Contents SIMCA 16.0.1 validation   **2020-06-09 12:27**

1. Validation report

2. Validation plan

	Role	Name	Date
Issued by:	Software quality	Lisa Gabrielsson	2019-05-23
Revised by:	Software quality	Anders Lindegren	2019-05-28
	Program manager	Therese Ringvall	2019-05-29
	Product manager	Stefan Rännar	2019-05-29
Approved by:	Head of Development	Jonas Andersson	2019-05-29
	Head of Quality	Andreas Norén	2016-05-29

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 paragraph 6.4 in the Validation plan.

This patch validation complements the full validation of SIMCA 16 (version 16.0.0.7738).

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 and listed in the Validation plan.

The CompareSimcaData report was saved and included in the validation package.

2.1 Validation package content

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

- Validation of SIMCA 16.0.1 pdf, which includes Validation report SIMCA 16.0.1 (this document).
- Bugs folder – Lists details for the bugs referenced in the validation package, if any.
- Projects folder – SIMCA project files (.usps) used during the validation.
- Numerical validation folder – Holding the background to the numerical comparisons.

3 Validation task results

3.1 Numerical comparison

In the numerical comparison versus SIMCA 16.0.0 and specification, using CompareSimcaData, no differences that require a corrective action were found.

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 16.0.1.7928
2. Open one of the .pdfs in the Graphical validation folder found in the full validation of SIMCA 16.0.0.7738.
3. Open the corresponding project 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
The bugs listed in paragraph 6.4 in the **Validation plan** were verified fixed and closed. Test cases were added for future automatic verification of these bugs.

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.

No differences were found. The used routines together with the validation ensure that SIMCA 16.0.1 gives correct results and is reliable.

		Name	Initial	Date
Issued by:	Software quality	Lisa Gabrielsson	LG	2019-05-23
Revised by:	Software quality	Anders Lindegren	ALi	2019-05-24
	Software quality	Andreas Norén	AN	2019-05-24
	Product manager	Stefan Rännar	SR	2019-05-27
Approved by:	Program manager	Therese Ringvall	TR	2019-05-27

Contents

1. Introduction

The purpose of this validation plan is to specify the validation activities to be performed for the SIMCA life cycle.

The validation plan describes the process of producing documented evidence that SIMCA gives correct results according to specification.

2. Background

SIMCA 16.0.1 will be released to address recently found bugs as listed under paragraph 6.4. SIMCA 16.0.1 will be numerically validated versus SIMCA 16.0.0 for all old functionality, and versus specification for known numerical changes.

3. Validation assessment and validation risk assessment

No validation assessment is carried out. Risk assessment, for changes done that may affect the validation outcome, is carried out and revalidation activities performed.

4. Overview of the System

SIMCA stores data electronically at a, by the user, specified location. While running SIMCA, temporary data are also stored in a temporary directory on the local hard drive.

5. Roles, responsibilities, and time plan

5.1 Validation group

The validation will be performed by the Software Quality group, SQ, consisting of Lisa Gabrielsson (LG), Thomas Jonsson (TJ), Anders Lindegren (ALi) and Andreas Norén (AN).

5.2 Responsibilities

Software Quality is responsible for performing the activities according to this validation plan and that documentation is produced and updated according to **Table 2**.

5.3 Initials

Initials are found on the first page of the validation plan. Jonas Andersson, JA, is Head of development. Andreas Norén, AN, is Quality Assurance Manager.

5.4 Time plan

The validation of SIMCA 16.0.1 should be completed by June 1, 2019.

6. Validation process

The validation process will follow the procedure described in the **Validation phase document** in the Quality manual available upon request.

6.1 Electronic Data/Electronic Signatures

SIMCA creates electronic data. Electronically generated data are defined in **Table 1**. Electronic Signatures (ES) are not handled by the system.

Table 1. Electronic data in SIMCA.

Data/File	File type/Folder	Content
Project	*.usp	File holding dataset spreadsheets, models, and results.

6.2 Version control

Version control during the validation will be partly applied. Version control is applied throughout the development of the system.

6.3 Handling of issues, logging of errors and actions

Changes and actions that influence the validation progress will be handled but not documented. Such changes can be that other projects takes priority and the validation of SIMCA is therefore delayed.

6.4 Validation tasks

For SIMCA, the validation will be completed according to the validation documents and tasks listed in **Table 2**. The acceptance criteria will be met upon the completion of the tests described.

All identified deviances from expected test results found during the validation life cycle will be reported and classified according to criticality. All deviations requiring a corrective action will be listed in the **Validation report**.

The following validation tasks will be performed to verify the correctness of SIMCA 16.0.1.

1. **Numerical verification** – vectors for the validation projects will be verified to be identical to those in SIMCA 16.0.0.

2. **Verification of bugs** - the bugs listed will be verified and test cases added for future automatic verification.

   a. 25047 Newsfeed makes SIMCA crash

   b. 25069 Predictionset not stable

   c. 25119 Incorrect predictionset for batch model with excluded observations in BEM

6.4.1 Validation traceability matrix

Table 2 shows the documents, files and test cases with validation tasks that will be produced/included and completed during the validation of SIMCA 16.0.1. Note that only documents that require approval have an entry in the Approved by column. All documents are revised, this is documented in the individual document. The document number used in this section is not used in other documents, but in the more thorough description of the table content in the last paragraph of this document.

Indented rows list resulting files when completing that section. All test cases are positioned in test suite: Validation documents and tasks, Suite ID 25122.

Table 2. Documents and test cases to produce and complete.

Doc. No.	Document	Reference	Approved by
1.	Validation plan	TC 18265.	TR
2.	Numerical validation	TC 20993.	
	a) usp-file	SIMCA files.	
	b) .docx, .txt result-files	Result files from CompareSimcaData.	
	c) .pjs, .scpp	N/A	
3.	Graphical validation	N/A	
	a) Content...	N/A	
	b) Plot files	N/A	
4.	Validation of new functionality summary	N/A	TR
	a) .xlsx-file, .m-file	N/A	
	b) VTC	N/A	SR
	c) VTC log	N/A	
5.	Projects, models	See the SIMCA 16 full validation	

Doc. No.	Document	Reference	Approved by
6.	Validation task results	N/A	TR
	a) Task results bugs	N/A	
7.	Validation report	TC 18266.	JA, AN
	a) Report bugs	TFS bugs mentioned in the **Validation report**.	
8.	Validation revision	TC 25123.	
9.	Validation risk assessment	TC 21019.[1]	TR, LG
10.	Validation package	A compilation of the files produced in steps 1-9.	
	a) Content	Content of the validation package.	

6.5 Prerequisites, exceptions, limitations and dependencies

6.5.1 Prerequisites
SIMCA creates electronic data according to Table 1.

6.5.2 Exceptions
No validation assessment (note [1] in **Table 2**) will be carried out.

User guide/help-file, listed under paragraph 11 Reference documents, is available from the website. The user guide holds information concerning the system and no additional documentation will be produced.

6.5.3 Dependencies
SIMCA is completely independent software.

6.6 Acceptance criteria
The general Acceptance criteria are described in detail in Validation phase, paragraph 6.7, in the quality manual stored in TFS.

6.6.1 Accepting the validation
The validation package is made available to the Head of Development and Quality Assurance Manager for revision and acceptance. The two will approve the validation provided that the acceptance criteria are met and specifically in this case:

1. **Numerical verification** – vectors for the validation projects are identical to the previous version.

2. **Verification of bugs** - the bugs listed were verified and test cases added for future automatic verification.

   a. 25047 Newsfeed makes SIMCA crash

   b. 25069 Predictionset not stable

   c. 25119 Incorrect predictionset for batch model with excluded observations in BEM

All differences, compared to previous version or specification, should be described in detail and include planned action.

The Head of Development and Quality Assurance Manager approve the validation by signing the validation report electronically using TFS.

7. Education
The members of the validation group are familiar with the routines concerning the validation work.

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[1] Validation risk assessment is carried out if applicable.

8. Tools

During the validation, the following tools will be used:

- CompareSimcaData written by Sartorius Stedim Data Analytics. Compares .dif-files with matrices extracted from SIMCA using the COM-interface under Windows.

- MATLAB from Mathworks.

- Team Foundation Server, TFS, and Excel from Microsoft.

9. Revalidation criteria

When a change of the system SIMCA is made during the validation activities, this is handled according to paragraph 3.

10. Validation report

The validation report should hold a summary of the validation work, documentation of the found deviations versus the validation plan, acceptance criteria and conclusions. It should also hold summarizing information concerning outcome of performed validation tasks, documented separately in detail in **Validation task results**.

In the validation report, any criteria not met should be documented. Software may not be released with known critical bugs.

11. Reference documents

Document	Description
SIMCA help file	User guide in the form of a help-file (.chm-file) is included with the software. The help-file holds information concerning the system. No additional documentation will be produced.
Validation phase	Describes the validation process.
Quality manual list	Lists all documents in the quality manual. Available upon request.

12. Appendix: Validation traceability matrix details

Description of documents and files in the Validation traceability matrix.

Doc. No.	Document	Explanation
1.	Validation plan	An overview of the validation of the specific software version. TC 18265.
2.	Numerical validation	Verification of numerical correctness versus previous version or specification. TC 20993.
	a) usp-file	SIMCA file holding the datasets and all models. One .usp for each selection of datasets.
	b) .docx, .txt result-file	A summary of comparisons made by CompareSimcaData[2] for each project. A set of dif-files are saved for each project to support future comparisons, but not included in the validation package.
	c) .pjs, .scpp	The project suite file (*.pjs) in TestComplete is the main file type for the automatic testing of SIMCA. The actual script.files (*.scpp) are included in the project suite. These files are created, but not included in the validation package.

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[2] Reference documents for CompareSimcaData: C:\devroot\common\smallapps\CompareSimcaData\Manual.doc and userguide.doc.

Doc. No.	Document		Explanation
3.	Graphical validation		Verification of correctness of plots versus previous version or specification. TC 19969, 19997.
	a)	Content...	A file showing which copied plots are included in the graphical validation.
	b)	Plot files	Files holding the printed-to-pdf plots in the graphical validation for the specific project and model.
4.	Validation of new functionality summary		A document listing the implemented features including a summary of the validation results. TC 18289 .
	a)	.xlsx-file, .m-file	New vectors are calculated from the specification either in Matlab or in Excel. The result is saved in an excel-file or a .dif-file to compare against in the future.
	b)	VTC	PDF of the executed the Validation Test Cases (VTC) for the new features. All in Test suite VTC with Suite ID 21634.
	c)	VTC log	Result log from running the VTC.
5.	Projects, models		A document describing the projects and models selected for the validation. TC 21036.
6.	Validation task results		A summary of the outcome of points 2-4. TC 18267.
	a)	Task results bugs	Bug descriptions extracted from TFS of the bugs mentioned in **Validation task results**.
7.	Validation report		An overview of the performed validation tasks and a conclusion of the outcome. This document includes a description of how the user can verify that the installed software was correctly installed. TC 18266.
	a)	Report bugs	Bug descriptions extracted from TFS of the bugs mentioned in the **Validation report**.
8.	Validation revision		Lists all components to revise.
9.	Validation risk assessment		Validation risk assessment is carried out if applicable. TC 21019.
10.	Validation package		A compilation of the files produced in steps 1-9.
	a)	Content	Content of the validation package.