

Technical Features of MODDE 9.1

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.

Design Generation

- Design Wizard guides the design generation.
- Up to 32 factors.
- Quantitative, quantitative multilevel (24 levels), quantitative constant and quantitative uncontrolled factors.
- Formulation (mixture), filler, constant and uncontrolled factors.
- Linear constraints on factors.
- Qualitative factors (24 levels).
- Combination of process and formulation factors.
- 128 responses possible.
- Linear, Log, Neglog, Logit, Exp and Power transformations of factors and responses.
- A wide variety of designs: Plackett Burman, L9, L18, L27, L36, Fractional Factorial, Full Factorial (2 levels, 3 levels and mixed), CCF, CCC, 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).
- Super saturated Plackett Burman Designs.
- Rectangular Experimental Designs for Multi-Unit Platforms, RED-MUP. Supports designs for up to 4 plates with sizes 8x12 and 16x24 plates, and one with 32x48 size plate. RED-MUP specific designs.
- D-Optimal designs using state-of-the-art D-Optimal algorithm.
- Blocking of classical and D-Optimal designs.
- D-Optimal designs including combinations of quantitative, qualitative and formulation factors.
- Inclusions imported and edited in the design wizard.
- Candidate sets can be read from file.
- Import Design data from external files.
- Complementing designs, using classical and D-Optimal approaches.
- Multivariate design using Onion designs from scores generated in SIMCA-P/P+.

- Onion design in ordinary factors, both with imported candidate set and candidate set generated by MODDE.
- Onion Plot and 3D Scatter Onion Plot.
- 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, at the press of a button.

Analysis and Modeling

- Color-coded cube plots for displaying results
 - 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
- Analys Guidance
- Analysis Wizard guides the user through the analysis step by step allowing model customization from the graphs.
 - Analysis advisor, explains Analysis plots and results, and advises you on what to do next.

Reviewing the Model

- Summary of the model fit – plot and list with Q2, R2, Model validity (LOF) and Reproducibility.
- 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.
- Multiplots and lists displaying selected responses.
- Box Cox plot.

Refining the Model

- Interactive toolbar allows on-screen deletion of model terms with automatic model fitting and updating of all open plots and lists. Changes apply to the current response only.
- Separate models for each response.
- Edit model buttons for adding squares and interactions of factors for selected responses.

Predictions

- Contour and Prediction Plot Wizards for simple generation of plots
- New graphics for Contour, Sweetspot and Surface plots
- 2D, 3D and mixture Contour plots
- 4D Contour plots make it possible to display up to 5 factors simultaneously
- 4D Contour plots with qualitative factors on the outer axes
- 4D Sweet Spot plot
- Sweet Spot plot for optimization
- Option to lock contour levels in contour plot
- Overlay prediction plots for multiple responses
- Response Prediction Plots and lists including confidence intervals
- Prediction Scatter Plot updated with changes in the Prediction List

Optimizer

- Uses a multidimensional Simplex method.
- Desirability function handles up to 128 responses.
- Possible to set target values and optimization criteria.
- Weighting according to the importance of the responses.
- Optimization of multiple responses, regular or derived.
- Sensitivity analysis of the optimal setting.
- Option to set response limits as absolute in Optimizer.
- Design Space estimation with Monte Carlo simulation.
- **Design space can be presented as a 2 or 4D contour probability plot**

Colored bullets are new features in MODDE 9.1

Design Space Validation

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

Plots and Lists

- Create List from plots.
- Color-coding in lists to highlight suspicious values.
- Plots can be customized and settings saved.
- Interchangeable plot labels.

Reports

- Flexible and automatic report generation.
- Report file (HTML format) from open lists and plots.

Quality

- 21 CFR part 11: Authority check, Audit Trail and validation to comply with FDAs regulation on electronic records.
- Lock and encrypt investigation.
- Validation binder available on request.
- Automation with COM interface.

Connectivity for MODDE 9.1

- M-Link.

System Requirements

- 1.5 GHz processor.
- 256 MB RAM, 100 MB free hard disk space.
- 800x600 screen resolution color display.
- Windows 7, XP or Vista.
- Graphics card with 3-D acceleration and which supports OpenGL.
- Internet Explorer version 6.0 or later.

Activation

- Activation with license file.