



MODDE®

Design of Experiments Solution

Technical features for MODDE® 12.1

27 March 2018

Design of Experiments (DOE) is the most effective method to achieve product and process efficiency and optimization. MODDE is a state-of-the-art design of experiments software package that is used by scientists, engineers, and statisticians alike to help understand complex processes and products. Features reserved for MODDE Pro highlighted.

New in MODDE 12/12.1

- Generalized subset designs, generates a complementary sequence of design sets.
- One-Click analysis feature, including automatic outlier detection, transformation and model tuning.
- Definitive screening design for 4 to 30 factors.
- Qualitative factors with missing levels supported.
- Response correlation effect optionally included in Design Space calculations.
- Export and open in SIMCA.
- Default individual response models with PLS regression.
- Reduced combinatorial designs available for optimization design generation.

Design generation

- Design Wizard guides the design generation.
- Up to 32 factors.
- Factor ranges (scaling) can be updated retroactively.
- Factor types:
Quantitative, quantitative multilevel (24 levels) factors.
Formulation (mixture), Filler, Qualitative factors (24 levels).
- Constant and uncontrolled factors.
- Linear constraints on factors.
- Combination of process and formulation factors.
- 128 responses possible.

- Linear, Log, Neglog, Logit, Exp and Power transformations of factors and responses.
- Power estimation of designs.
- A wide variety of designs: Fractional factorial, Full factorial (2 levels, 3 levels and mixed), L9, L18, L27, L36, CCF, CCC, CCO, Reduced CCF and CCC, Box Behnken, Rechtschaffner designs in 2 and 3 levels, Doehlert designs in 2-20 factors. Axial (reduced, normal, and extended), Cubic centroid (Mod, Mod w/face, Special and Full), regular and Super saturated Plackett Burman designs. Definitive screening design for 4 to 30 factors.
- Reduced combinatorial designs (J2)
- Generalized subset designs - optimal and balanced multilevel designs.
- Stability testing designs.
- Rectangular Experimental Designs for Multi-Unit Platforms, RED-MUP. Supports designs for up to 4 plates with sizes 8x12 and 16x24, with 32x48 size plate. Includes RED-MUP specific designs.
- D-Optimal designs using state-of-the-art algorithm.
- Blocking of classical and D-Optimal designs.
- Inclusions can be imported and edited.
- Candidate sets can be read from file.
- Import design data from external files.

- Complementing designs, using classical and D-Optimal approaches.
- Onion designs from scores generated in SIMCA.
- Onion design in ordinary factors, both with imported candidate set and candidate set generated by MODDE.
- Analysis of worksheet including Scatter Plots, Histogram, Descriptive Statistics, Correlation Matrix, Replicate Plots and condition number.
- Investigations can be sent by e-mail, directly from MODDE.
- Export and open in SIMCA

Analysis and modeling

- Fit with MLR or PLS
- Cox and Scheffé Mixture models.
- Handles process and mixture models and their combinations.
- Cross validation of models
- Indication of confounded model terms for fractional factorial designs.

Analysis guidance

- Analysis Wizard guides the user through the analysis step by step allowing model customization from the graphs.
- One-Click analysis feature, including automatic outlier detection, transformation and model tuning.
- Automatic Square and Interaction tests in the Analysis wizard.





- Advisor pane which explains analysis plots and results, and advises you on what to do next.

Reviewing the model

- Multiplots and lists displaying selected responses.
- Summary of the model fit – plot and list with Q2, R2, Model validity (LOF) and Reproducibility.
- Customizable model overview multiplot.
- ANOVA plots and lists.
- Residual vs Run Order, Predicted, Variable Plots and Lists.
- Normal Probability of residuals, Observed vs Predicted and Distance to Model plots.
- Coefficient plots and lists.
- Effects and Interaction plots.
- Variable importance (VIP) plots and lists.
- Score and Loading plots.
- Box Cox plot.

Refining the model

- Interactive pruning of model terms with automatic model fitting and updating of all open plots and lists.
- Automated model tuning feature.
- Separate models for each response.

Predictions

- Contour, Sweet Spot, Design Space probability and Prediction Plot Wizards for simple generation of plots
- 2D, 3D (mixture) and 4D plots make it possible to display up to 5 factors simultaneously.
- 4D plots with qualitative factors on the outer axes.
- Contour surface with multiple responses.
- Option to lock contour levels in Contour plot.
- Prediction plot interval estimates include

confidence, prediction and tolerance options.

- Prediction plots display raw data.
- Overlay prediction plots for multiple responses.
- Factor Effects Plot including confidence intervals.
- Prediction Scatter Plot updated with changes in the Prediction Spreadsheet.
- Transformed factors by default displayed in original units in prediction plots.

Optimizer

- Uses a multidimensional Simplex method.
- Customizable desirability functions.
- Possible to set target values and optimization criteria.
- Optimizer predicts possible ranges for all responses.
- Weighting according to the importance of the responses.
- Optimization of multiple responses, regular or derived.
- Risk analysis of the optimal setting.
- Option to set response limits as absolute in Optimizer.
- Robust optimization feature presenting the most robust setpoint.

Design Space Explorer

- Export of complete Design Space as a data matrix.
- Design space explorer plot expansion with hypercube to facilitate communication of the Proven Acceptable Range (PAR).

Setpoint validation

- Statistical robustness validation of the investigated system.
- Interactive GUI and automatic functions for robust range establishment.

Plots and lists

- Predefined plot sizes when copying to various presentation types.

- Create list from plots.
- Color-coding in lists to highlight suspicious values.
- Plots can be customized and templates saved.

Reports

- Customizable report generator for fast and standardized documentation.
- Report integrated in the MODDE *.mip file

General

Information about the use of functionality in MODDE is available at our website:

<http://umetrics.com/product/modde-pro>

Installation

Administrator permissions are necessary to install MODDE 12.

Trial limitations

MODDE Pro can be run as a trial for 30 days.

Minimum system requirements

- Microsoft Windows 7, 8 or 10
- 1024x768 screen resolution color display

Support

For technical support, contact umetrics_support@sartorius-stedim.com

The latest information and support questions can be found in [Sartorius Stedim Data Analytics Knowledge base](#).

