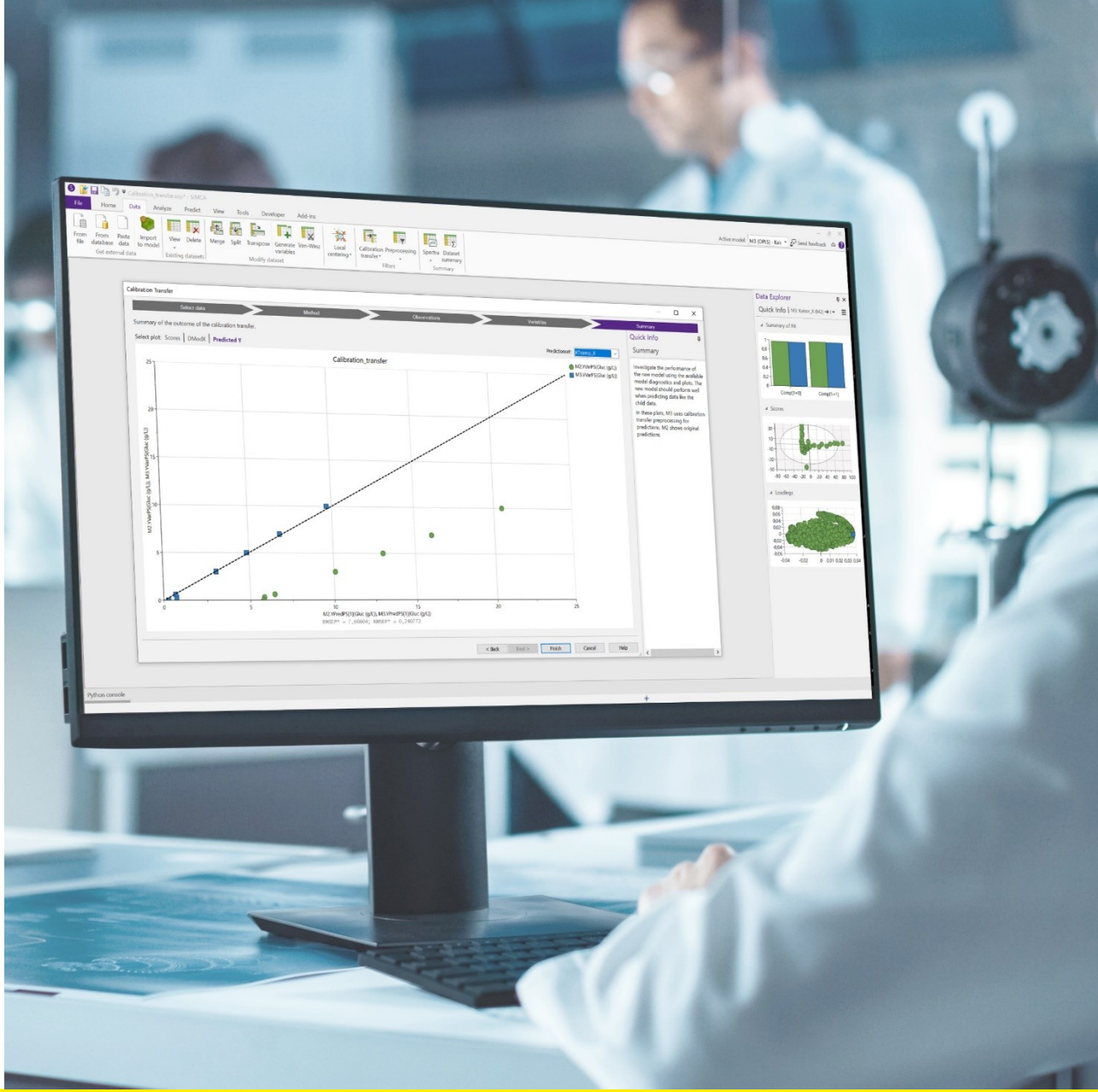
- Added guided workflow for calculating Calibration Transfer weights to set up a model for new multivariate calibration solution

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



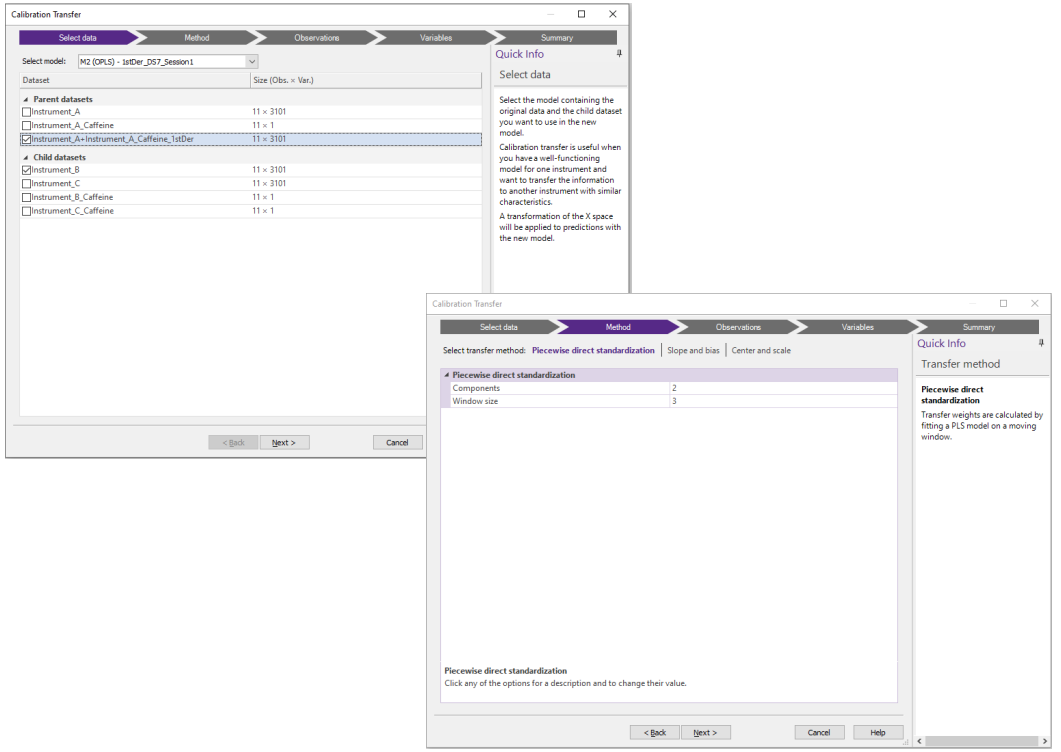
Calibration Transfer – Guided Workflow

Select data

- Parent dataset – original dataset that calibration model was built on
  - Raw data
  - Preprocessed data (in case it exists)
- Child dataset - spectra from
  - Additional/New instrument
  - Instrument after service/maintenance
  - Latest time period - instrument drift

Method

- Calculate calibration transfer weights with Piecewise Direct Standardization
- Slope and bias
- Centering and scale
- Or add custom Python function



Calibration Transfer – Guided Workflow

Observations

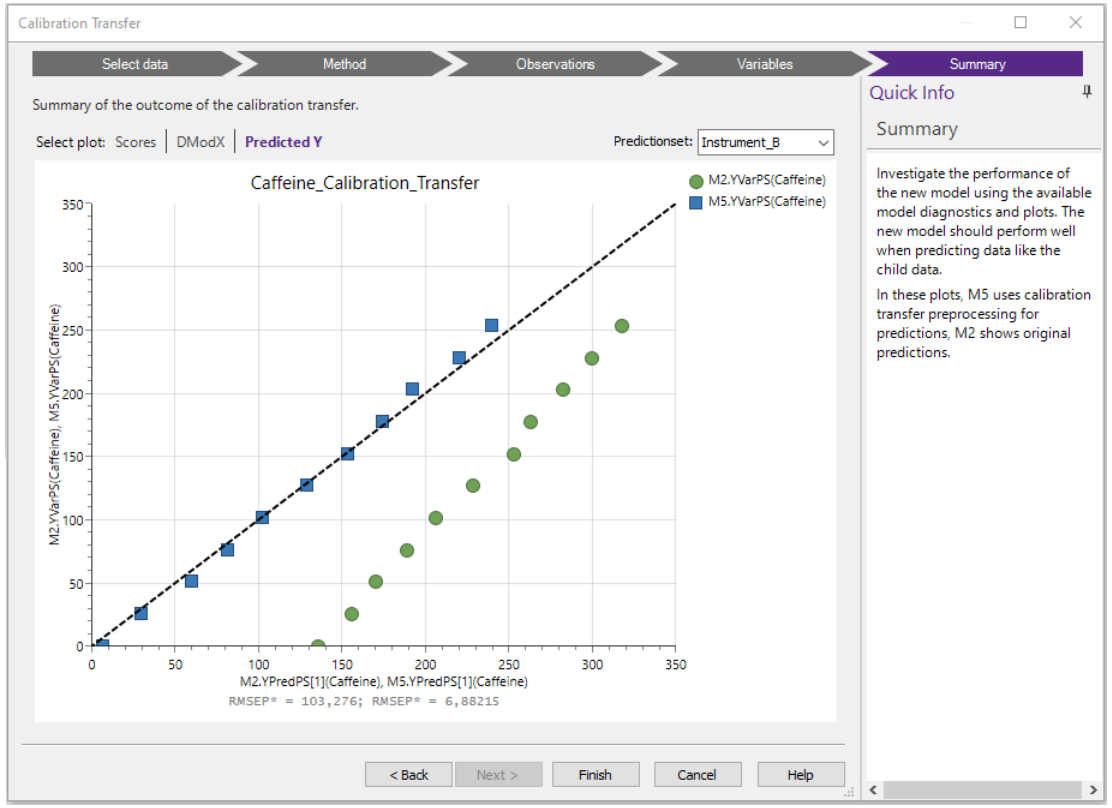
- Match observations in the calibration model (parent) to representative new observations (child)
- Match button
- Match ID

Variables

- Exclude/include variables to be used in new setup
- Align variables if necessary

Summary

- Model statistics
- Adjust transfer weights calculation?



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

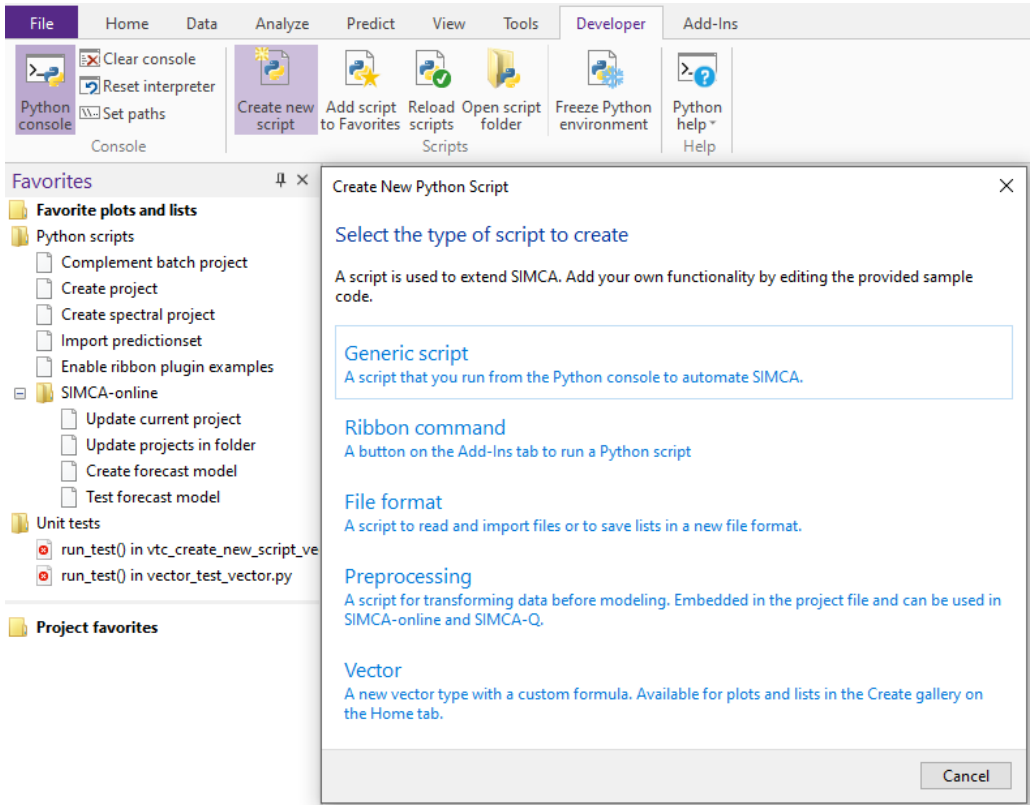
- Better dialog texts explaining the different options
- Improved Python sample scripts
- Python Help overhaul in included SIMCA® Scripting Guide

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

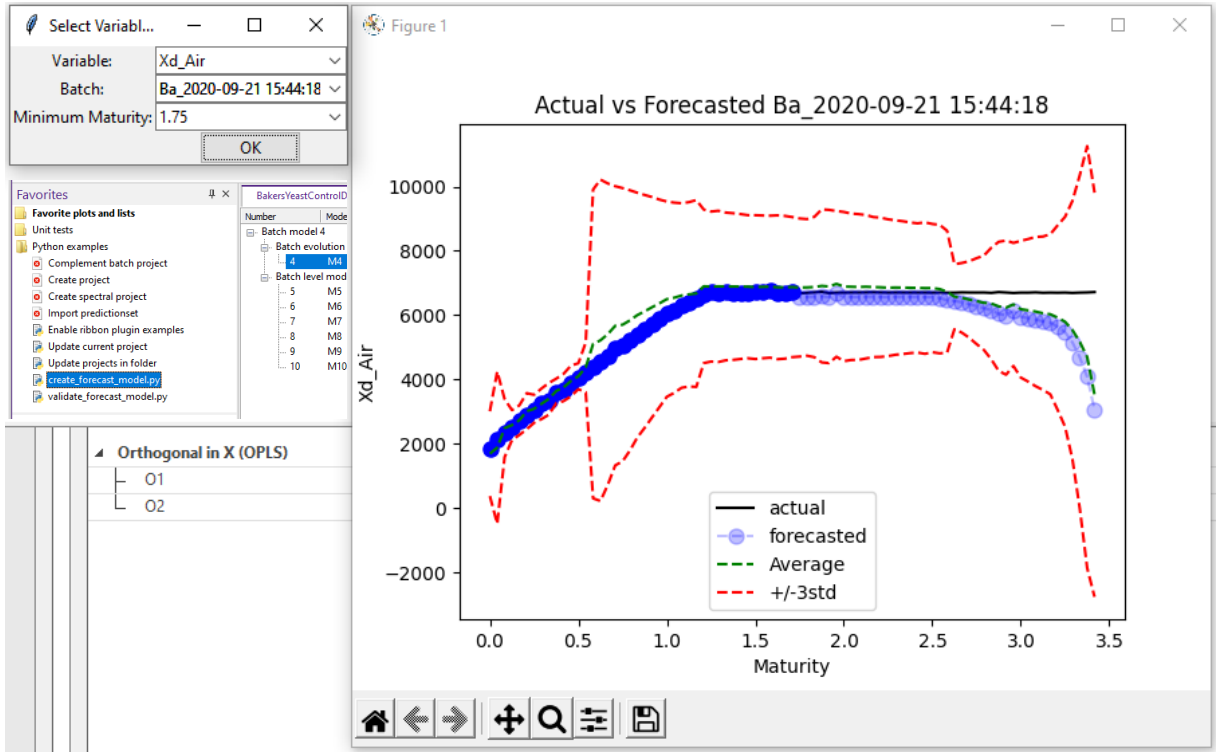
- Create forecast model Python script*, for creating datasets and models for SIMCA®-online

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

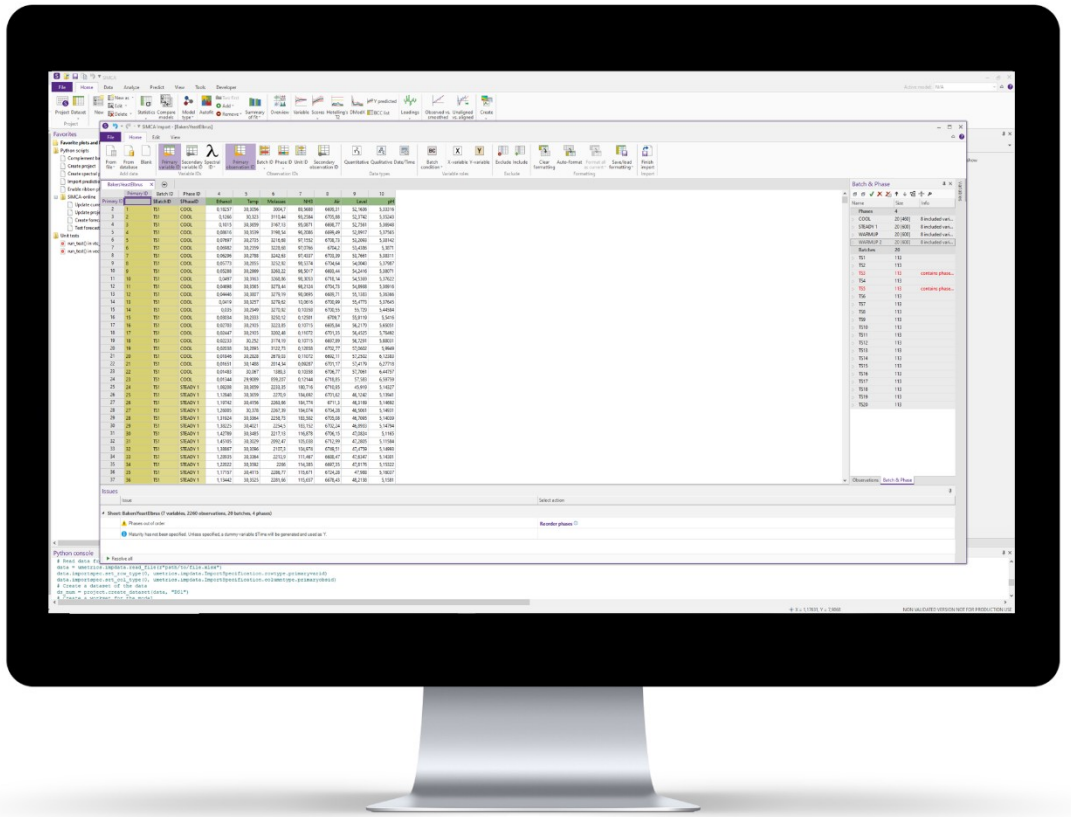


*All bundled scripts are provided as is and customers are encouraged to modify

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



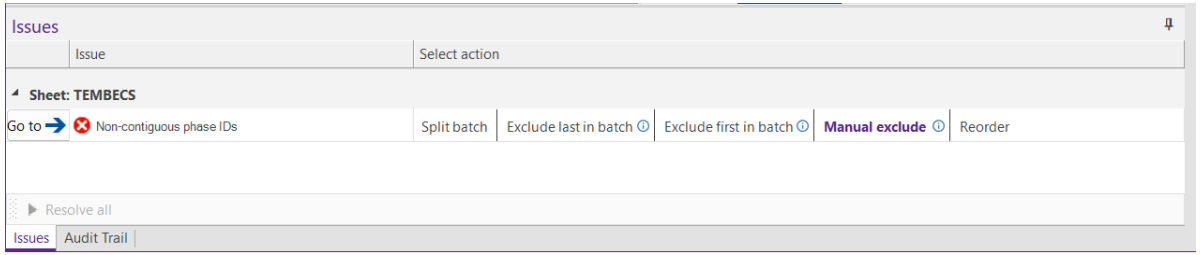
Import of Batch and Phase Data

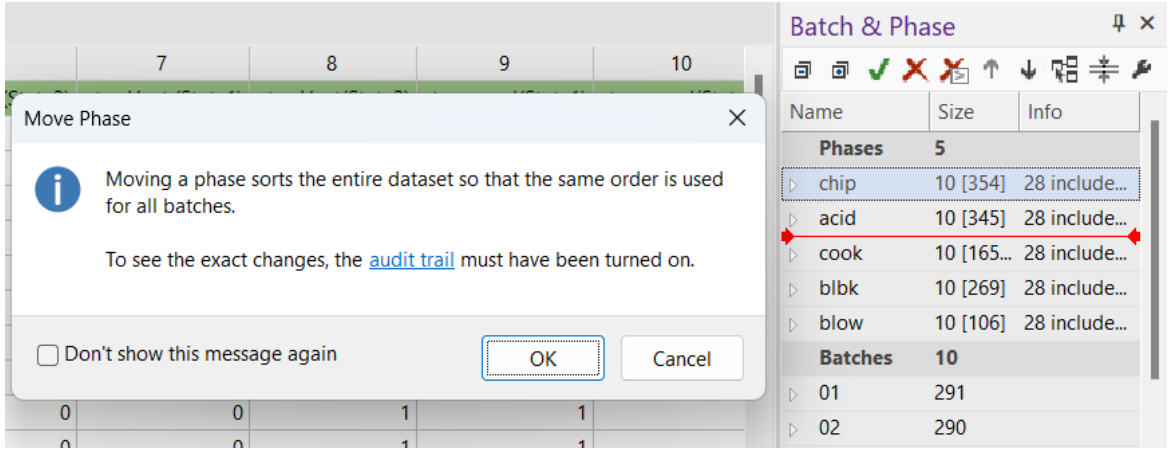
Problem Statement

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

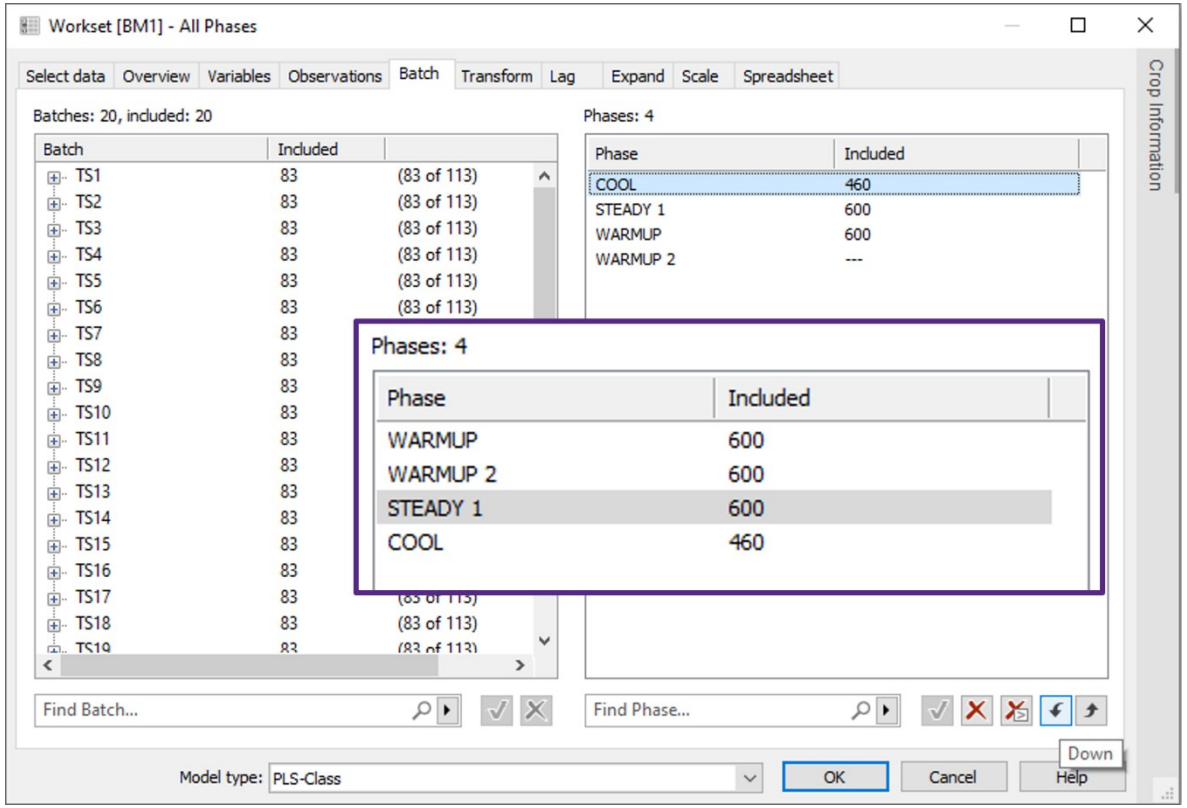
Problem Statement

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



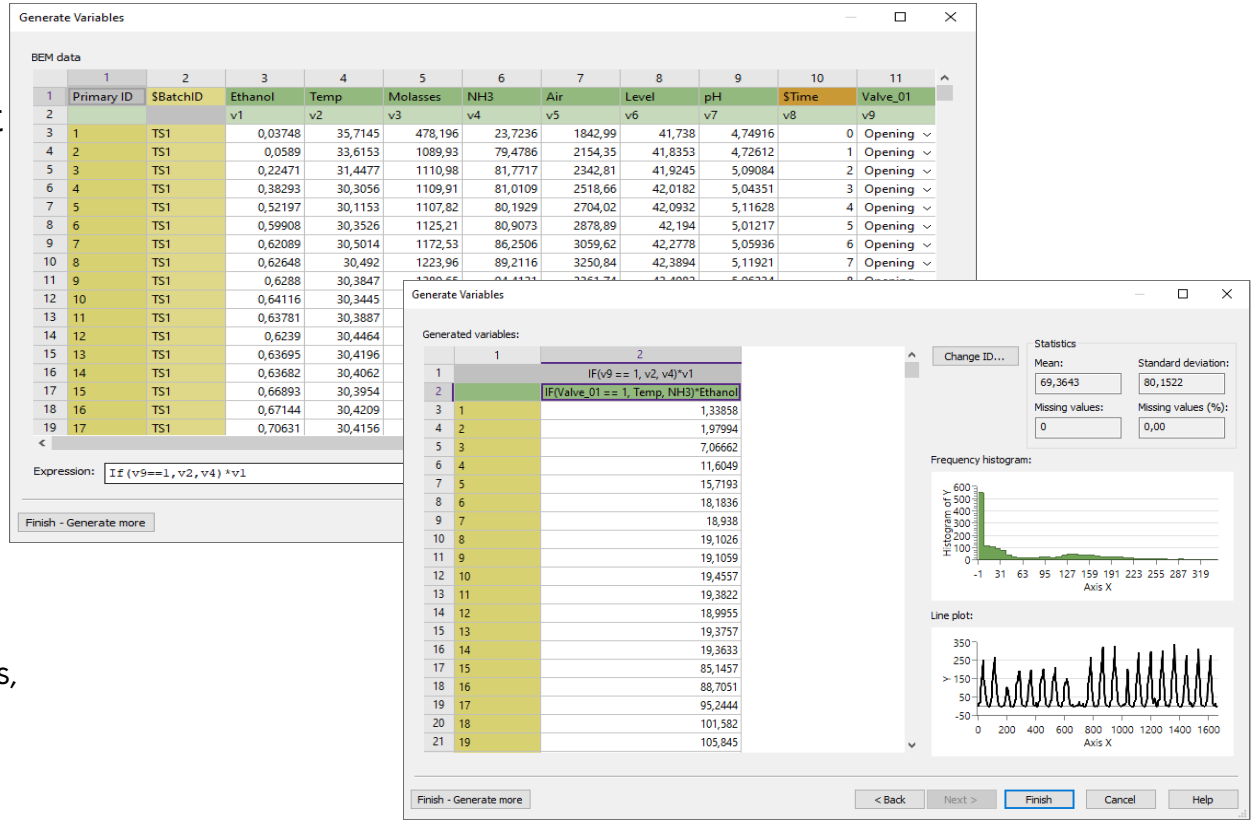
Generated Variables From Qualitative Variables

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



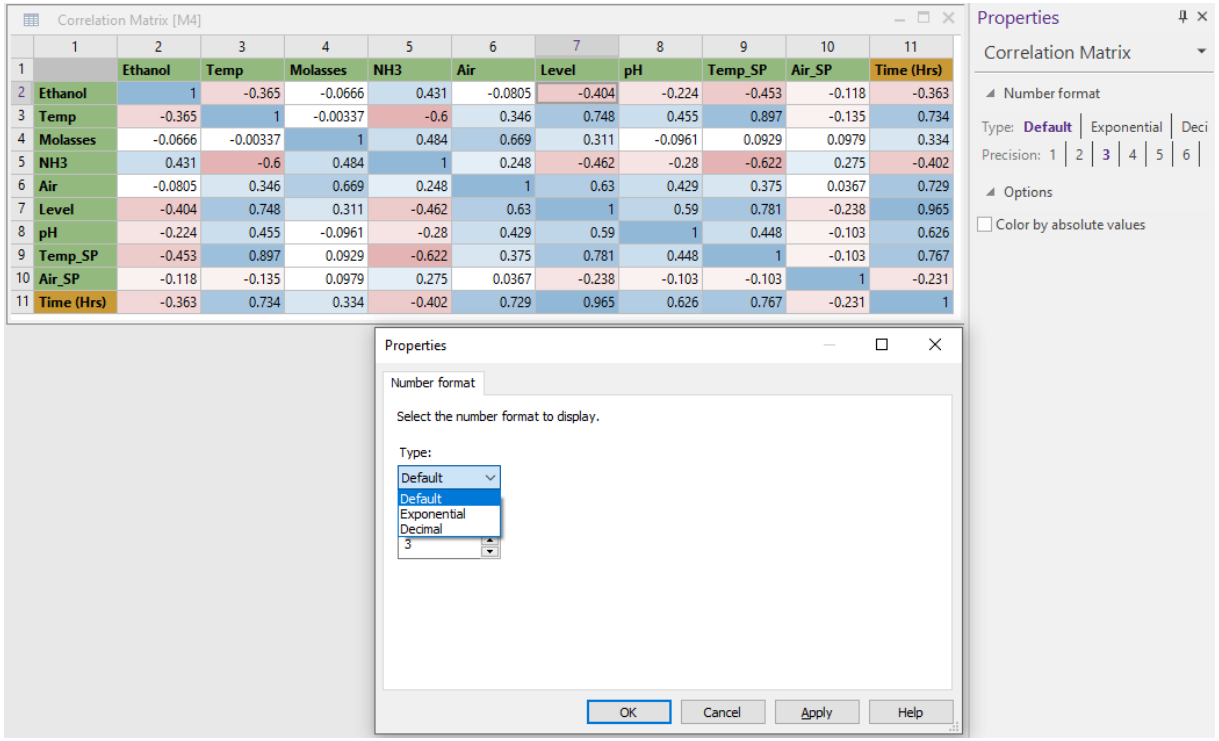
Correlation Matrix Update

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



		1	2	3	4	5	6	7	8	9	10	11
1		Ethanol	Temp	Molasses	NH3	Air	Level	pH	Temp_SP	Air_SP	Time (Hrs)
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

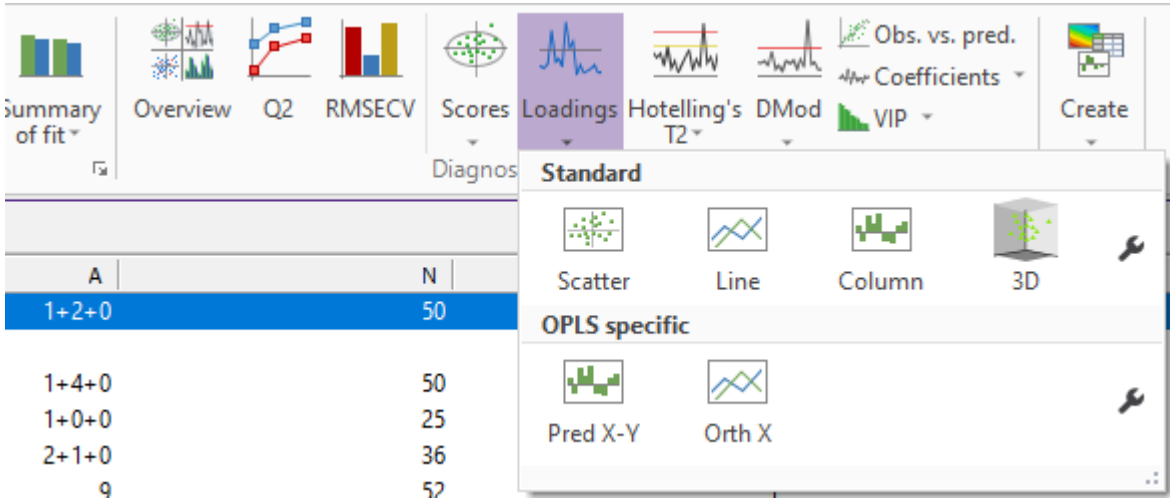
Orthogonal Component Visualization

Problem Statement

Not straightforward to visualize orthogonal component of trademark method OPLS®

New | Change

- Default line plot for Spectroscopy projects
- Makes model interpretation straightforward



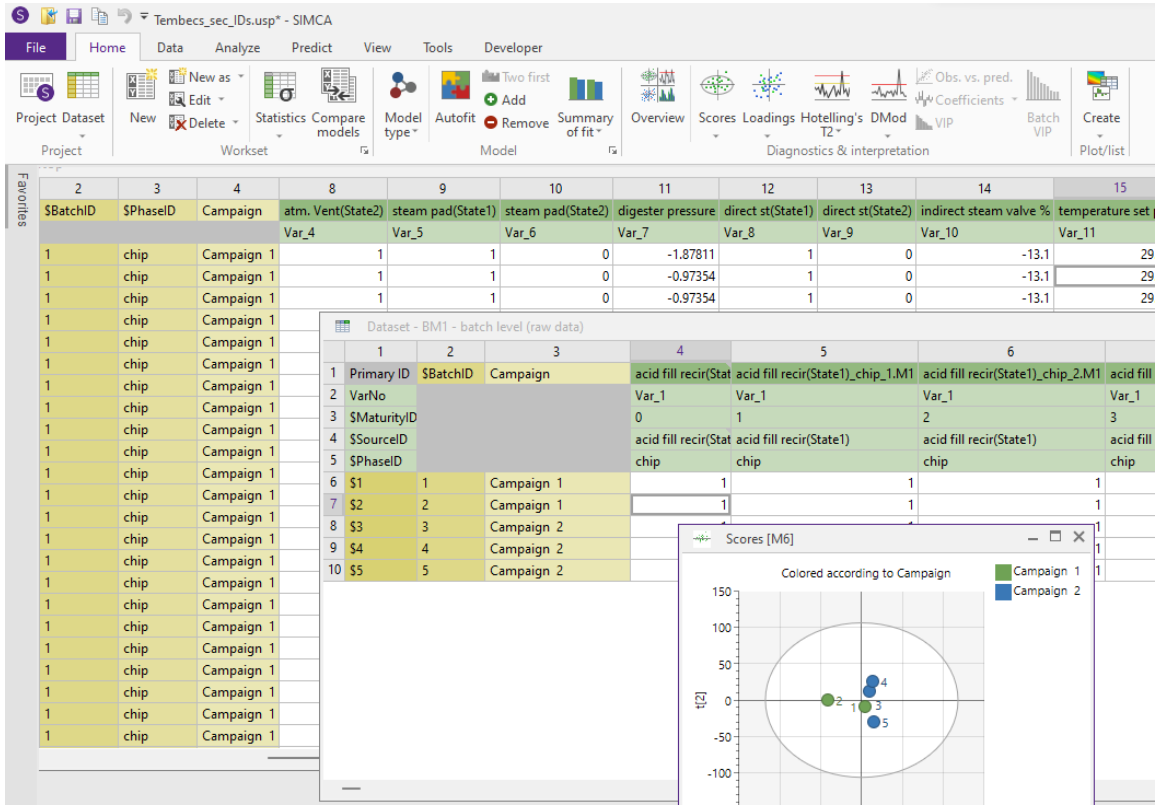
Secondary Batch ID for Batch Level Models

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

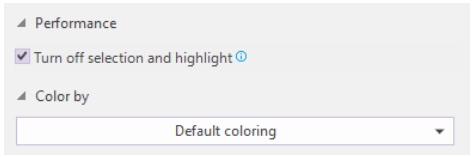
Open a project that needs to be recovered

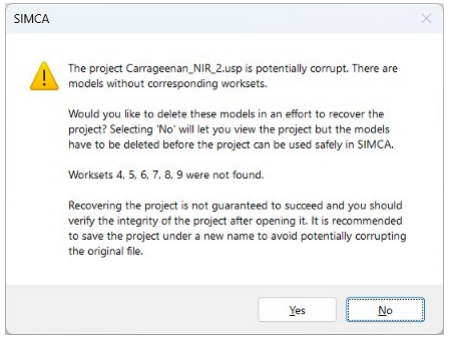
- Now possible to open possibly corrupt project with option to remove the datasets | models that makes SIMCA® unstable

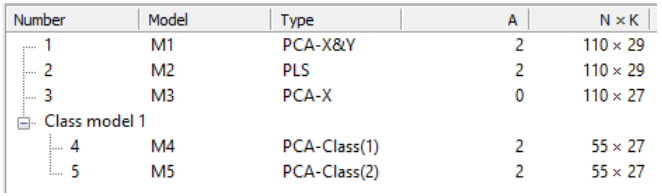
All customer reported stability issues have been fixed

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.

Specifications subject to change without notice.

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