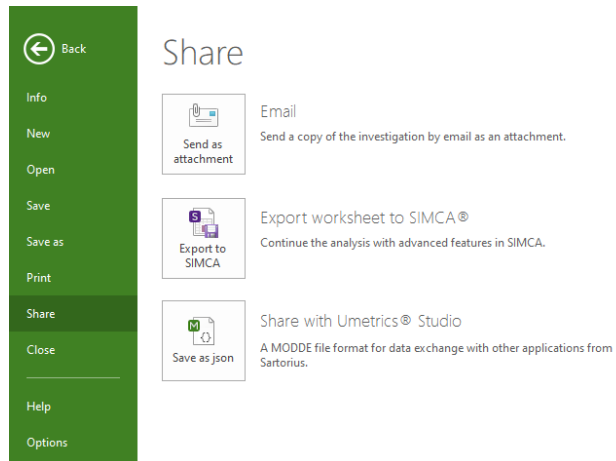# SARTORIUS

## Simplifying Progress

# MODDE® 13 – What's New?

Release March 28, 2024

# MODDE® 13.1 Highlights

- Umetrics® Studio compatibility
  - Share with Umetrics® Studio cloud solution using new json file format
  - Offer templated solutions for Sartorius equipment



- Design wizard
  - Information text for all objectives
  - Option set order of Responses and Factor according to preference
  - Select design page has updated Recommended designs that better reflect Application Engineering expert advice

- Miscellaneous
  - Licensing aligned with other Umetrics® Suite products and updated with the latest version
  - Stability improvements from customer and internal reports

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# MODDE® 13.1 Compatibility – Umetrics® Studio and Beyond

- Share a DOE investigation in json format for use in other applications
  - Facilitate collaboration on DOE projects
  - Create basis for templated solutions leveraging our knowledge of production and capabilities of the instrument used

- Refine json DOE investigation
  - Open investigation created in other DOE applications
  - Provide detailed analysis and predictions for investigation updated in cloud DOE or other Sartorius applications

- Currently supported in json file
  - Factors
  - Responses
  - Constraints
  - Reference mixture
  - Fit method (when custom selected)
  - Worksheet
  - Model terms
  - Excluded variable per response
  - Design name
  - Candidate set
  - Setpoints
  - Options/settings that affect model
    - E.g. Replicate tolerance

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# MODDE® 13 Overview

- Umetrics® suite MODDE® is focused on delivering a full Design of Experiments solution, from creating an investigation plan to analyzing results and support decision making based 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 functions and customizations can now be accessed in the Properties pane making it easier than ever to succeed with design of experiments.

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# 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 with existing settings for contour like plots
  - Performance

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# 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

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MODDE® 13 What's New
Design Selection

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# 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
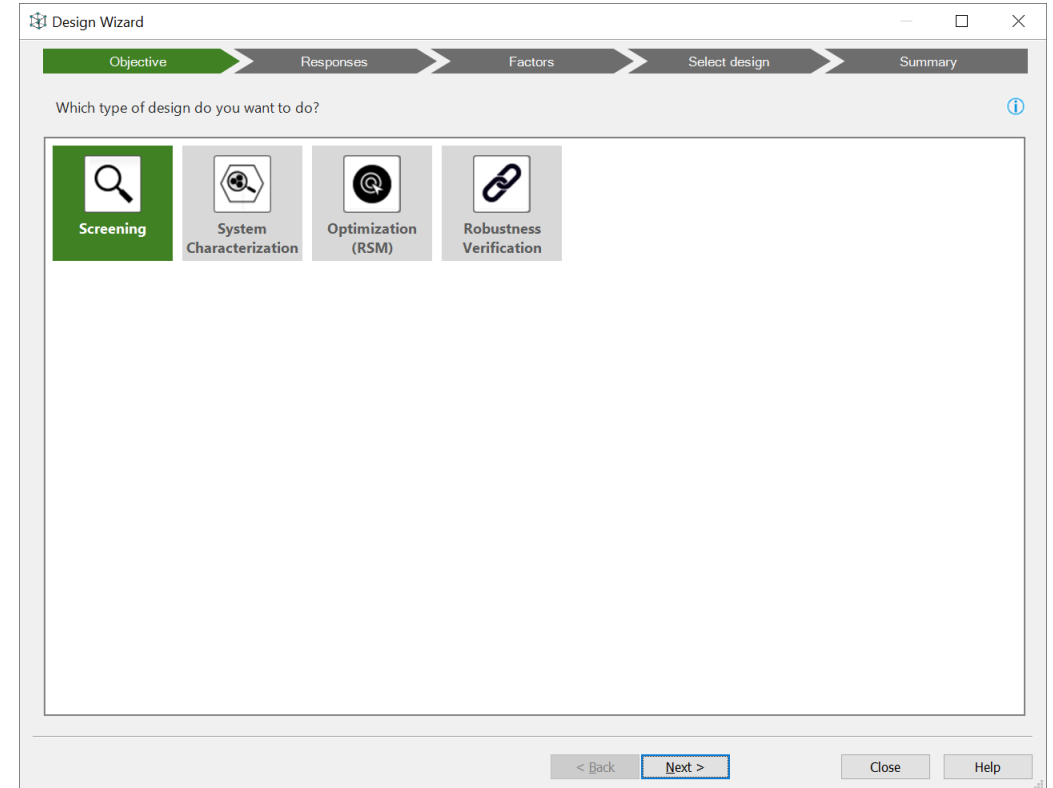
# Design Wizard – Responses definition dialog

- 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

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# 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
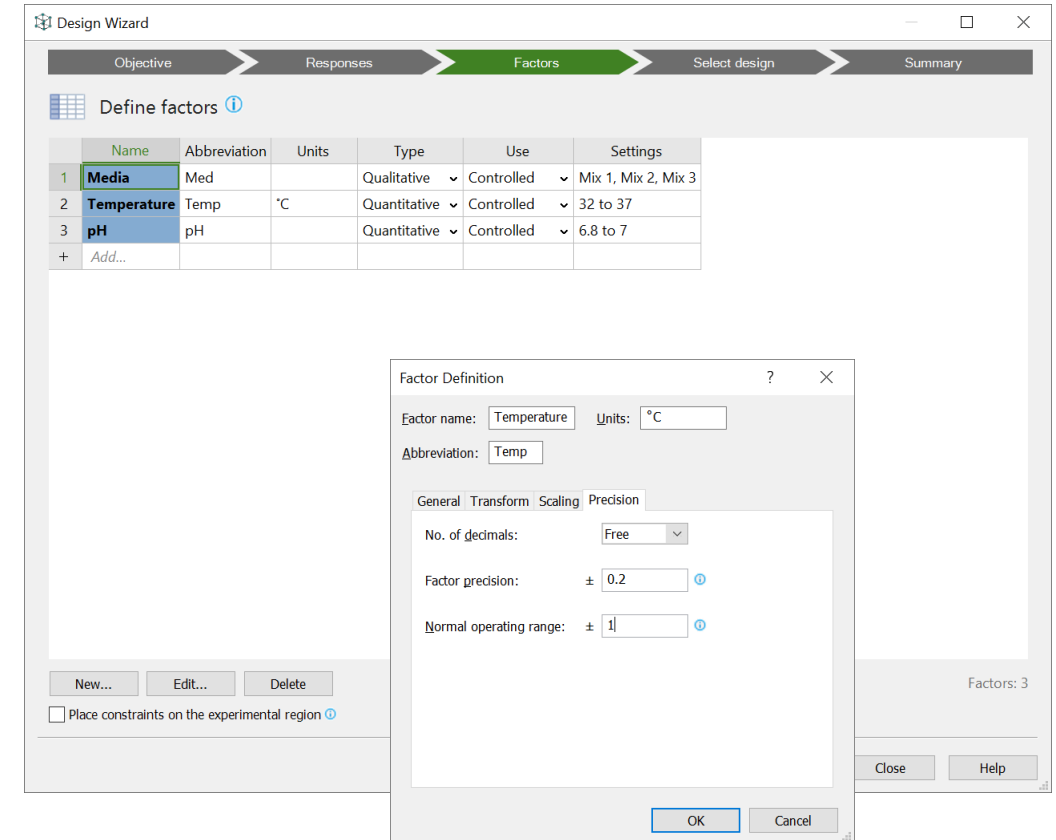
# Design Wizard – Select Design

- 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

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MODDE® 13 What's New
Optimization

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# Optimization Wizard – Inspect Response Settings

- 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.

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# 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
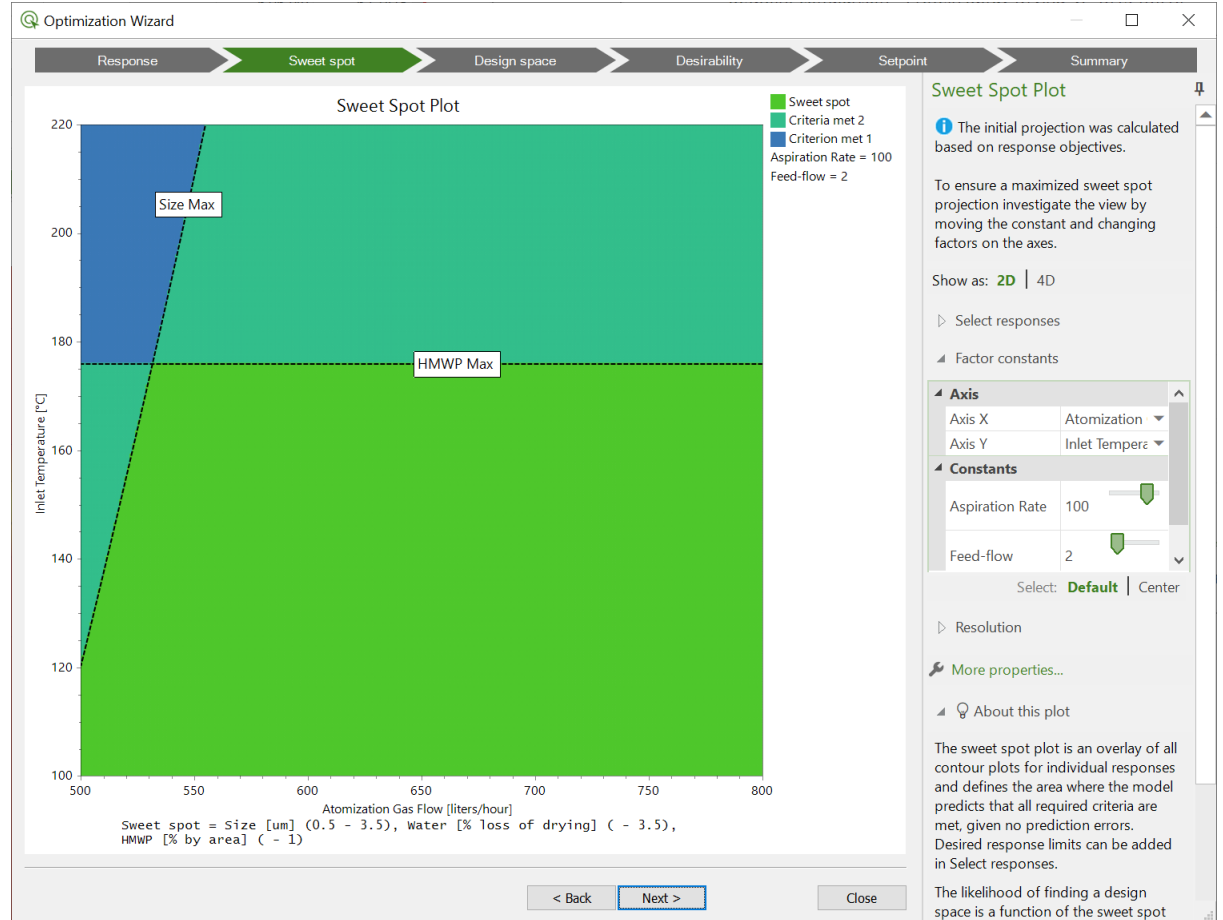
# Optimization Wizard – Design Space

- 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
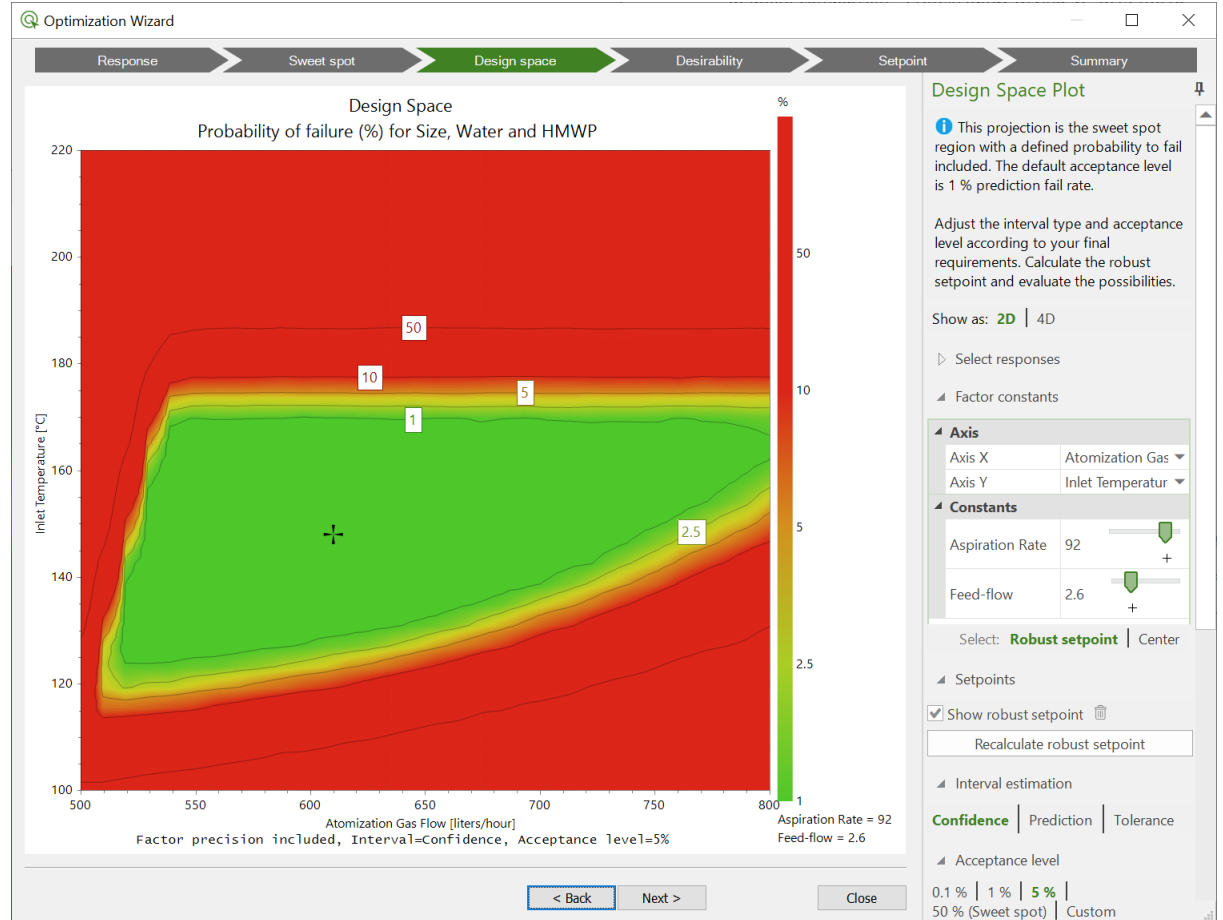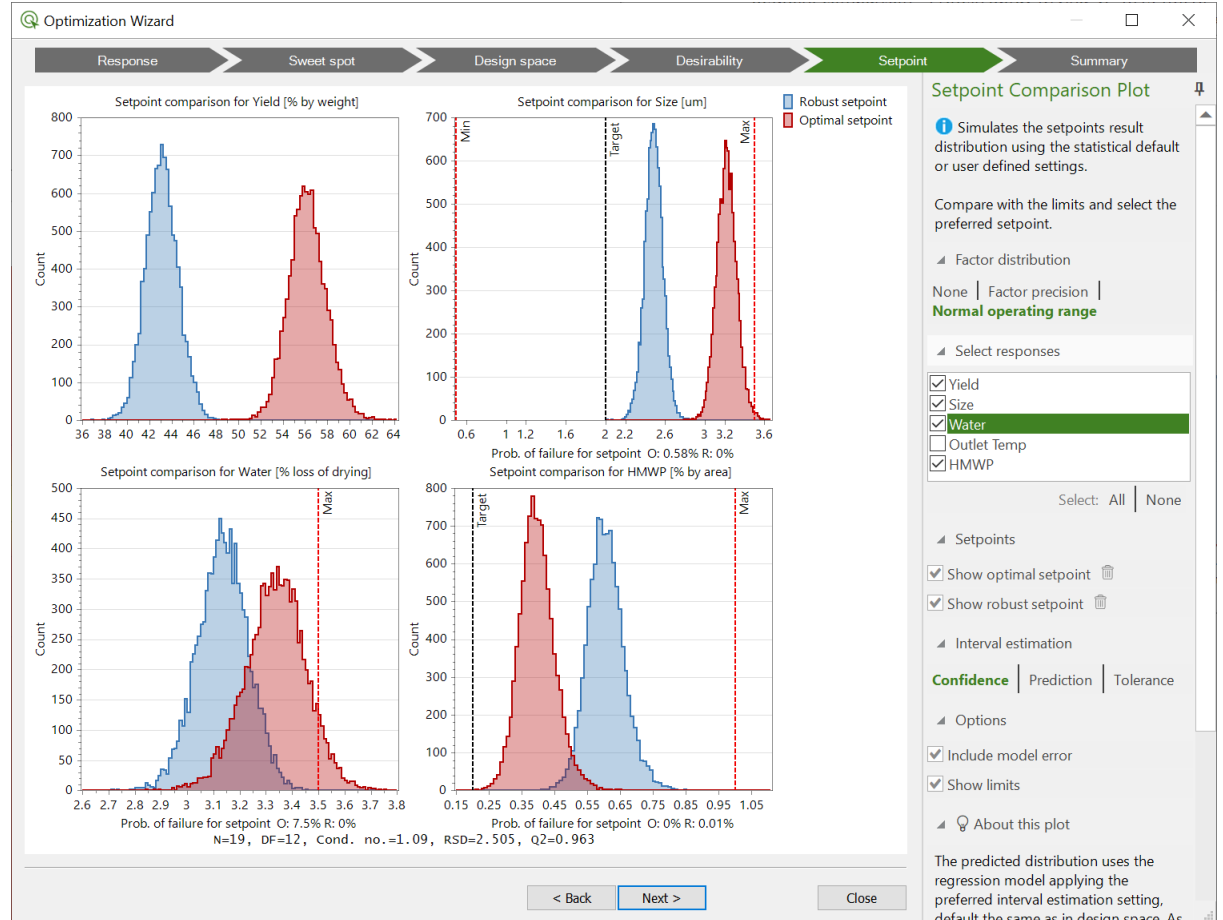
# Optimization Wizard – Desirability

- 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

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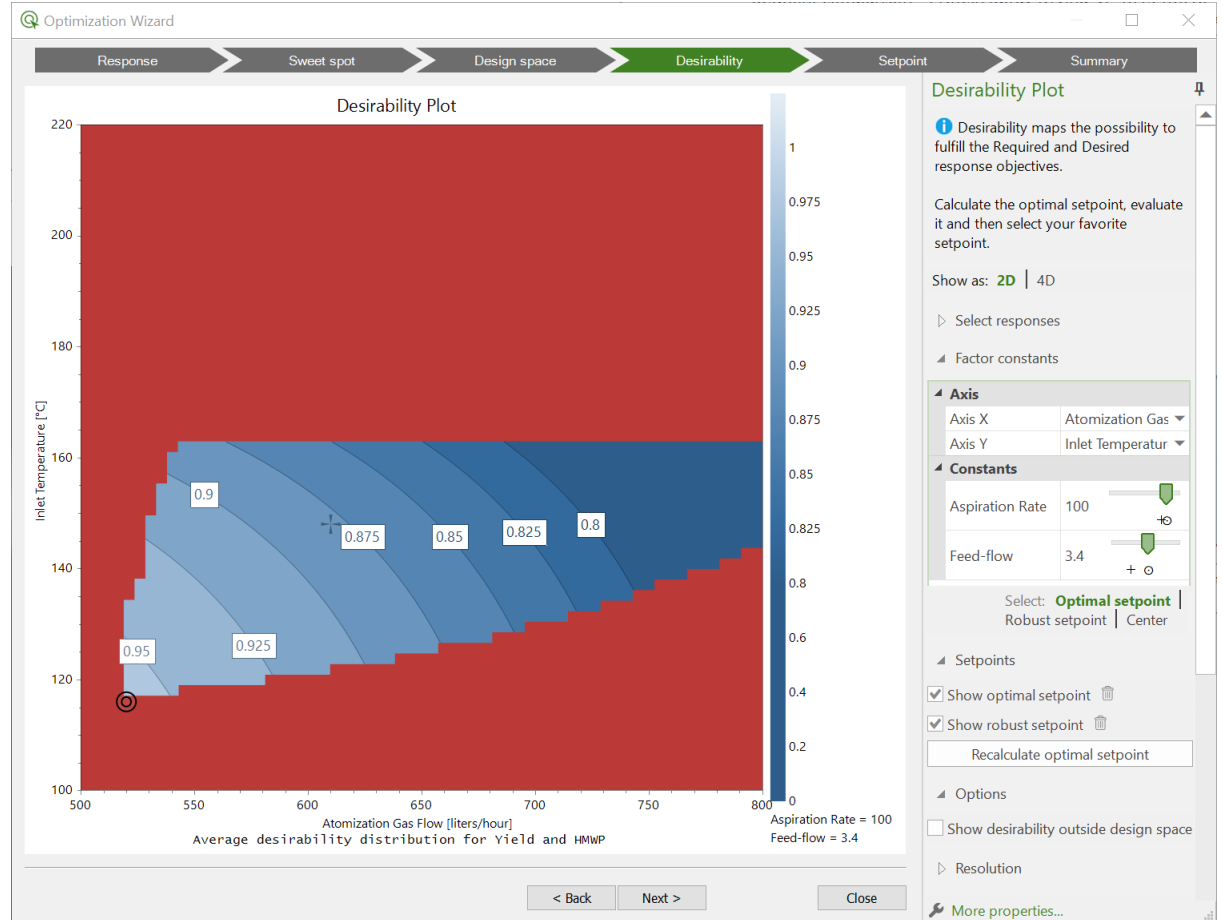
# Optimization Wizard – Setpoint Comparison

- 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

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MODDE® 13 What's New
Features and improvements

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# User interface

- Properties pane with most used settings
  - Available for all plots
  - Select or deselect responses
  - Select axis and adjust constants with slide bars
  - 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 design space plot with the current axis and constant settings

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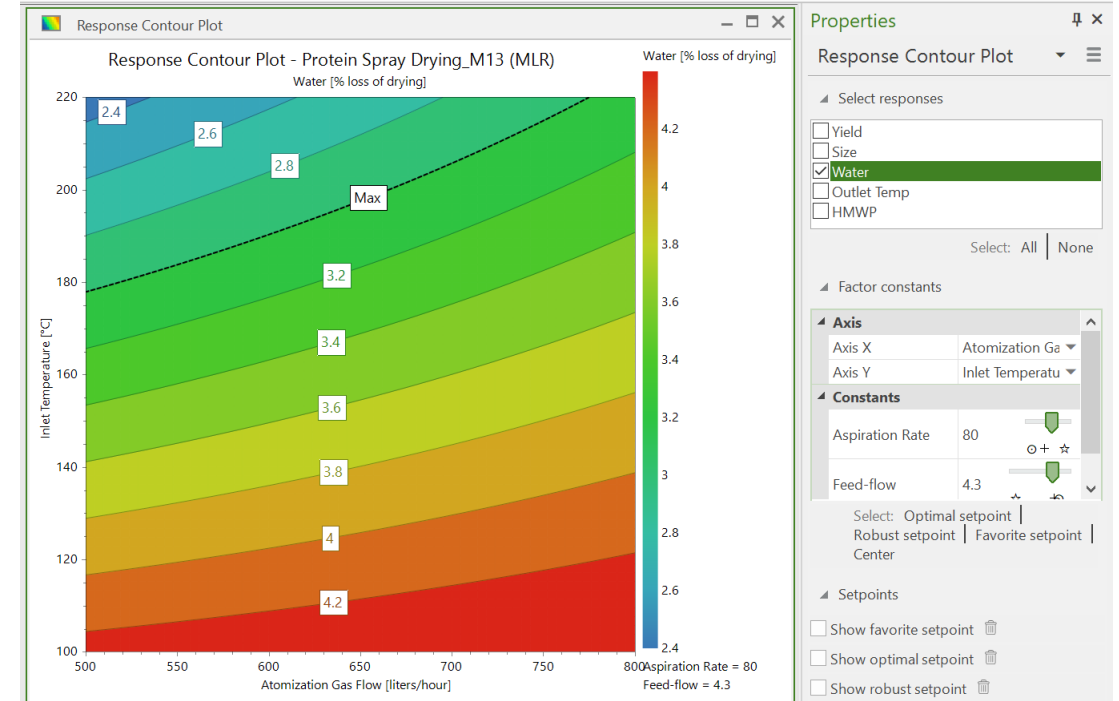
# Robust, Optimal, and Favorite setpoint

- MODDE® 13 has three different setpoints and can be used in all types of 2D and 4D contour 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

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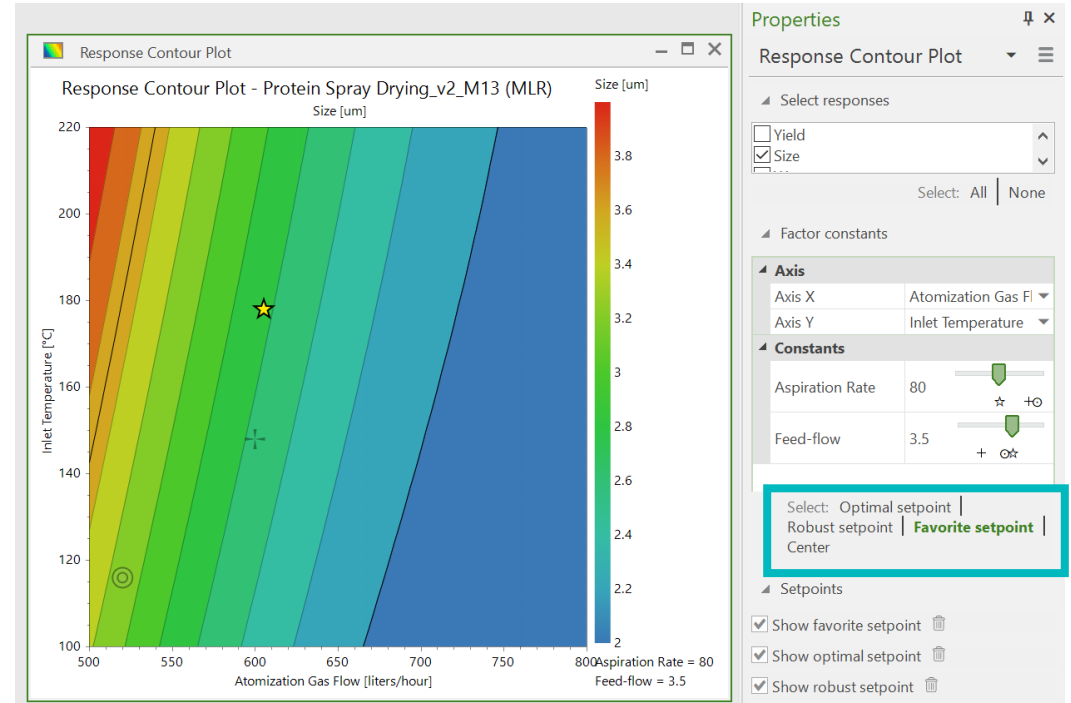
# Analysis Wizard

- 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

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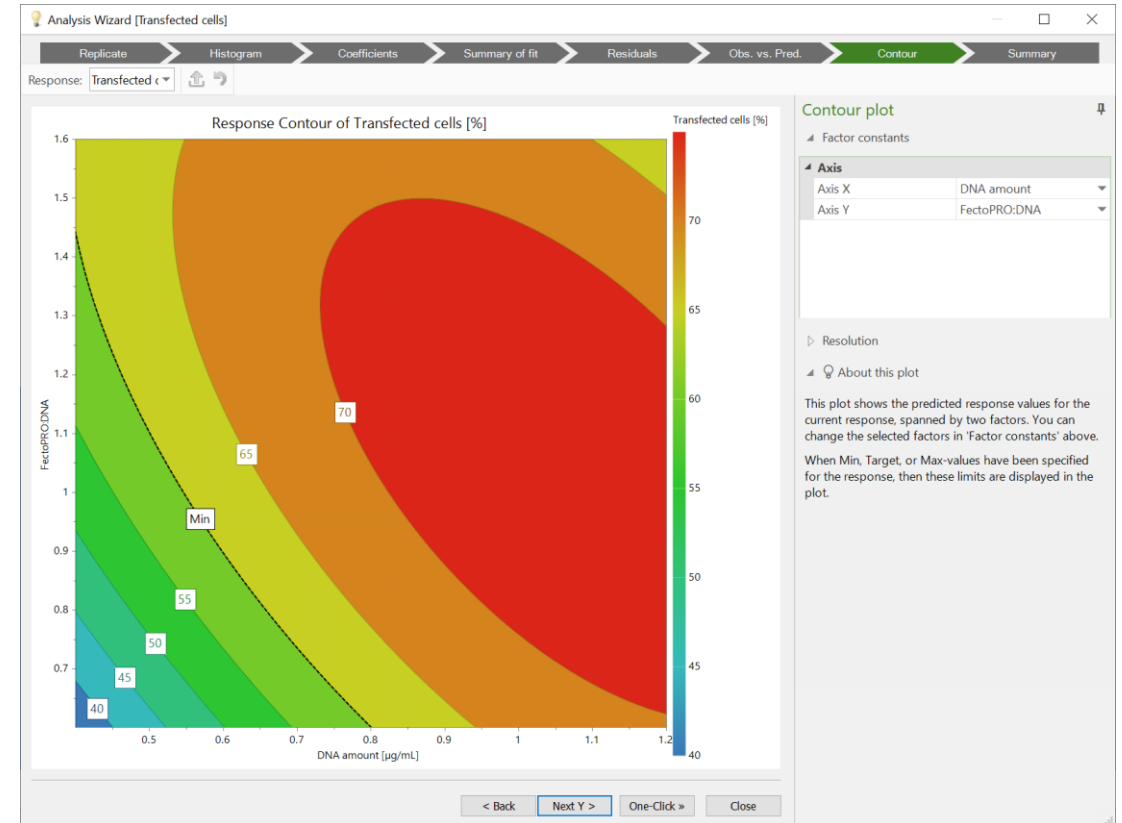
# Desirability plot

- 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
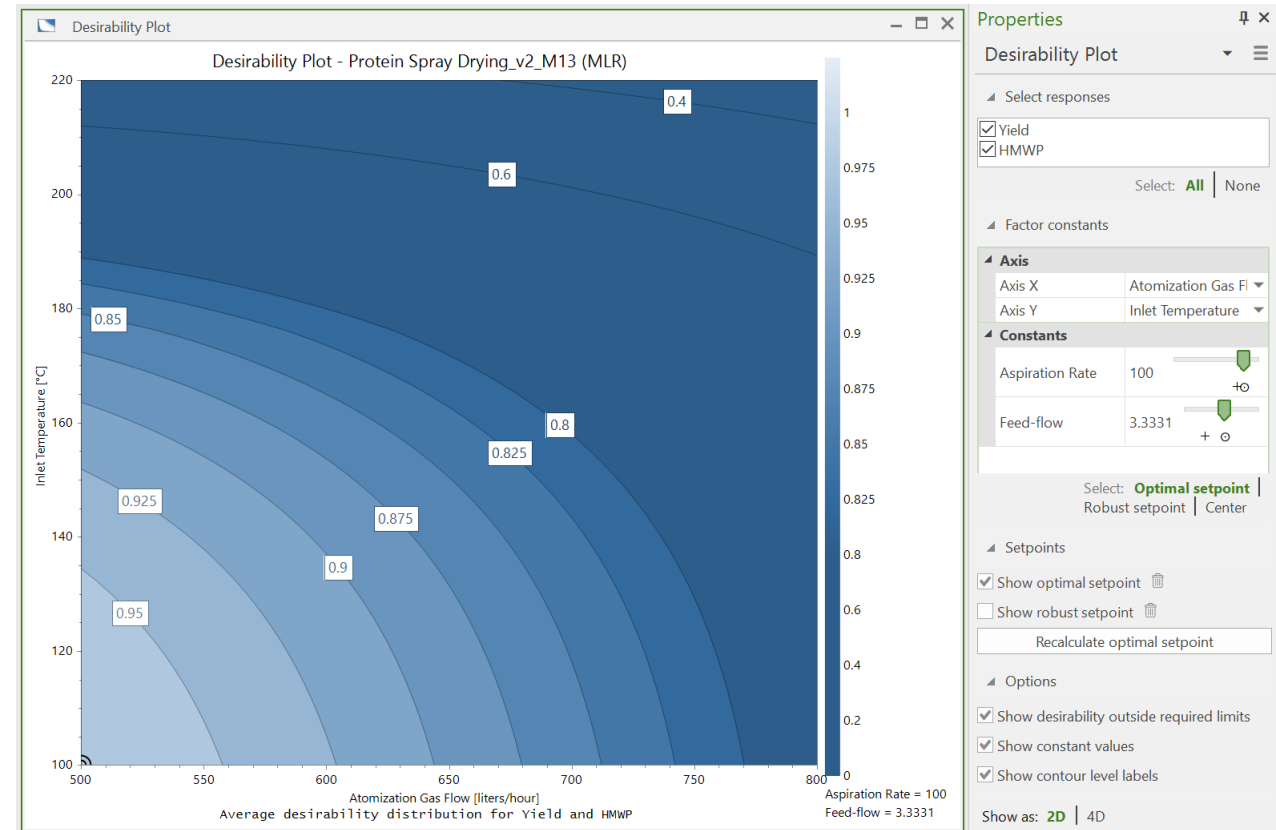
# Optimization within design space

- When a design space has been calculated, MODDE® can identify the factor combination with the 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.

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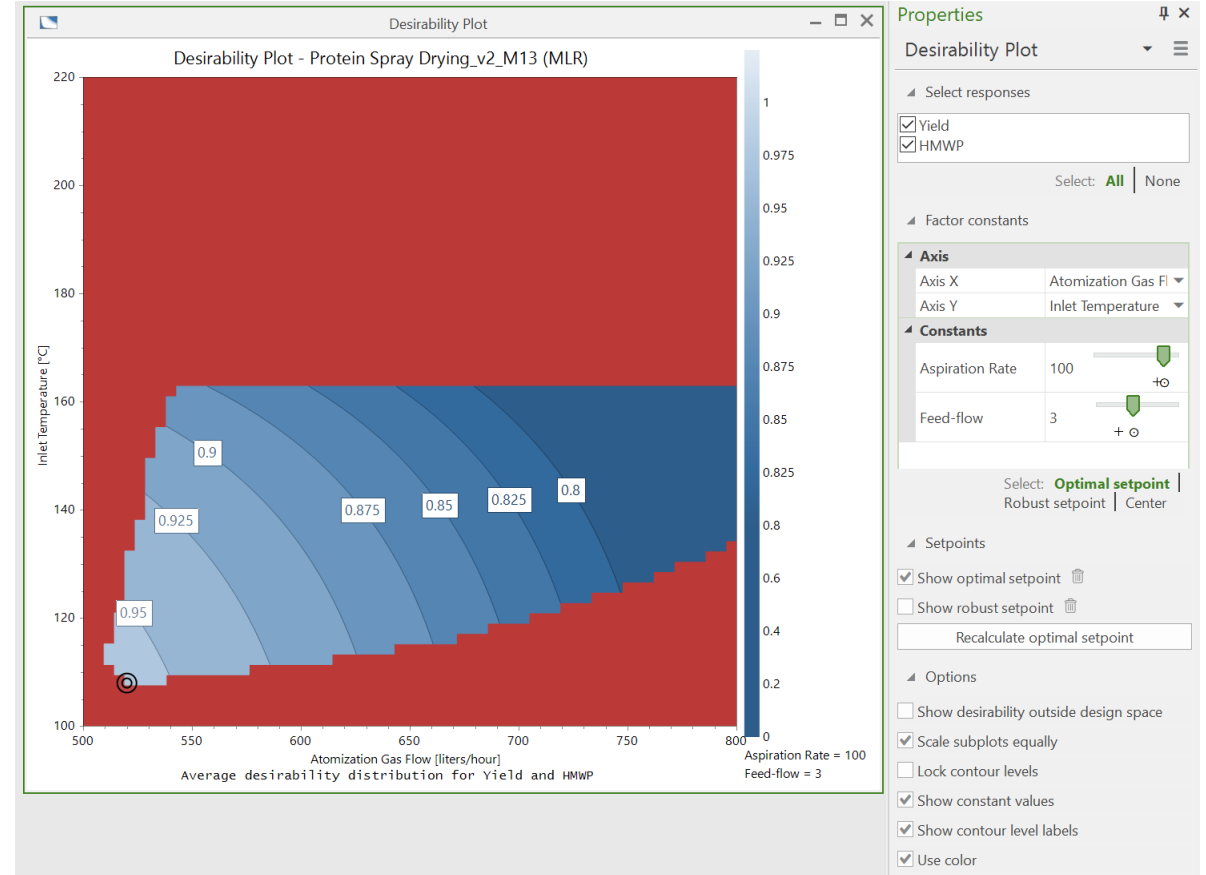
# Setpoint comparison

- 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 individual for each response are shown for selected setpoints

- Normal Operating Range, NOR, is the default setting
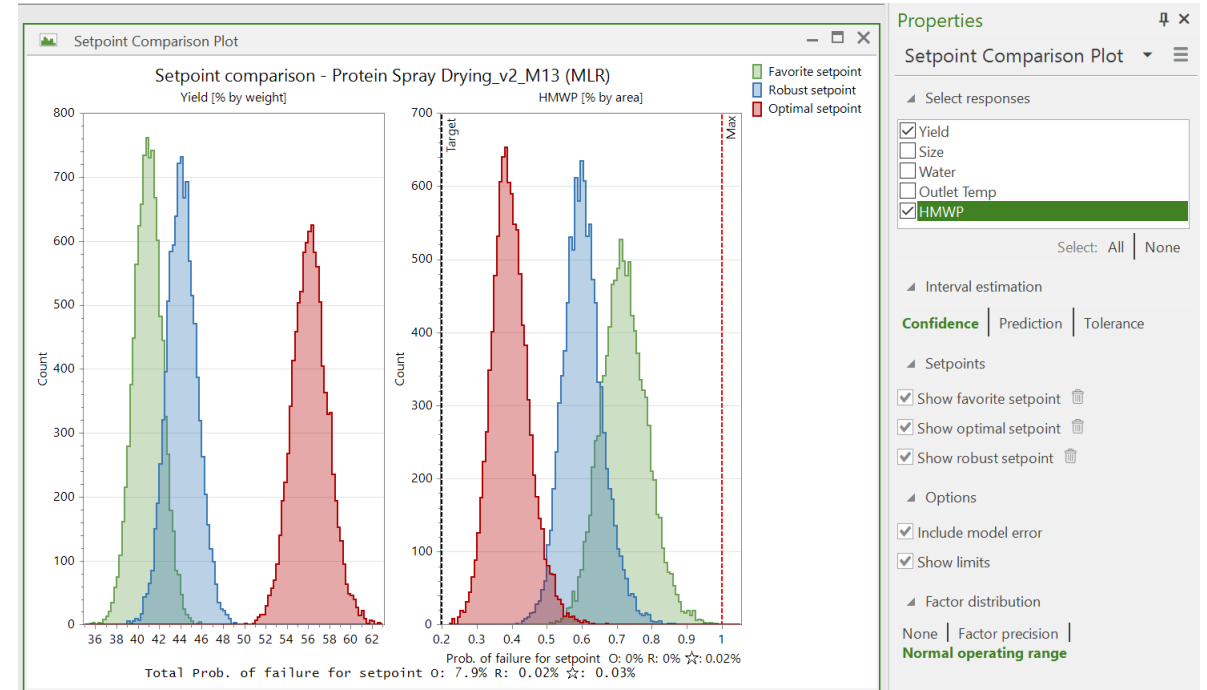
# Design Wizard – Detailed power in Responses definition dialog

- 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



Detailed Power ×
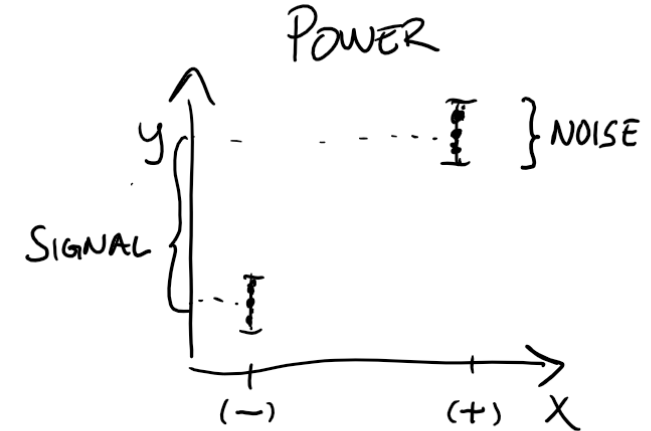
| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | Name | Unit | Signal to det | Noise/std. de | S/N ratio | Alpha level | L/h | ms | cm | L/h*ms | L/h*cm | ms*cm |
| 2 | Yeild | mg/l | 4 | 2 | 2 | 0.05 | 81.5326 | 81.5326 | 81.5326 | 81.5326 | 81.5326 | 81.5326 |
| 3 | Impurity | ug/L | 40 | 5 | 8 | 0.05 | 100 | 100 | 100 | 100 | 100 | 100 |

OK

# 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

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# Thank You for Your Interest in MODDE® 13

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

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