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Prepared by	Andreas Norén	2018-03-01 13:52
Revised by	Lisa Gabrielsson, Therese Ringvall, Stefan Rännar	2018-03-07, 2018-03-26, 2018-03-29
Approved by	Jakob Mohr Christensen, Johan Trygg	2018-04-04, 2018-04-04

Content

1	Validation report summary.....	2
1.1	Validation package content.....	2
2	Validation task results.....	2
2.1	Numerical comparison.....	2
2.2	MODDE-Q functionality.....	2
2.3	New functionality.....	2
3	Verification of installed software.....	2
4	Source code.....	3
5	Routines.....	3
6	Bug handling.....	3
7	Validation conclusion.....	3



1 Validation report summary

The numerical validation of MODDE 12.1 64-bit under Windows 10 was done versus MODDE 12.0 using MODDECompare. The comparison report is included in the validation package together with compared files for the selected models as well as all investigations.

New functionality was validated versus specification.

The details of the validation tasks performed are described in the **Validation plan**.

1.1 Validation package content

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

- Validation of MODDE 12.1 pdf which includes Validation report MODDE 12.1 (this document).
- Bugs folder – Lists the bugs referenced to in the validation package.
- Investigations folder – MODDE investigations (.mip) used during the validation.
- MODDE-Q folder – files and documentation connected to the MODDE-Q validation.
- Numerical validation folder – holding the background to the numerical comparisons.

All new functionality verifications were included in the MODDE-Q and Numerical validation folders.

2 Validation task results

2.1 Numerical comparison

In the numerical comparison versus MODDE 12.0, using TestComplete, no differences were found.

2.2 MODDE-Q functionality

MODDE-Q was numerically validated versus MODDE 12.1 using MODDEcompare.

The differences listed below were found.

No.	Vector/List	Investigations	Explanation	Action
1	Response limits in optimizer	All	The response limits could not be set correctly using the COM interface	Bug 16907. This bug may be fixed in a future release.
2	All model results and predictions	Larsmod7trm_III, Valena, Valhpc11	The “Fit equal PLS models as one model” option could not be set with the COM interface	Bug 21212. This bug may be fixed in a future release.

2.3 New functionality

New functionality described in features closed during the development of MODDE 12.1 was validated and can be found in **Validation of new functionality summary** and New functionality folder.

No differences that other than those listed in paragraph 2.2 were found.

3 Verification of installed software

To verify that your license of the software has been correctly installed follow the instruction found in **Verification of installed software**. In short:

1. In SIMCA, click **File | Help** and under About SIMCA ..., verify that the version is MODDE 12.1.0.5491.
2. Open one of the .pdfs in the validation folder
3. Open the corresponding investigation in the software, found in the Investigations 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.

4 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.

5 Routines

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

6 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 2.

7 Validation conclusion

All bugs found between the release of MODDE 12.0 and the release of MODDE 12.1 that remain not fixed were considered unimportant and therefore deferred.

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 2, and the WIs referenced to are stored TFS and available in the Bugs-folder.

None of the found differences are serious. The used routines together with the validation ensure that MODDE 12.1 gives correct results and is reliable.

Jakob Mohr Christensen, 2018-04-04
Managing Director, Sartorius Stedim Data Analytics AB

Johan Trygg, 2018-04-04
CTO, Sartorius Stedim Data Analytics AB

