SIMCA® 17 – What’s New?

Release February 9, 2021
SIMCA® 17 Overview

- Umetrics® suite SIMCA® is focused on delivering a full data analysis experience, from data organization to data based decision making supported by multivariate models.
- SIMCA® 17 is focused on improving spectroscopy data analysis by providing tools to make multivariate calibration easy and reliable
- With SIMCA® 17 you get a complete solution for preprocessing your spectral data to enhance prediction performance
  - Extended library of preprocessing algorithms in an easy-to-use wizard
- Calibration wizard providing instant model quality visualization after each preprocessing choice helping you chose the best prediction model
SIMCA® 17 Highlights

- **Spectroscopy Project**
  - Set, or generate Spectral ID at import
  - New spectra visualization
  - Extended library of preprocessing algorithms
  - Preprocessing wizard
  - Calibration wizard for 1 Y models

- **Batch Data and Database Import**
  - Possibility to control Batch alignment
  - BCC from dataset
  - SimApi:s available at installation and database interface improvements

- **Plot Interactivity**
  - Color by Rank – new option for better vector coloring
  - Reverse and log axis control in properties pane
  - Color BCC by batch condition vectors

- **Other Improvements**
  - Multiple file import for CSV, TXT and DIF files
  - Import configuration template
  - Python news and additions
  - Dataset properties
  - Dataset merge to keep un-matched content
  - New bias vectors (MBE)
  - SIMCA® 16 compatibility
  - Performance
Learning What’s New in SIMCA® 17

- In the following slides you will get an overview of the changes and additions made in SIMCA® 17

- For more details on how to use the features, please watch the what’s new videos that you can reach from the start page of SIMCA® 17

- Please also check out more videos on SIMCA® and other Umetrics® suite products by looking up Sartorius Data Analytics on YouTube
SIMCA® 17 What’s New – Spectroscopy Project
A new integrated Spectroscopy project
- Requires a Spectral ID vector
- X-data (spectra) and Y-data are split in separate datasets

Set your Spectral ID at import
- Spectral ID will be used as X-axis in plots
- Triggers access to the Calibration wizard

Select your spectral ID, or type in a custom name
- Generate your own numerical vector if none exist

Center (ctr) scaling is set as default for spectral data
Spectroscopy Project – New Spectra Visualization

- New selection tool in spectra plot
  - Spectra selection instead of variable selection
  - ctrl click to select more than one spectrum
  - Tooltip follow selected spectra for easy comparison

- SIMCA® recognizes spectra as observations and links the plot selections accordingly
Preprocessing Library Additions

SIMCA® 16 preprocessing

- Smoothing
  - Savitzky-Golay
  - EWMA (left filter)
  - Wavelet denoising

- Normalization
  - SNV

- Baseline correction
  - Row center

- Other (Spectra enhancement)
  - MSC
  - Wavelet compression
  - Derivatives (Savitzky-Golay) 1st–3rd
  - OSC

SIMCA® 17 additions

- Smoothing
  - Moving window
    - average and median
  - EWMA (symmetric filter)
  - AsLS

- Normalization
  - peak height
  - peak area

- Baseline correction
  - Offset, linear baseline, AsLS

- Other (Spectra enhancement)
  - Derivatives (Savitzky-Golay) 4th
Preprocessing Wizard

- Extensive selection of spectral preprocessing
  - Individual or chained filters
- Interactive, graphical, wizard for filter settings
  - Direct visualization of filter transformation effect
- Python based preprocessing filters are easily added to any of the categories in the wizard
- All filters are automatically applied to predictions
  - Also in SIMCA®-Q and SIMCA®-online
Calibration Wizard

- Wizard for creating and comparing multivariate calibration models with 1 Y
  - Automatically available for spectroscopy projects
    - Spectral ID required
  - Creates a calibration session of models
    - Similar to Class models and Phase models
    - Workset observations consistent over session
  - Existing calibration sessions can be opened and new data can be added
    - But only new prediction (validation) data
  - Session report template available
Calibration Wizard – Filter & Compare

- Same filter selection as in Preprocessing wizard
  - Select zero or many filters to apply
- Fit PLS or OPLS models
  - Access to cross validation group definition
- Model performance pane display model parameters and statistics
  - Calibration view (workset statistics)
  - Validation view (prediction set statistics)
SIMCA® 17 What’s New – Batch Data and Database Import
Batch Alignment – New Batch Alignment Option

- New option to control the batch alignment vector
- The default SIMCA® alignment algorithm has been complemented with the possibility for user defined alignment vector
- For short batches (< 20 observations) there sometimes is a desire to control the alignment vector in detail
- In SIMCA® 17, it is possible to align Y according to an existing batch
  - Y alignment option in Workset dialog
  - Same batch for all phases
  - Short batches (<20 observations) have this as default
Batch Modelling Related Additions

- Variable BCC from dataset
  - No need to first create a model
  - Also in Quick info
  - Select and Exclude batches possible
SimApi:S and Database Interface Improvements

- To assist users with process data to extract data directly from the process database some common SimApi:s have been made available during installation
  - No need to download and install the SimApi after SIMCA® installation
- More SimApi:s are available on Sartorius Data Analytics webpage (link in SIMCA® Help)
- Database interface improvements
  - Hierarchies and node trees visible in database import
  - Database import of batch data where the process node is missing a Batch ID tag is now possible
SIMCA® 17 What’s New – Plot Interactivity and Other Improvements
Plot Interactivity - Color by Rank

- Color by rank added as an alternative for Continuous coloring
- Ranked color is useful when the coloring vector values have a skewed distribution
  - Ranked color distributes the colors linearly over the full vector range
  - Available in the properties pane
Plot interactivity

Plot Interactivity – Axis Options

- Reverse and Log axis available in the properties pane
- Not only for spectra plot
Plot Interactivity – BCC Coloring

- BCC can be colored by batch conditions
Import multiple CSV, TXT and DIF files
- SIMCA® supports multiple file import of text style file formats

Template functionality during import
- Template configures columns and rows
- Copy current tab configuration to selected tabs
- Save and load templates
Python News and Additions

- Python updated to version 3.7.9
- NumPy, SciPy, and Pandas are pre-installed in the default virtual environment
  - Versions aligned with SIMCA®-Q and SIMCA®-online
- Python security improvements
  - User to trust new or updated Python scripts and Plugins
- New Python functionalities
  - Create, copy, and save generic plots
  - Plot properties in BCC
  - Labels and colors in plots
  - All new SIMCA® 17 added functionality
In dataset properties you can
- Change the name of the dataset
- Changing X and Y assignment
- Set, or rename, Spectral ID

Add qualitative variables to an existing dataset
In SIMCA® 17 un-matched content is retained in a new dataset.
New Vectors – Mean Bias Error

- **Mean Bias Error (MBE)**
  - Average prediction error in original unit and with sign
  - Indicates if model has a bias in the predictions
    - i.e. over or under predicts
  - The new Identity line (1:1) helps to visualize bias

- **Available bias vectors**
  - MBEE
    - Estimated from workset observations
  - MBEcv
    - Calculated from the CV-round predictions of Workset observations
  - MBEP
    - Calculated from (true) prediction set observations

- **Compare models list found in Home and Predict tabs**
  - Prediction performance for models with same Y
  - Best value in each column in green
### SIMCA® Compatibility

- **SIMCA® 17 is compatible with**
  - SIMCA® -Q 17 and SIMCA® -online 17

- **Save as SIMCA® 16 introduced**
  - But not available for preprocessing functionality added in SIMCA® 17

- **SIMCA® Qpe format**
  - A special format for embedded predictions. Need special implementation to be used
  - Only for OEM customers

- **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
Performance – Some Examples

- Many aspects of SIMCA® performance and responsiveness have been addressed in SIMCA® 17
  - Plot creation and interactivity
    - e.g. line plots and coloring of line plots
  - Opening of projects is approximately 67% faster
  - Drop-down lists get populated with values in a fraction (<1%) of the time
  - And many more things to improve the SIMCA® experience
Thank You for Your Interest in SIMCA® 17

Don’t forget to check out the instructional videos