Simplifying Progress

MODDE® 13 – What’s New?
Release March 2, 2021
MODDE® 13 Overview

▪ Umetrics® suite MODDE® is focused on delivering a full design of experiment solution, from creating an investigation plan to analyze results and support decision making base on scientific principles.

▪ MODDE® 13 is focused on improving Design Selection and making Optimization easier and more powerful.

▪ With MODDE® 13 you get the new Optimization Wizard that complements the reworked Design Wizard and updated Analysis Wizard.

▪ The most frequently used function and customizations can now be accessed in the Properties pane making it easier than ever to succeed with design of experiments.
MODDE® 13 Highlights

- Design Selection
  - New response Objectives and Conditions
  - Factor setting for Normal Operating Range
  - Detailed design Power per factor and response
  - Optimal selection of replicated design points
  - Interactive design selection view
  - New investigation objectives

- Model and Analysis
  - Model verification in Analysis Wizard
  - Visualization of desirability

- Optimization
  - Optimization Wizard
  - Optimization within design space
  - Setpoint comparison

- Other Improvements
  - Access to most used functions in new Properties panes
  - Define favorite setpoint
  - Create new plot from with existing settings for contour like plots
  - Performance
Learning What’s New in MODDE® 13

- In the following slides you will get an overview of the changes and additions made in MODDE® 13

- Please also check out more videos on MODDE® and other Umetrics® suite products by looking up Sartorius Data Analytics on YouTube
Design Wizard – Investigation Objective

- **Screening**, first stage of an investigation when little is known
- **System characterization**, investigate the influence of the most influential factors, including their two-factor interactions and quadratic effects
- **Optimization (RSM)**, optimization using the most influential factors and focus on low prediction error
- **Robustness verification**, investigate the system’s sensitivity to changes in certain critical factors
Design Wizard – Responses definition dialog

- **Condition** - importance of response
  - Required responses are quality attributes with hard limits that must be fulfilled. They define sweet spot, design space and are used in robust setpoint calculations
  - Desired responses are influencing optimal setpoint
  - Observed responses are predicted but do not influence design space or optimization

- **Objective** - what you want to do with the response.
  - Minimize the response, often with max limit
  - Maximize the response, often with min limit
  - Target set the response close to a value
  - Inside, not influencing optimal setpoint

- **Power to detect a coefficient as significant**
  - Signal to noise ratio
Design Wizard – Factor definition dialog

- Precision is the uncertainty in measurement of the factor setting
  - If set, it complements the prediction uncertainty range in Design Space estimation and Setpoint Exploration estimation

- Normal Operating Range, NOR, is defined as the common range during daily use of the application
  - Use the model to simulate response distributions
  - NOR can be used in Setpoint Comparison and Setpoint Exploration
Design Wizard – Select Design

- **Requirements**
  - Used to filter the design alternatives
  - Max number of runs, Design Power and Degrees of freedom
  - Model complexity

- **Design options for selected design**
  - Replicated runs, add best replicated design points
  - Edit model of a design
  - Add to comparison to add the current design to Compare designs section

- **Other improvements**
  - Create D-Optimal design directly from select design page
  - Detailed Power for each factor and response combination
  - Sort design on Design power or I-optimality
MODDE® 13 What’s New
Optimization
- Verify that response Condition, Objective and limits are set correctly
- Response condition, objective and limits are automatically fetched from the response definition. Green values are tooltips that indicate the range of values valid when considering the model.
- Set desirability type
  - Target, reach a solution close to target
  - Limit, reach a solution within limits
- Weight can be used to limit the influence of some responses in order to find a compromise between many.
Optimization Wizard – Sweet spot

- Automatically sets factor constants to display the largest sweet spot.
- When no sweet spot can be found there is guidance in pane to the right.
- Sweet spot plot is shown when there is at least one response with Condition: Required.
Optimization Wizard – Design Space

- Calculate the robust setpoint by clicking “Find robust setpoint”
  - Factor constants are adjusted to match the robust setpoint
  - Robust setpoint is marked by a crosshair
- Customization of Design Space calculation in the properties pane
- When no Design Space can be found, there is guidance in pane to the right
Optimization Wizard – Desirability

- Interpreting the desirability plot:
  - Red: outside the design space
  - Blue: inside the design space. The lighter the blue, the higher the desirability

- Calculate optimal setpoint by clicking “find optimal setpoint”
  - Factor constants are adjusted to match the optimal setpoint
  - Optimal setpoint is marked by a double circle

- When Design Space can be found there is guidance in pane to the right
- Compare predicted distribution of selected responses. Can be used to simulate future process output
- Probability of failure for each setpoint for all responses with Objective: Required
- Adjustment of factor distribution and Interval estimation settings in pane
Optimization Wizard – Summary

- Summary of setpoint characteristics
  - Response settings
  - Factor settings
  - Predicted value
  - Probability of failure
  - Cpk

- Proven acceptable range calculated for robust setpoint
  - Robust low/high edge
  - Hypercube low/high edge
MODDE® 13 What’s New
Features and improvements
User interface

- Properties pane with most used settings
  - Available for all plots
  - Select or deselect responses
  - Select axis and adjust constants with slide bars
  - In the pane to the right specific settings for current contour plot are available and alternatives can be activated by point and click.

- Right-click any contour plot and select “... from this” creates the selected sweet spot, contour plot desirability or designs space plot with the current axis and constant settings
Robust, Optimal, and Favorite setpoint

- MODDE 13 have three different setpoints and can be used in all types of 2D and 4D contour like plots
- Robust setpoint – crosshair symbol
  - Calculate in design space plot and optimizer
- Optimal setpoint – double circle symbol
  - Calculate in Desirability plot or optimizer
- Favorite setpoint identified by star symbol
  - Position your own favorite setpoint (right-click, Set as favorite setpoint)
- Select factor constants by clicking a setpoint in Properties pane
- When factor constants don’t match exactly for a setpoint, that setpoint symbol is displayed in grey
Features and improvements

Analysis Wizard

- Contour plot added in Analysis wizard for model verification by user
  - Is the model in line with expectations and prior knowledge
- 4D contour plot available, customize axis in properties pane
- Improved Interaction test-dialog for reduced factorial designs
The desirability plot shows how well the response objectives are fulfilled
- Visualization of desirability function
- Used to identify optimal setpoint
- Find optimal setpoint function in properties pane to identify the optimal setpoint
- Combine with sweet spot or design space if there are required responses
When a design space has been calculated, MODDE can identify the factor combination with best desirability within the design space.

- Optimal setpoint marked with double circle symbol
- For full view of desirability, select “Show desirability outside of design space” in Properties pane
- Create desirability plot from a sweet spot plot to calculate optimal point inside the Sweet spot.
Setpoint comparison

- Setpoint comparison plot shows histograms of simulated process output profiles based on factor distribution
- All defined setpoints can be visualized in the same histogram
- Total Probability of failure and individually for each response are shown for selected setpoints
- Normal Operating Range, NOR, is the default setting
Features and improvements

Design Wizard – Detailed power in Responses definition dialog

- A measure of the DOE’s ability to detect an effect as significant. Power is expressed in percent.
- Ratio between expected noise and the size of the effect to be detected
- Intended mainly for screening investigations
- MODDE provides detailed power for each factor per response
Design Wizard – Optimal selection of replicated design points

- Repeated design creates a DOE with 22 experiments and Power of 96
- Add replicated design runs to create a DOE with sufficient power
  - Original design (full fac) : 11 runs Power 57
  - Repeated design : 22 runs Power 92
  - Optimal replicated runs : 15 runs Power 82
Thank You for Your Interest in MODDE® 13

Don’t forget to check out the instructional videos in Sartorius Data Analytics YouTube channel