SARTORIUS

MODDE

Design of Experiments Solution

Technical features for MODDE 13

2 March 2021

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. Highlighted rows are new in MODDE 13.

Feature	MODDE Go	MODDE Pro
Design generation		
Design Wizard guides the design generation	■	■
Four design objectives: Screening, System Characterization, Optimization (RSM), Robust Verification	■	■
Split objective	-	■
Up to 48 factors	■	■
Factor ranges (scaling) can be updated retroactively	■	■
Factor types: Quantitative, quantitative multilevel (24 levels) factors, qualitative factors (24 levels),	■	■
Factor types: Formulation (mixture), Filler	-	■
Constant and uncontrolled factors	■	■
Linear constraints on factors	-	■
Combination of process and formulation factors	-	■
128 responses possible	■	■
New response objective and condition	■	■
Linear, Log, Neglog, Logit, Exp and Power transformations of factors and responses	■	■
Detailed design power estimation	■	■
Optimal selection of replicated design points	■	■
A wide variety of classical 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, regular and Super saturated Plackett Burman designs. Definitive screening designs.	■	■
Axial (reduced, normal, and extended), Cubic centroid (Mod, Mod w/face, Special and Full) designs	-	■
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	-	■

Feature	MODDE Go	MODDE Pro
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	-	■
Paste design to import it	-	■
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	■	■
Qualitative factors with missing levels supported	■	■
Export and open in SIMCA	-	■
Analysis and modelling		
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	■	■

Feature	MODDE Go	MODDE Pro
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 model for each response with all fit methods	■	■
Predictions		
Contour, Sweet Spot and Prediction plots wizards for simple generation of plots	■	■
Design Space plot wizard to find design space and robust setpoint	-	■
Visualization of desirability	■	■
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 Predictions spreadsheet	■	■
Transformed factors by default displayed in original units in prediction plots	■	■
Optimization guidance		
Optimization wizard guides the user through the optimization step by step	-	■
Visualization of simulated process output	-	■
Favorite setpoint defined by user	■	■
Summary of alternative setpoints and statistics	-	■
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	-	■
Response correlation effect optionally included in Design Space calculations	-	■

Feature	MODDE Go	MODDE Pro
Optimization within design space	-	■
Design Space Explorer		
Design space explorer plot expansion with hypercube to facilitate communication of the Proven Acceptable Range (PAR)	-	■
Export of complete Design Space as a data matrix	-	■
Setpoint validation		
Statistical robustness validation of the investigated system	-	■
Interactive GUI and automatic functions for robust range establishment	-	■
Setpoint comparison histogram	-	■
Plots and lists		
Contextual properties pane for easier access to plot properties	■	■
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	■	■