Simplifying Progress

What's new
SIMCA® 15 Multivariate Data Analysis Solution
June, 2020

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Overview

- Time in analysis of continuous process data

- Managing recurrence of batches and phases in batch processes

- SIMCA-online synergies

- SIMCA Import updates

- Minor fixes

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Time in analysis of continuous process data

Time consideration in continuous processes

Changes has been made to the following functionalities:

- Lags
  - in relation to time
  - in relation to speed/distance

- Introduction of Leads (negative lags)

- Control charts grouped in time range

- Cross validation groups based on time range

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Lag on time and "distance"

- Time = constant time lag
  - Relevant if process speed is static
- Distance = constant distance, varying time
  - Relevant if process is dynamic/changing speed
  - Distance the material travels through the process

"Distance" = 7 m

Measurement A   Measurement B   Measurement C
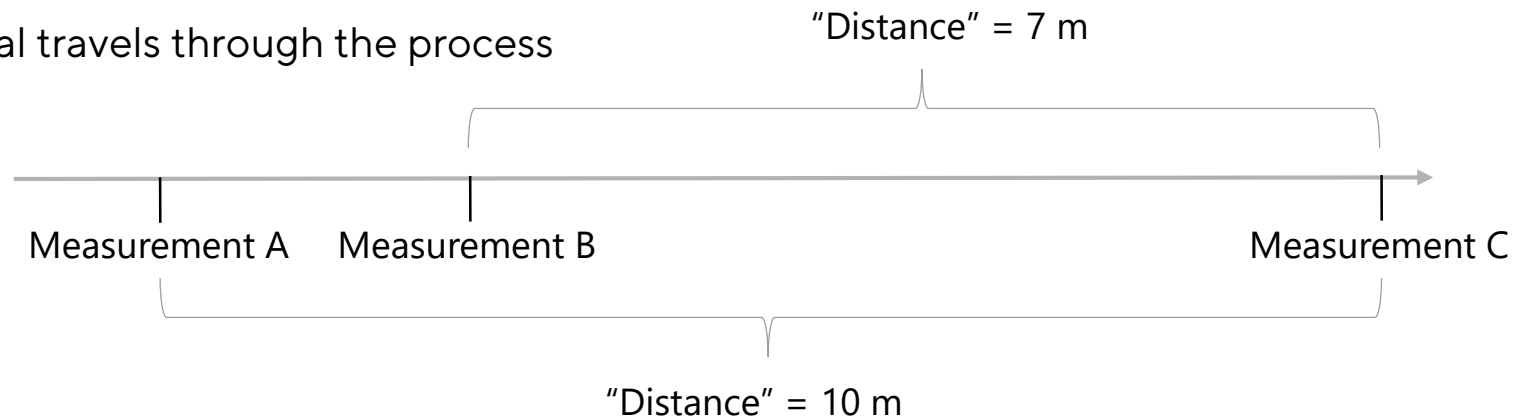
"Distance" = 10 m

- Constant speed of 1 m/s → Time lag of 10 s A to C and 7 s B to C
- Varying speed → Distance lag of 10 and 7 m respectively calculated from Time and Speed tags

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Lags

- New design of Lag page in Workset

- Lags can be based on a time variable or any variable

  - Observation index = how SIMCA 14.1 and previous worked

  - Time variable → Fixed time structure

  - Variables → Fixed "distance" structure

    - Requires a time variable. A distance is calculated meaning that the lag time adjust by changes in process speed.

- Lags in relation to variable / distance

- For guidance, median step length is given

  - For Time and Distances
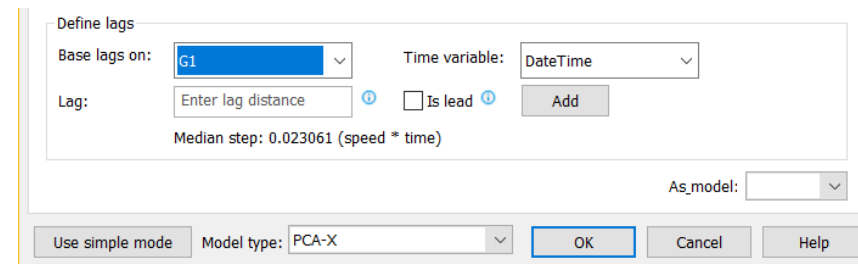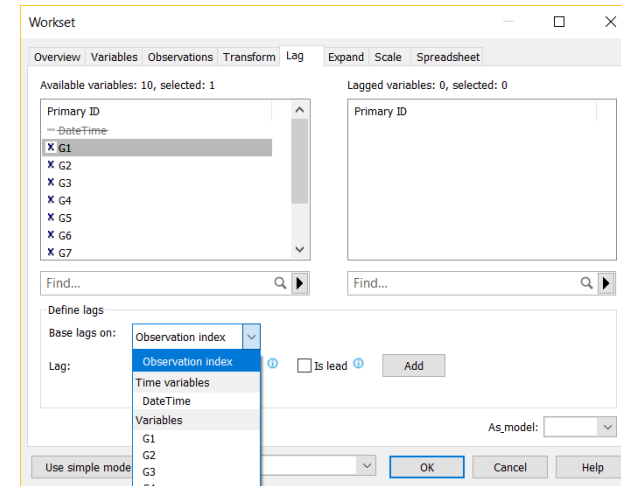
Leads

- Leads are negative lags, i.e. lags into the future.

- Useful when creating models for SIMCA-online Control Advisor.

- Mark the Is Lead Checkbox to switch from Lag to Lead mode

- Lags and Leads can be combined in the same project

  - Leads with -time

- Due to their nature, leads are set as Y variables
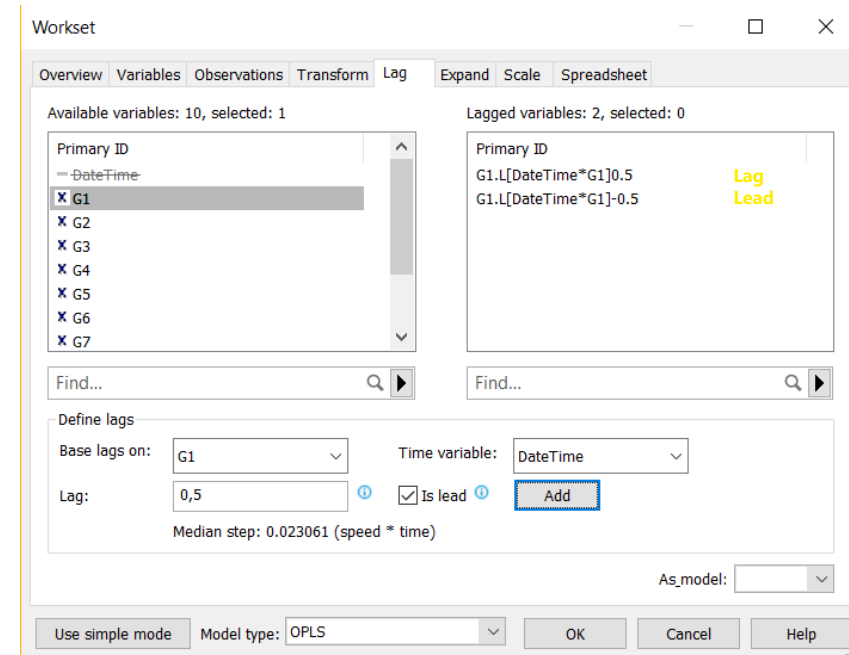
Control charts in Time or variable range

- Group on observations, time or another continuously increasing or decreasing variable.

- Ex Shewhart Mean/Std.Dev.
  - Left: Group size 10
  - Right: Group range 24h
    - Group range unit relates to parsed time unit at import
    - Group size vary, statistics are adjusted. Std.Dev. cannot be calculated when group size <2
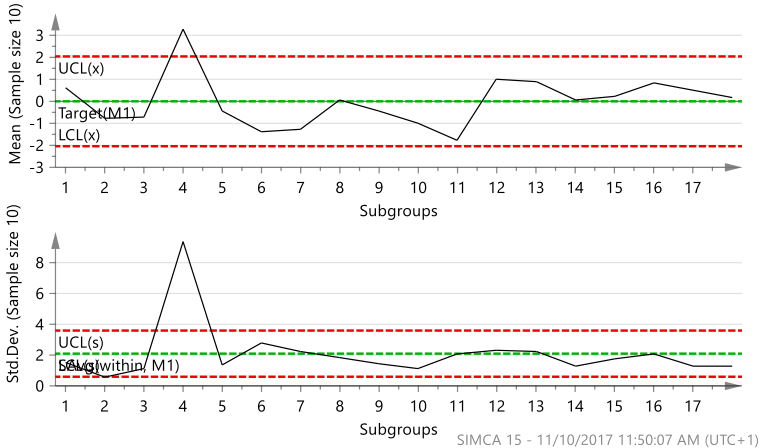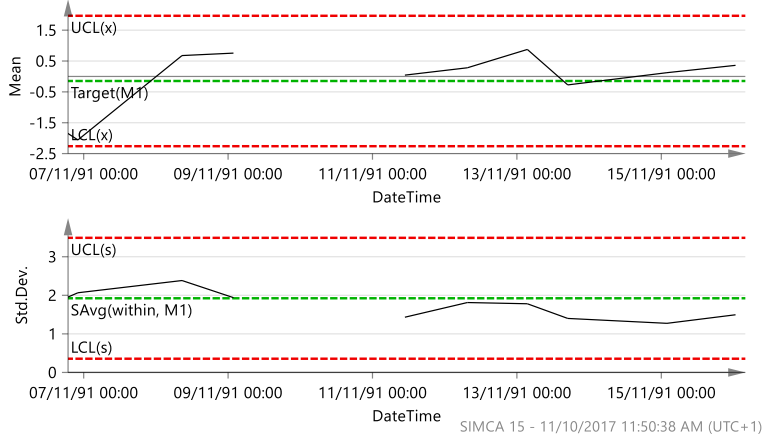
Cross validation groups on time

- Cross validation groups must be changed prior to model fitting

- Access from Model Options
  - Right click on model or Options.. button in Model window.
  - CV-groups tab

- Variable range in dataset shown for guidance

- Max range is 99 hours

- Number of CV groups cannot exceed number of variables in dataset
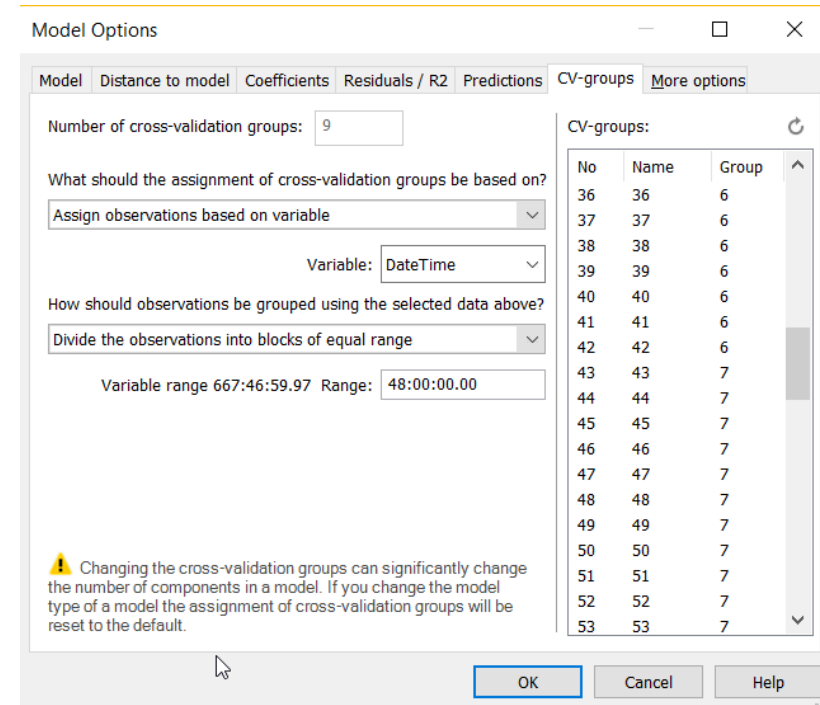
Customer challenges addressed

- Lagging based only on observations can be erroneous
  - As in SIMCA 14.1 and previous
  - Gaps in data was disregarded, actual lag structure in relation to time unknown

- Need support for changes in Lag structure as process dynamics vary
  - Changed speed of process → change in lag time

- Control charts should optionally be in relation to time ranges
  - Grouping by observations may hide time gaps in data

- Cross validation difficult to trust
  - Even with options for group similar etc. it was unknown if CV groups spanned over varying time gaps

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Managing recurrence of batches and phases in batch processes

Managing recurrence of batches and phases in batch processes

- Two main cases:

- The complete batch is processed in one phase more than once
  - Failure to meet Q / reworks
  - Processing failure

- The batch is divided into sub-parts (sub-batches) which are separately processed
  - In parallel in different process units
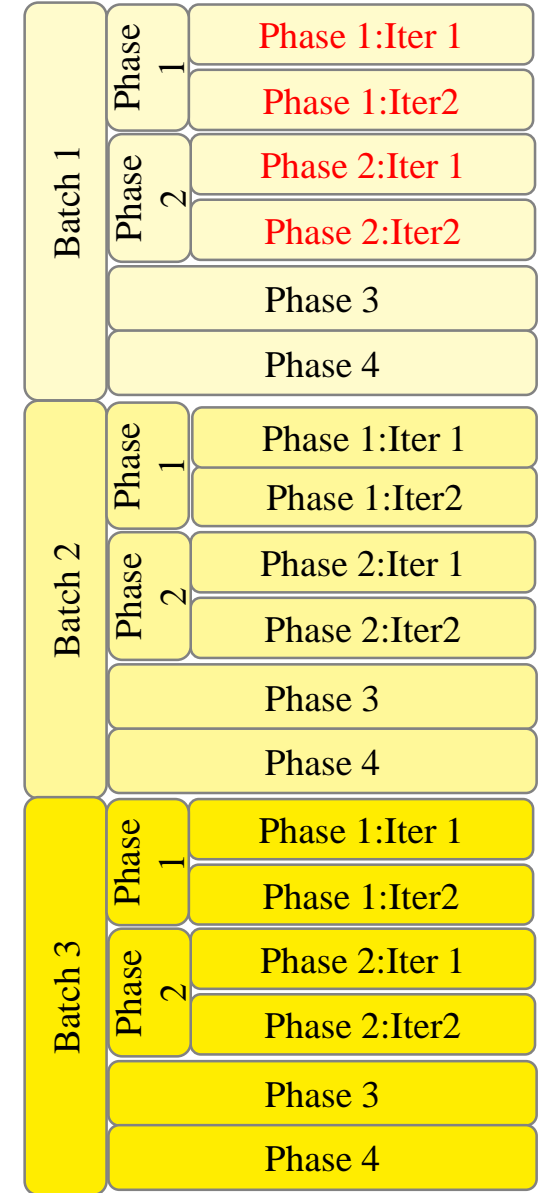 - In series in same process unit
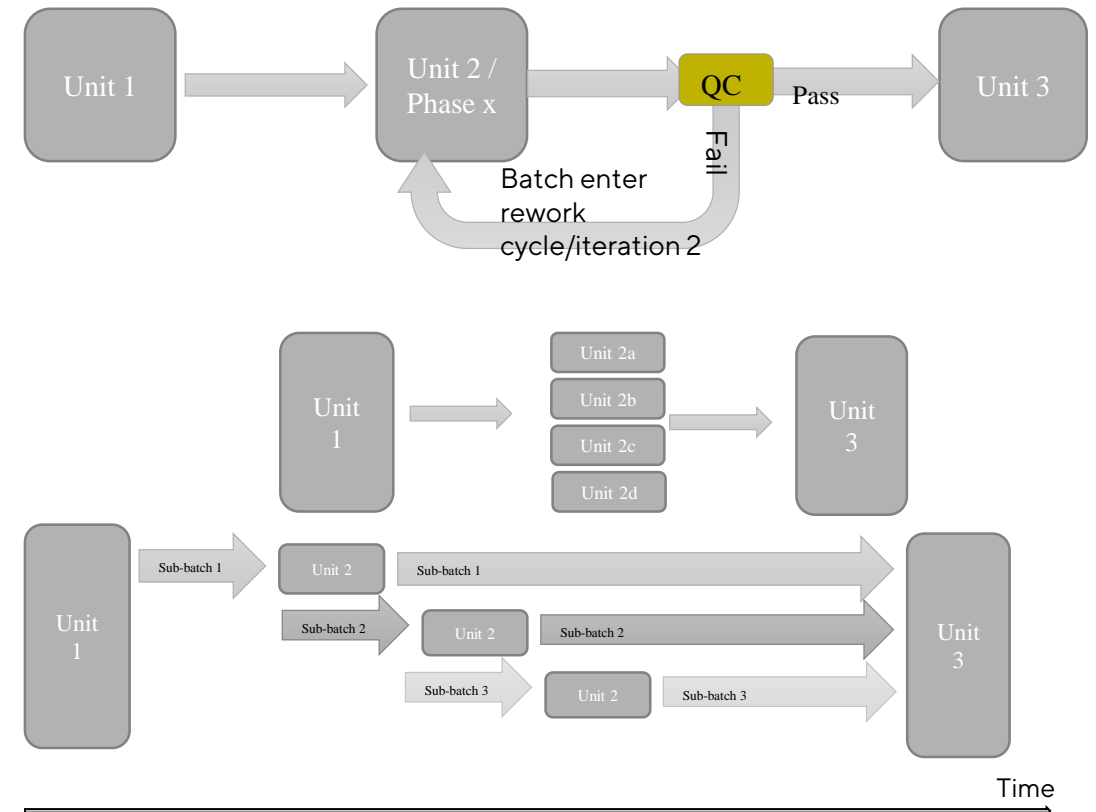
Data structure requirements

Process setup

Phase 1 and phase 2   Phase 3   Phase 4
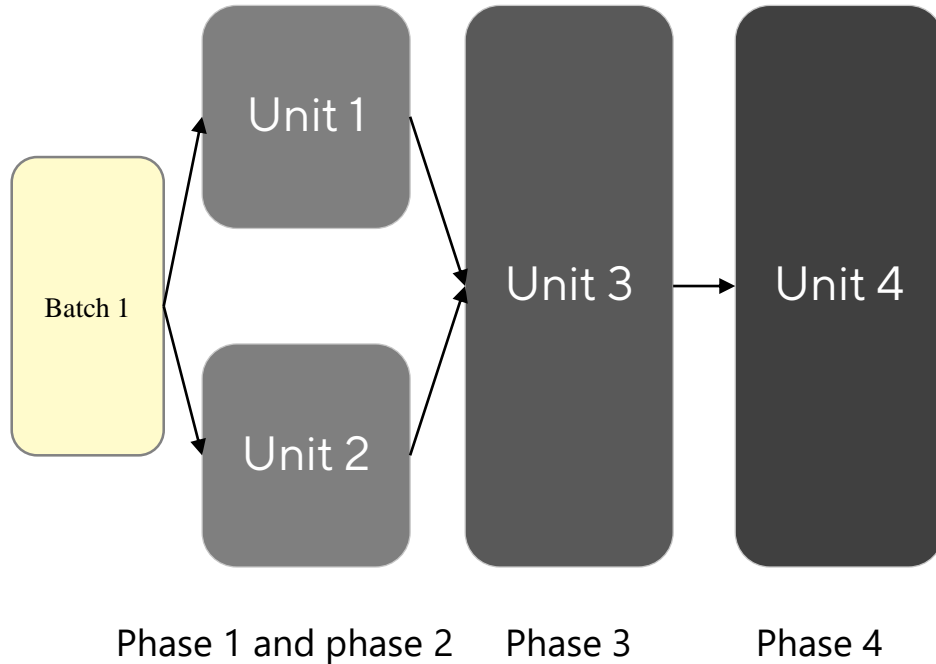
- Data structure
  - Hierarchy:
    - Batch
    - Phase
    - Phase iteration

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Impact of recurring batches

- A new ID has been introduced to recognize the different occurrences of the batch

  - Phase Iteration ID

- Batch evolution models with phase iterations will include several instances of the same batch

  - Number of batches varies between phases

  - Control limits are based on total number of iterations (sub-batches) in that phase

- For projects with phase iterations, separate batch level datasets will be created per phase

- There are options on how to treat phase iterations at batch level

- Max number of iterations of a phase limits prediction capabilities on Batch level

  - Prediction sets including more iterations than the workset will be cut at the number matching workset

    - First and last will not be affected.

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Data import

- New observation ID for Phase iterations (slide 30)

- Hierarchy is Batch-Phase-Phase iteration
  - All data from one batch contiguous within a dataset
    - Different phases could be in different datasets
  - All data from on batch and phase must be contiguous
  - All data from on batch, phase and phase iteration must be contiguous
  - If Issues pane complains, sort on (in this order)
    1. Phase iteration ID
    2. Phase ID
    3. Batch ID

- Batch, phase and phase iteration conditions
  - First value - from a continuous dataset – in each batch, phase and phase iteration
  - Phase and phase iteration conditions from a discrete dataset requires batch, phase and phase iteration ID

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Batch evolution models – BEM Workset Batch tab

- Batch tree structure

  - Batch ID

    - Phases

      - Phase iterations

- Include/exclude Batches/ phases/ phase iterations

- A specific phase iteration can be removed from the workset

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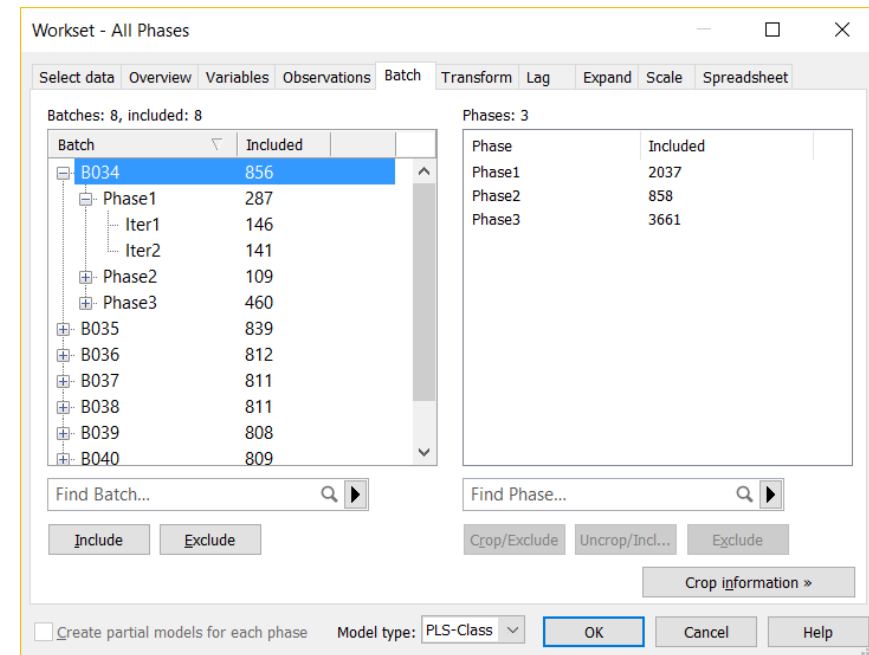
Batch evolution models – the plots

- Example has 2 phase iterations

- For one batch there are two lines in all BC charts

  - Statistics are based on actual number of batches/iterations in that specific phase

- Use Marking mode to select batches with specific iteration ID, Unit ID etc.

  - Tools ribbon, Plot tools group, Select
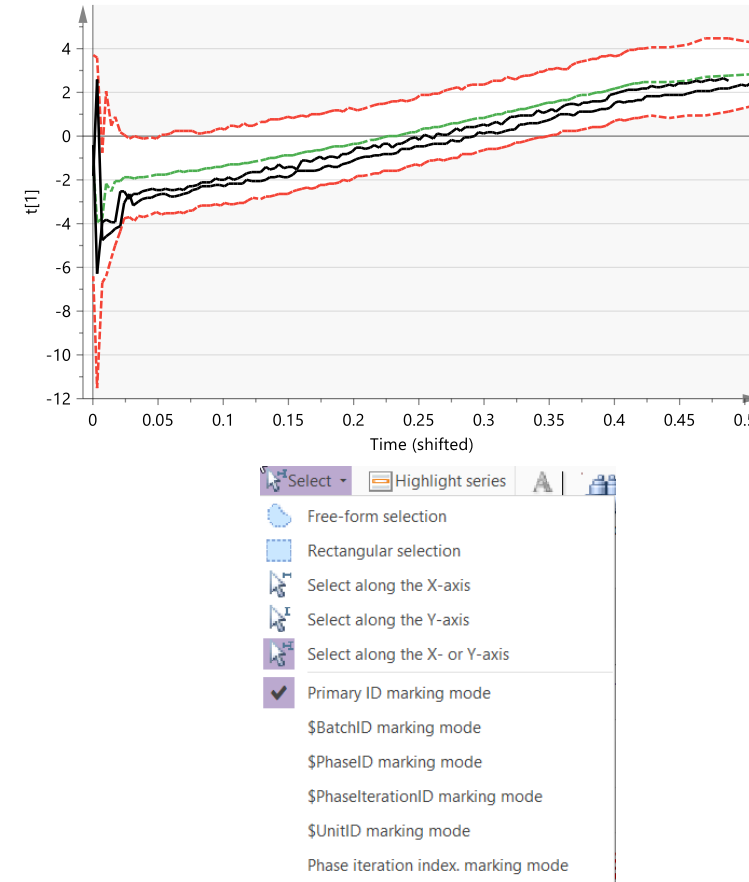
The batch level datasets

- Batch level dataset with phase iterations differ from normal BL datasets

- Primary ID is a combination of BatchID, PhaseID and PhaseIterationID

- One row per Batch, phase and phase iteration
 - Several rows per batch for phases with phase iterations

	Dataset - BM1 - batch level (raw data):Phase1													_ □ ×
	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	Primary ID	$BatchID	$PhaseID	$UnitID	$PhaseIterationID	Number	Agitation_	Agitation_	Agitation_	Agitation_	Agitation_	Agitation_	Agitation_	Agitation_
2	$PhaseID						Phase1	Phase1	Phase1	Phase1	Phase1	Phase1	Phase1	Phase1
3	$MaturityID						0	0.0034838	0.0069732	0.0104675	0.0139618	0.0174408	0.0209351	0.0244446
4	$SourceID						Agitation	Agitation	Agitation	Agitation	Agitation	Agitation	Agitation	Agitation
5	$B034$Phase1$Iter1	B034	Phase1	Unit1	Iter1	1	50.382	46.163	5.77551	5.77551	5.77551	5.77551	7.05546	87.218
6	$B034$Phase1$Iter2	B034	Phase1	Unit2	Iter2	1	47.2689	47.2689	−1.5565	−1.5565	−1.5565	0.425929	116.411	115.711
7	$B035$Phase1$Iter1	B035	Phase1	Unit1	Iter1	2	52.2662	52.2662	2.58055	2.58055	2.58055	2.9794	67.2096	165.708
8	$B035$Phase1$Iter2	B035	Phase1	Unit2	Iter2	2	46.8593	46.8593	0.204803	0.204803	1.68845	135.465	123.214	104.441
9	$B036$Phase1$Iter1	B036	Phase1	Unit1	Iter1	3	49.7675	1.61926	186.458	137.573	172.609	154.505	163.188	163.188
10	$B036$Phase1$Iter2	B036	Phase1	Unit2	Iter2	3	46.9822	3.56361	3.8974	156.006	134.261	151.903	161.061	152.275
11	$B037$Phase1$Iter1	B037	Phase1	Unit1	Iter1	4	46.9003	0.344669	0.204803	209.75	125.309	177.449	151.133	167.918
12	$B037$Phase1$Iter2	B037	Phase1	Unit2	Iter2	4	48.9483	.0409698	0.815293	177.107	118.951	174.825	147.859	165.092
13	$B038$Phase1$Iter1	B038	Phase1	Unit1	Iter1	5	53.0444	6.8972	15.4859	222.412	123.322	181.825	148.97	165.139
14	$B038$Phase1$Iter2	B038	Phase1	Unit2	Iter2	5	46.0811	0.73822	0.204803	225.572	121.49	185.763	159.169	167.407
15	$B039$Phase1$Iter1	B039	Phase1	Unit1	Iter1	6	51.7746	−1.18787	0.433041	183.84	120.114	172.985	146.835	155.037
16	$B039$Phase1$Iter2	B039	Phase1	Unit2	Iter2	6	35.2674	1.78002	27.6576	136.031	115.069	142.912	125.334	133.492
17	$B040$Phase1$Iter1	B040	Phase1	Unit1	Iter1	7	45.7124	45.7124	0.626288	78.4288	161.183	161.551	161.837	161.824
18	$B040$Phase1$Iter2	B040	Phase1	Unit2	Iter2	7	44.6884	44.6884	2.68288	80.3108	146.787	171.053	157.904	157.904
19	$B041$Phase1$Iter1	B041	Phase1	Unit1	Iter1	8	58.0826	53.3059	5.09122	225.388	138.678	189.623	165.759	173.969
20	$B041$Phase1$Iter2	B041	Phase1	Unit2	Iter2	8	45.0161	44.802	8.67445	230.304	142.009	187.97	162.819	171.831

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The batch level workset and phase iteration options

- For BMs with phase iterations, Phase Iteration Options are available

  - Active option shown in info bar

  - Pay attention to Primary ID match
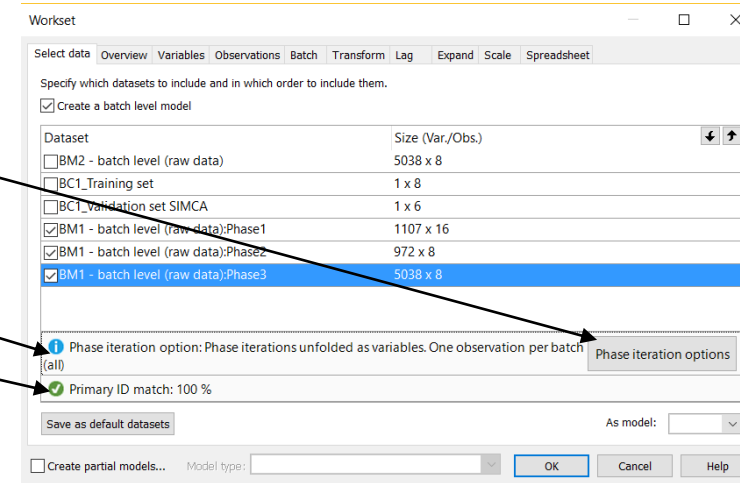
- Phase iteration options dialog – specify treatment of phase iterations
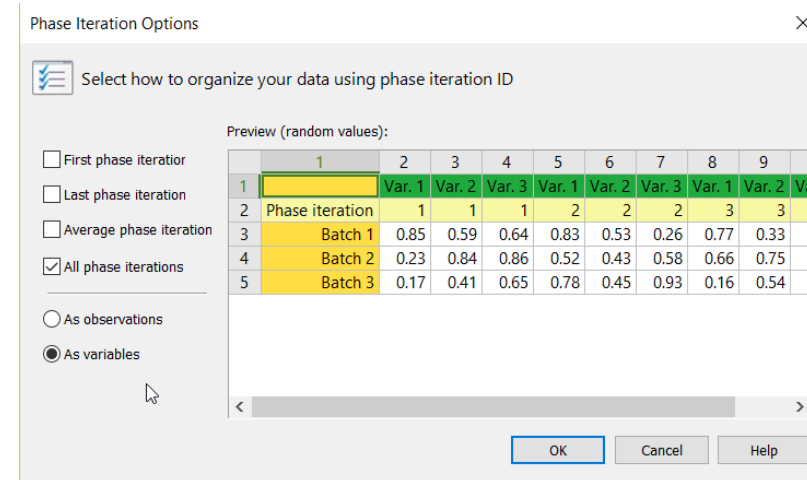
Phase iteration options

Which phase iterations to include

How to organize the data from phase iterations, if "All phase iterations" option is active

Option preview on dummy data

First, last or average phase iteration

- Gives only one iteration per phase meaning that these options equal a normal batch level model without iterations

- Examples of when these options make sense
  - First: When investigating differences between a successful first iteration with a failing one resulting in rework
  - Last: When you are only interested in modeling the final successful iteration (last and first can be equal)
  - Average: When there are varying numbers of phase iterations between batches or to scale down potential high influence of phases with many iterations in the model.
    - Block scaling can also be applied

	1	2	3	4
1		Var. 1	Var. 2	Var. 3
2	Phase iteration	1	1	1
3	Batch 1	0.26	0.03	0.25
4	Batch 2	0.85	0.59	0.82
5	Batch 3	0.31	0.25	0.37

	1	2	3	4
1		Var. 1	Var. 2	Var. 3
2	Phase iteration	Last	Last	Last
3	Batch 1	0.75	0.86	0.64
4	Batch 2	0.89	0.53	0.03
	Batch 3	0.29	0.92	0.88

	1	2	3	4
1		Var. 1	Var. 2	Var. 3
2	Phase iteration	Avg.	Avg.	Avg.
3	Batch 1	0.55	0.97	0.10
4	Batch 2	0.12	0.03	0.29
5	Batch 3	0.09	0.03	0.15

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All phase iterations

- As variables resembles normal batch level unfolding
  - One observation per batch
  - One block of variables per phase iteration instead of per phase
    - One phase is represented as many times as there are max number of iterations in workset
    - Workset limits how many phase iterations there can be in predictionset
    - Batches with fewer than max phase iterations are replaced with average phase iteration within that batch
      - Not beneficial to leave empty
- As observations resembles normal BL model of one phase only
  - One observation per batch and phase iteration
  - Only applicable when *one* dataset including phase iterations is selected
    - Otherwise warning
    - Low primary ID match
  - Allows investigation of drifts over time in phase iterations, differences between production units etc.
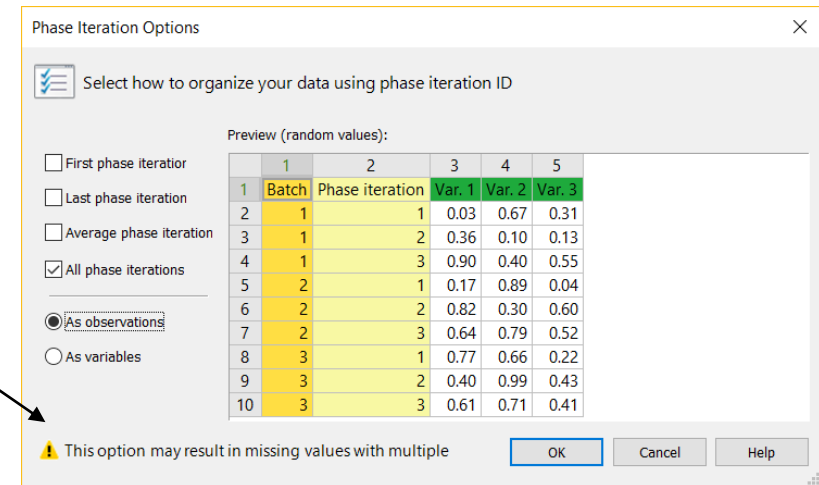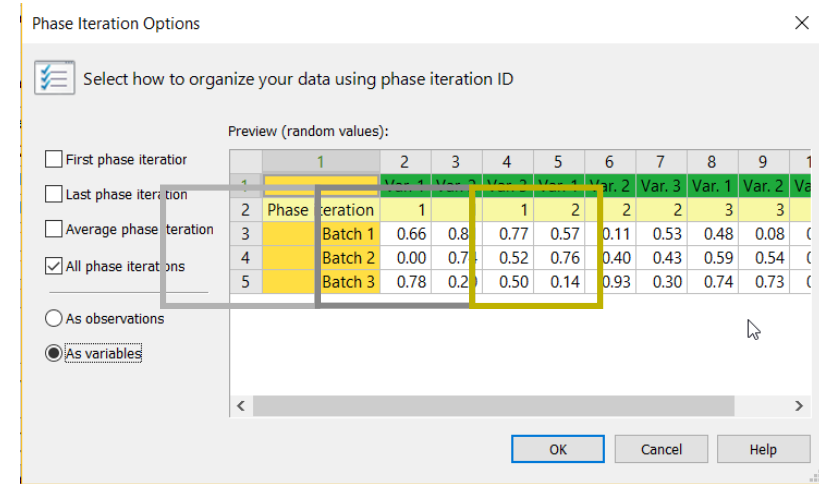
Customer challenges addressed

- SIMCA and SIMCA-online must support modeling/monitoring of recurring phases
  - Common in downstream processing but also occur in upstream

- Ability to combine all data for the batch at batch level
  - For CPV
  - Quality / output prediction
  - Compare production unit performance
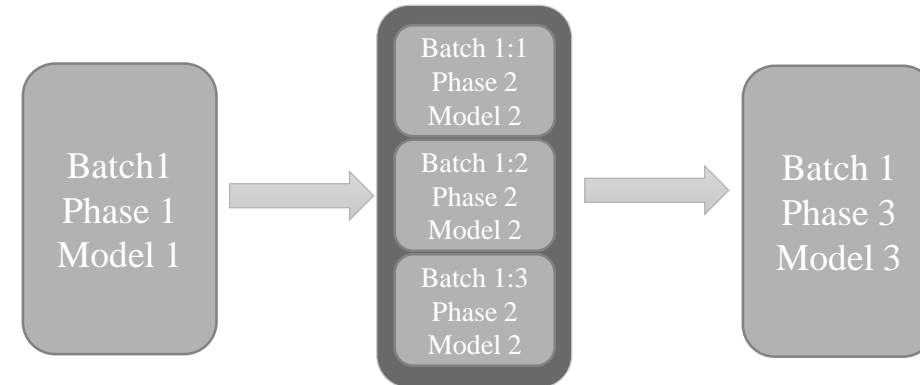
- All data from the process in One project
  - Phase and phase iteration conditions

Batch1
Phase 1
Model 1

Batch 1:1
Phase 2
Model 2

Batch 1:2
Phase 2
Model 2

Batch 1:3
Phase 2
Model 2

Batch 1
Phase 3
Model 3

| Unit1,Phase 1 | Unit2:phaseIt1 | Unit2:phaseIt2 | Unit2:phaseIt3 | Unit2:phaseIt4 | Unit3, Phase1 |

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SIMCA®-online synergies

The customer challenge

- It should be possible for the model builder to include information about limits and alarms to be used in SIMCA-online configuration

  - Not always same person building model as configuring in SIMCA-online

- Some steps in the SIMCA-online configuration is demanding, how could info in the model building dataset help?

  - If available in dataset, UnitIDs should be possible to help with Unit configuration. The models know which models that are run in which unit and which units there are in the system

- SIMCA-online can send additional data to a SIMCA project for model update, but the way back to SIMCA-online is manual.

  - SIMCA can now share projects directly with SIMCA-online. Either for model update – then applying original configuration - or as a completely new configuration

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SIMCA-online synergies

- Prepare SIMCA-online configuration file in SIMCA usp
  - Define alarm limits and rules
    - File|Info|Configure limits and alarms for SIMCA-online
  - Define UnitID at import greatly simplifies Unit configuration in SIMCA-online

- Push project from SIMCA to accessible SIMCA-online server
  - File|Share|Open in SIMCA-online
  - Review and complete configuration in SIMCA-online

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Configure limits and alarms for SIMCA-online

Configure Limits and Alarms

Configure limits and alarms for SIMCA-online.

	Type	Vector	LoLo limit	Lo limit	Target	Hi limit	HiHi limit	Alarm		
Batch evolution models (BEM)										
◢ M1:Phase1										
✕	DModX	DModX				3 std. dev.	4 std. dev.	3 outside or 10 …	⌄	📈
✕	T2Range	T2Range[1-4]				25	30	3 outside or 10 …	⌄	📈
▶	(New)								⌄	
◢ M2:Phase2										
▶	(New)								⌄	
◢ M3:Phase3										
▶	(New)								⌄	
Batch level models (BLM)										
◢ M4 - Phase iterations										
▶	(New)								⌄	
◢ M5 - Complete Batch										
▶	(New)								⌄	

☑ Show triggered alarms in plots

[OK] [Cancel] [Apply]
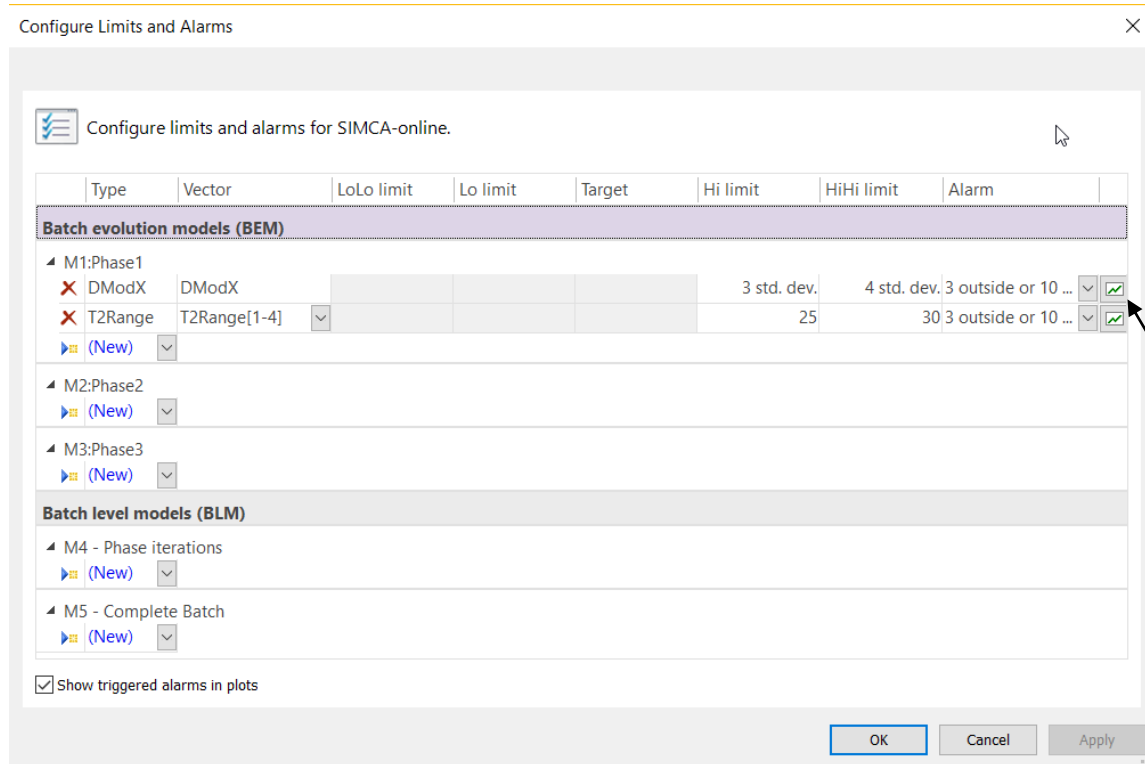
- Vector, limits and trigger

- Stored in SIMCA usp, copied to SIMCA-online

- Window is non-modal meaning that you can still access and work with plots in the main SIMCA window.

- Icon opens plot for vector showing active prediction set and triggered alarms

  - Note: Limits and alarms must be "Applied" before alarm triggers are visible

  - Note: Only the first triggered alarm for each phase, batch and vector will show.

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SIMCA® Import updates

SIMCA import updates

- Changed workflow in Home ribbon and File

- New variable and ID types

- Guidance in Issues pane

- Exchanged Excel parser for faster and more memory efficient import of Excel files

- SIMCA Import integrated into SIMCA
  - Earlier SIMCA Import was stand-alone, no visible difference in experience for user.

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Home Ribbon changes including New variable and ID types

Regular project import

Add data replace
File|New spreadsheed

Observation section

Variable section

Finish import
Cancel is replaced by
File|Discard import

Batch project import

Phase ID arrow includes Phase Iteration ID
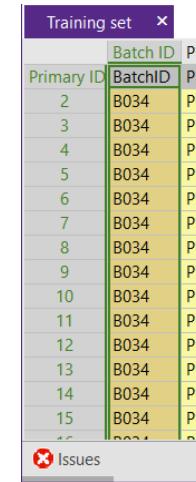
Phase ID
Phase iteration ID
Split column and set as Phase ID

New ID type

Batch condition arrow holds
Phase and Phase iteration conditions
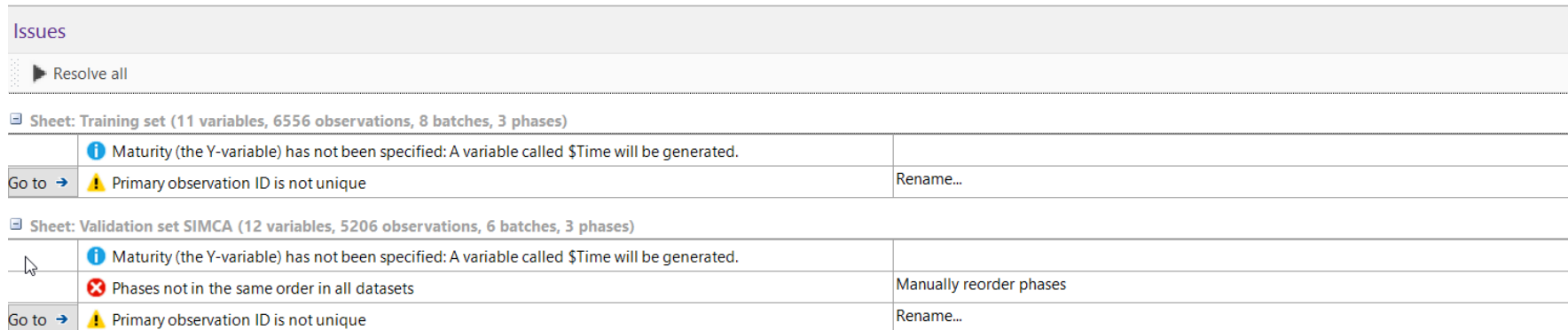
BC Batch condition
PC Phase condition
ItC Phase iteration condition

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Issues pane

- Hidden by default. Icon indicates issue

  - Click for more info

- If "Finish import" is clicked while warnings or critical issues remain, there will be a warning and the issues pane opens.

- Icons indicate severity or issue

  - ℹ️ Can be handled automatically by SIMCA

  - ⚠️ Issues with suggested actions

  - ❌ Critical issues that must be managed by manual action, e.g. sort dataset

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Minor fixes

Minor fixes summary

- Backstage New information

- Workset Select data page

- Batch marking mode → Mark on any secondary ID

- SoV drill down to BE BCC

- Secondary Observation Identifiers are brought to Batch level datasets

- Permutation plot axis titles, change in default settings and Python support for creation

- Support project restore in case of computer crash

- Improvements in DPI awareness for high resolution screens

- Send us Feedback or report bugs directly from SIMCA

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Backstage|New information

- Descriptions to assist new users set up relevant type of project

Workset Select data page

- Changed layout where any potential issues are shown at the bottom of the list
- Size of datasets is included for guidance
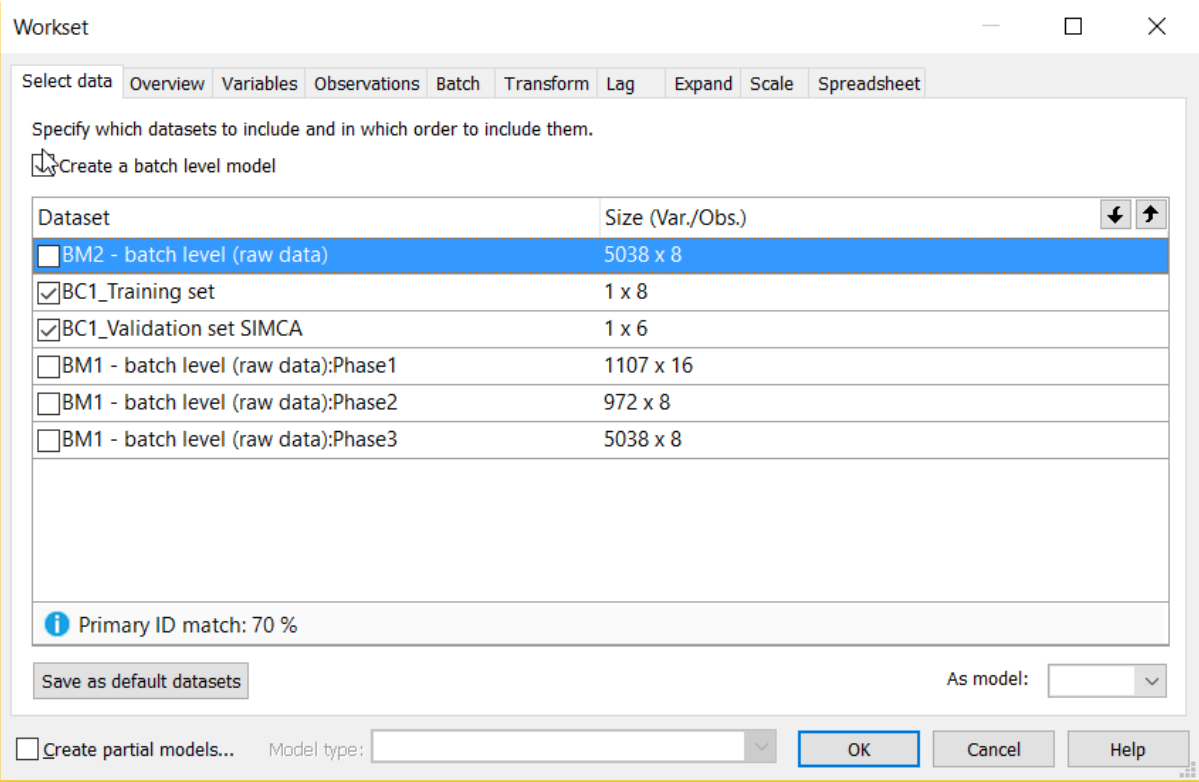
Batch marking mode → Mark on any Secondary ID

- Batch marking mode was replaced by a generic Secondary Identifier marking mode

- Available in Tools ribbon, Plot tools section, Select function

- Accessible for all project types with secondary IDs
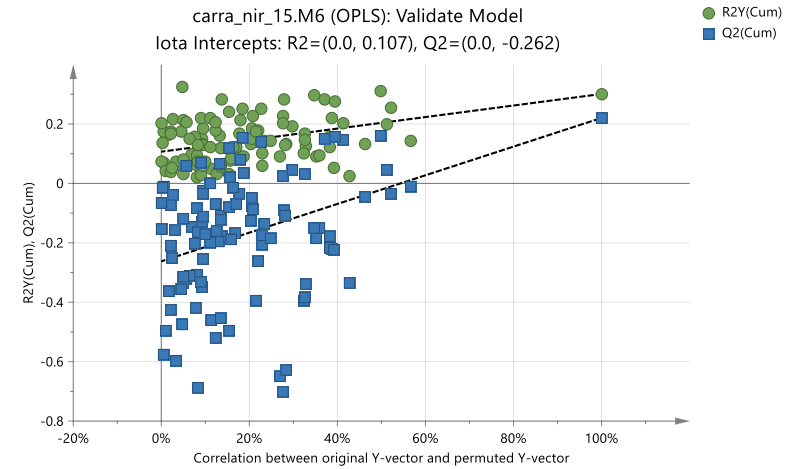
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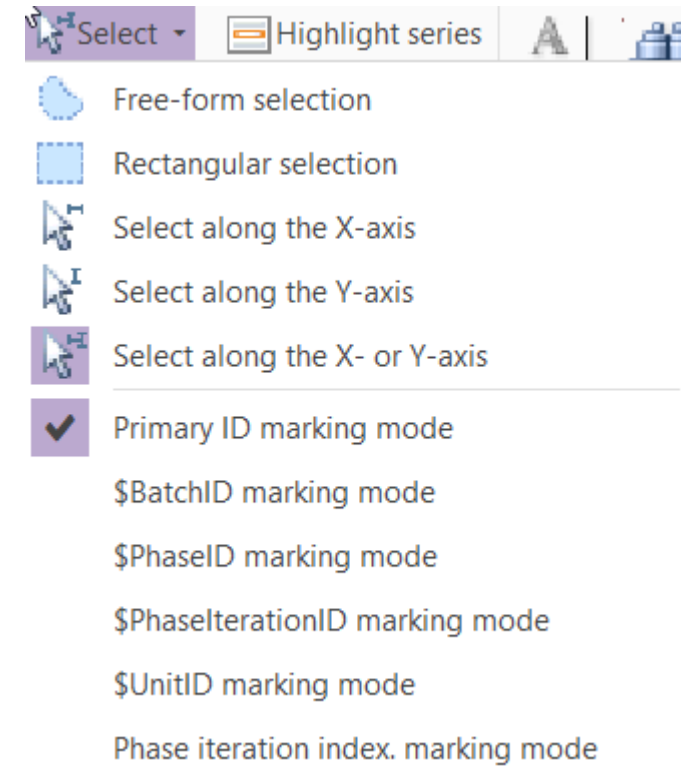
Variable plot drill-down from Batch level

- Variable plots like loading and contribution plots drill down to BE variable BC charts

  - Also Sources of variation

- For Loading plot / SoV Loading plot drill down all workset batches are shown in BCC

- For Contribution plot / SoV contribution plot

  - Group to group contribution shows batches from both groups in BCC

  - Group / point to average contribution shows batch(es) from group / point in BCC
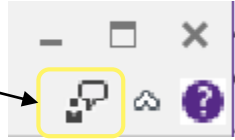
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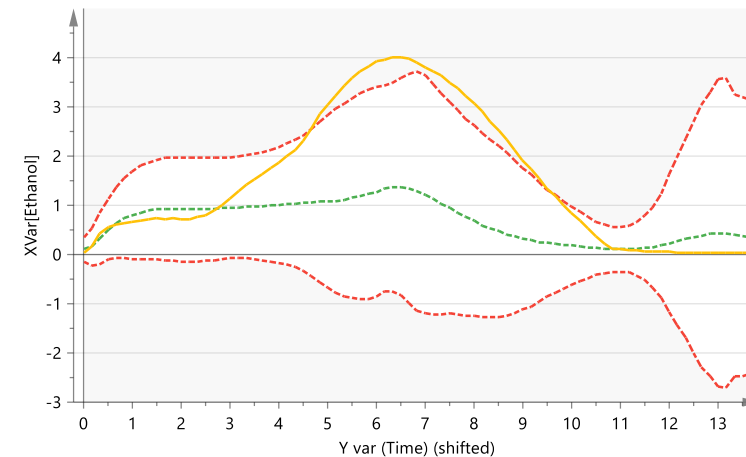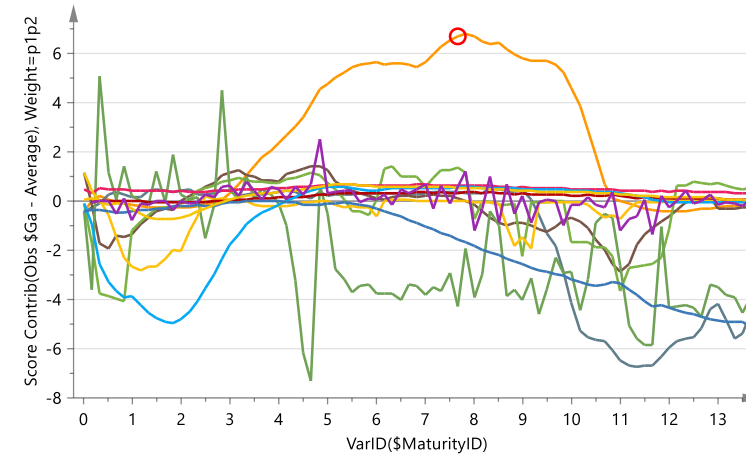
Permutation plot

- Axis titles added for clarity

- Default number of permutations changed from 20 to 100

- Permutation plot use same CV rules and groups as model

- Support to create permutation plots via Python interface

carra_nir_15.M6 (OPLS): Validate Model
Iota Intercepts: R2=(0.0, 0.107), Q2=(0.0, -0.262)

R2Y(Cum) Q2(Cum)

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Give us your feedback

- Link to feedback form in SIMCA
- Upper right corner

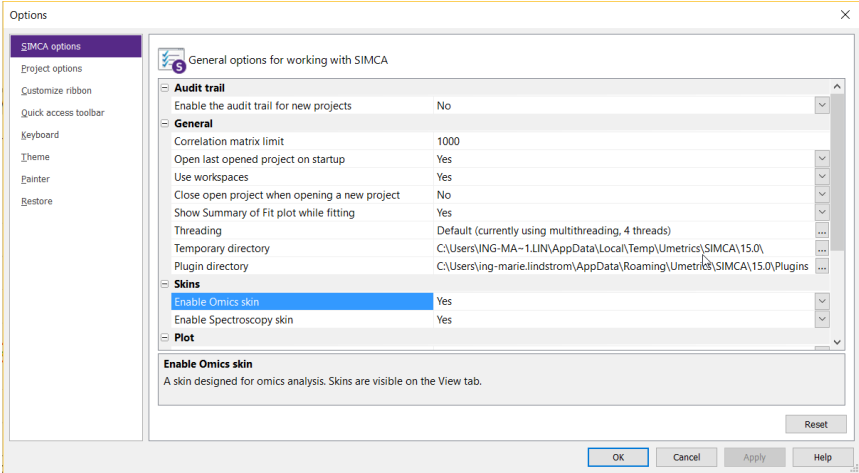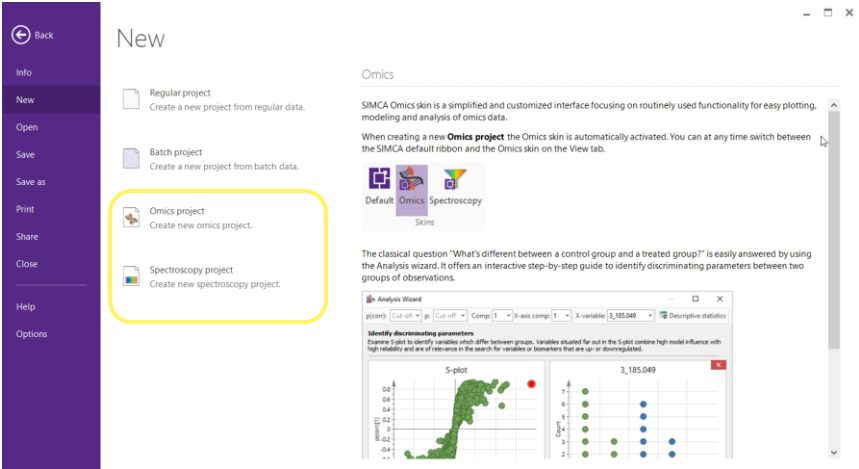- Report bugs, give suggestions for future improvements

Simplifying Progress

Skins for SIMCA® 15

Skins for SIMCA 15

- Omics skin and Spectroscopy skin are included in SIMCA 15 installation

- If not shown on the File|New page, enable them in File|Options|SIMCA options

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Thank you for your interest in SIMCA® 15

Don't forget to check out instructional videos
Search for "Sartorius data analytics" on YouTube

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