SARTORIUS

Validation report SIMCA 16   2020-06-09 16:45

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Content

1 Introduction

The purpose of the **Validation report** is to summarize and document the found differences that needs corrective actions from the validation activities performed.

The scope of the validation tasks performed are described in paragraphs 6.4 and 6.5 in the Validation plan.

1.1 Notation and notes

'US' followed by a number refers to a User Story in the TFS database.

'WI' followed by a number refers to a Work Item in the TFS database. May be Bug, User Story, Feature etc.

'VTC' followed by a number refers to a Test Case in the TFS database that has been written as a Validation Test Case, VTC. All files referenced here can be found in the New functionality folder in the validation package.

Note: Approving this document includes approval of all subdocuments and results referred to in this document.

2 Validation report summary

The purpose of the **Validation report** is to summarize and document the found differences that needs corrective actions from the validation activities performed.

The numerical validation of SIMCA 16 was done versus SIMCA 15.0.2 using CompareSimcaData. The CompareSimcaData report is included in the validation package together with comparison files for the selected models as well as all projects.

The graphical validation versus SIMCA 15 was done on a number of projects and models under Windows 10. The copied/printed plots and lists are included electronically in the validation package.

New functionality was validated versus specification.

2.1 Validation package content

The validation package includes files and folders, organized alphabetically as follows:

- Validation of SIMCA 16 pdf which includes Validation report SIMCA 16 (this document).

- Bugs folder – Lists details for the bugs referenced in the validation package, if any.

- Graphical validation folder – Documents containing the compared graphs, lists and tables.

- Projects folder – SIMCA project files (.usps) used during the validation.

- New functionality folder – New functionality and improvements have been validated and available in a folder named 'New functionality' in the validation package.

- Numerical validation folder – Holding the background to the numerical comparisons.

3 Validation task results

3.1 Numerical comparison

In the numerical comparison versus SIMCA 15.0.2, using CompareSimcaData and comparing lists in Excel, no differences that require a corrective action were found.

3.2 Graphical comparison

In the graphical comparison of plots and lists versus SIMCA 15, no differences that require a corrective action were found.

3.3 New functionality

New functionality described in features closed during the development of SIMCA 16 was validated and can be found in **Validation of new functionality summary** and New functionality folder.

The differences found are listed in the table below.

No.	Feature	Explanation	Action
5.	Quick Info	Coloring of the displayed variable plot in Quick Info was not by Batch ID.	Reported in bug 24106. May be fixed in a future release
6.	Quick Info	YObs is not supported in Quick Info. When marking a point in a DModY or DModY PS-plot, the YObs trend should preferably be displayed, but instead XObs is displayed.	Reported in Bug 24142. May be fixed in a future release
7.	Quick Info	The expanded term displayed in the Quick Info pane was created by multiplying the original variables. This is not what will be used in calculations where the variables are scaled and centered before multiplying to avoid variable range influence.	Reported in bug 24213. May be fixed in a future release

4 Verification of installed software

To verify that your license of the software has been correctly installed follow the instruction here:

1. In SIMCA, click **File | Help** and under About SIMCA …, verify that the version is SIMCA 16.0.0.7738.

2. Open one of the .pdfs in the Graphical validation folder

3. Open the corresponding project/investigation in the software, found in the Projects folder.

4. Create and compare one of the 2D plots (column, line, or scatter) and one 3D plot (3D scatter, response surface, or wavelet power spectrum). The plots should content wise be identical.

5 Source code

All source code for the final version of a full release is transferred to electronic media and kept both at Sartorius Stedim Data Analytics AB as well as in the safe of a local bank.

6 Routines

The relevant routines are stored in TFS in the QualityManual and QualityManagementSystem folders.

7 Bug handling

Work items describing bugs found are stored electronically in the database TFS. Bugs that require a corrective action are listed in the tables in paragraph 3.

8 Validation conclusion

All bugs found between the release of SIMCA 15.0.2 and the release of SIMCA 16 that remain not fixed were considered unimportant and therefore not fixed.

All differences found during the validation process are described in detail in the **Validation task results** document.

All differences that require a corrective action are listed under paragraph 3, and the WIs referenced to are stored in TFS and available in the Bugs-folder.

None of the found differences are serious. The used routines together with the validation ensure that SIMCA 16 gives correct results and is reliable.