SARTORIUS

MODDE

Design of Experiments Solution

Technical features for MODDE 13

27 March 2024

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 or 13.1.

Feature
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
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

Feature
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
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

Feature
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
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

Feature
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
Experimental Design sharing
Share DOE investigations in json file format