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Simplifying Progress

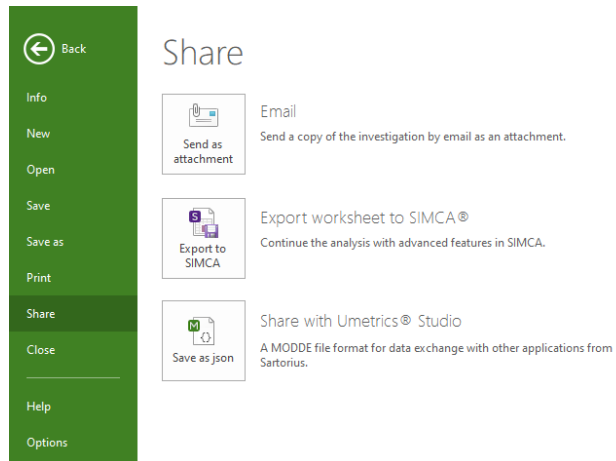
MODDE® 13 – What's New?

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

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

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.

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

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



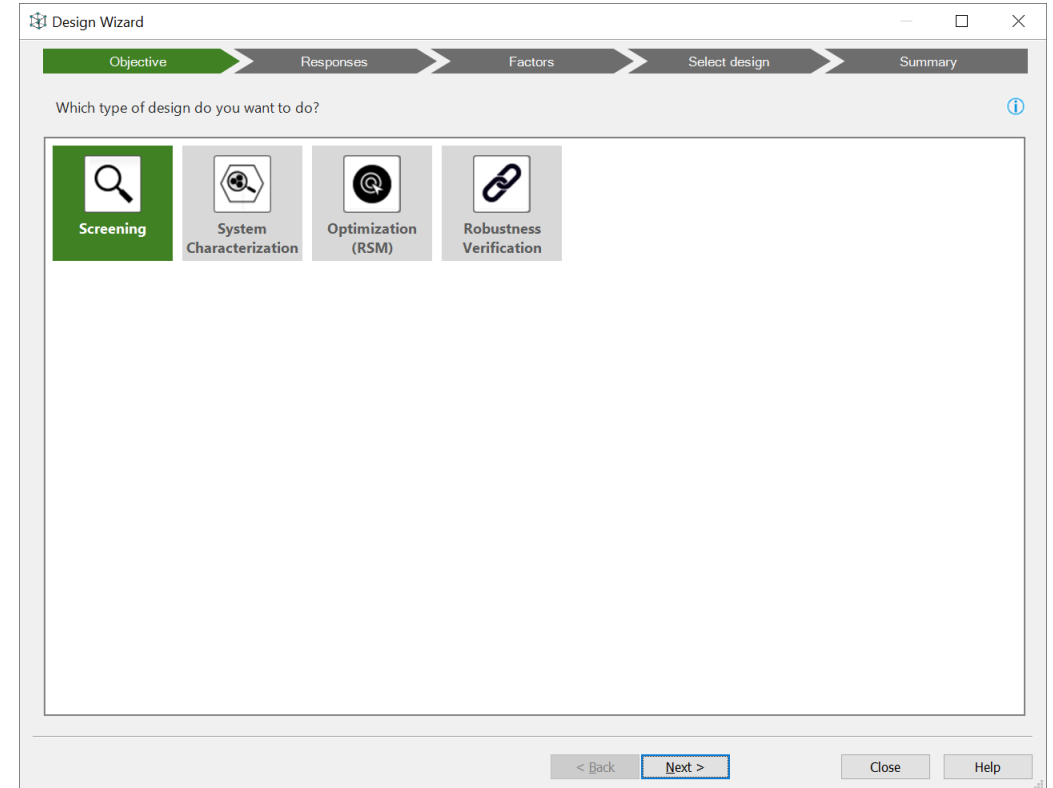
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MODDE® 13 What's New
Design Selection

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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

The screenshot shows the 'Design Wizard' software interface. The main window is titled 'Design Wizard' and has a progress bar with steps: Objective, Responses (highlighted), Factors, Select design, and Summary. Below the progress bar is a 'Define responses' dialog with a table of responses.

	Name	Abbreviation	Units	Condition	Objective	Min	Target	Max	Predicted min	Predicted max	R
1	Titer	Titer	mg/l	Required	Maximize	350	400		--	--	
2	VCC	VCC		Required	Maximize	4	4.5		--	--	
3	Viability	Via	%	Required	Maximize	70	100		--	--	
+	Add...										

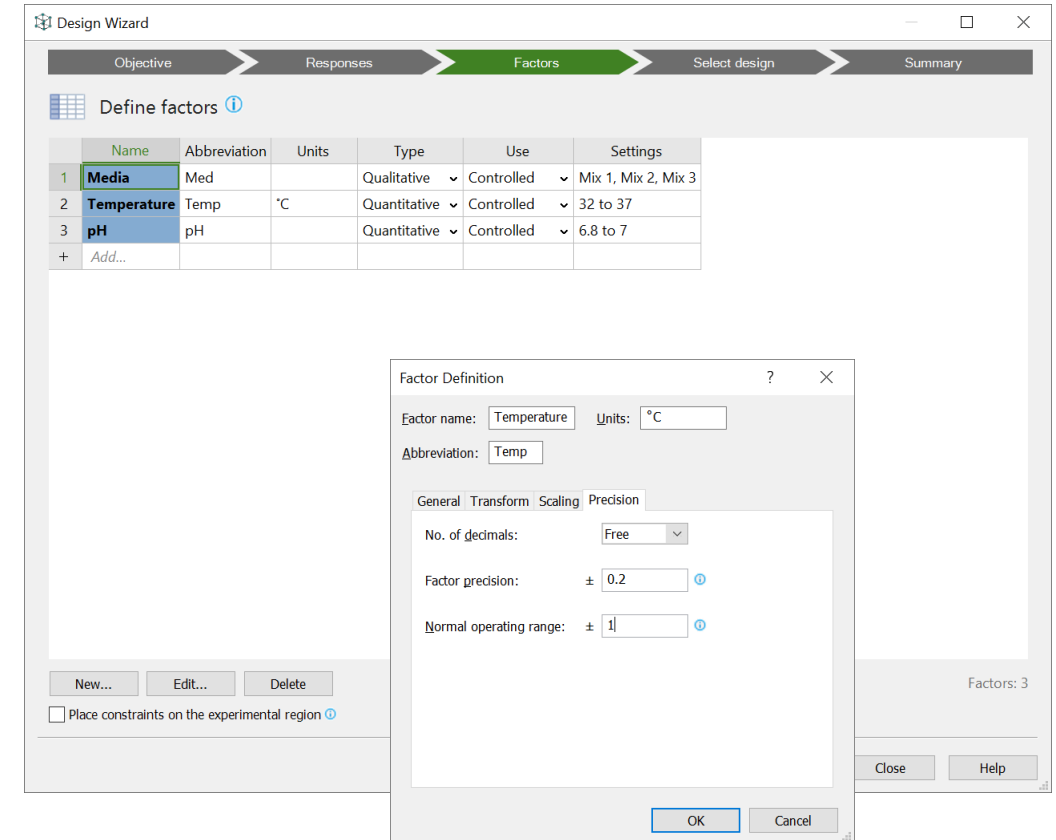
Below the table are buttons for 'New...', 'Edit...', and 'Delete'. A 'Response Definition' dialog box is open for the 'Titer' response. It contains the following fields:

- Response name: Titer
- Units: mg/l
- Abbreviation: Titer
- Settings: Power, Transform, Scaling
- Response type: Regular | Derived
- Response optimization settings:
 - Condition: Desired
 - Objective: Maximize
 - Min: 350
 - Target: 400
 - Max: (empty)

Buttons for 'OK' and 'Cancel' are at the bottom of the dialog.

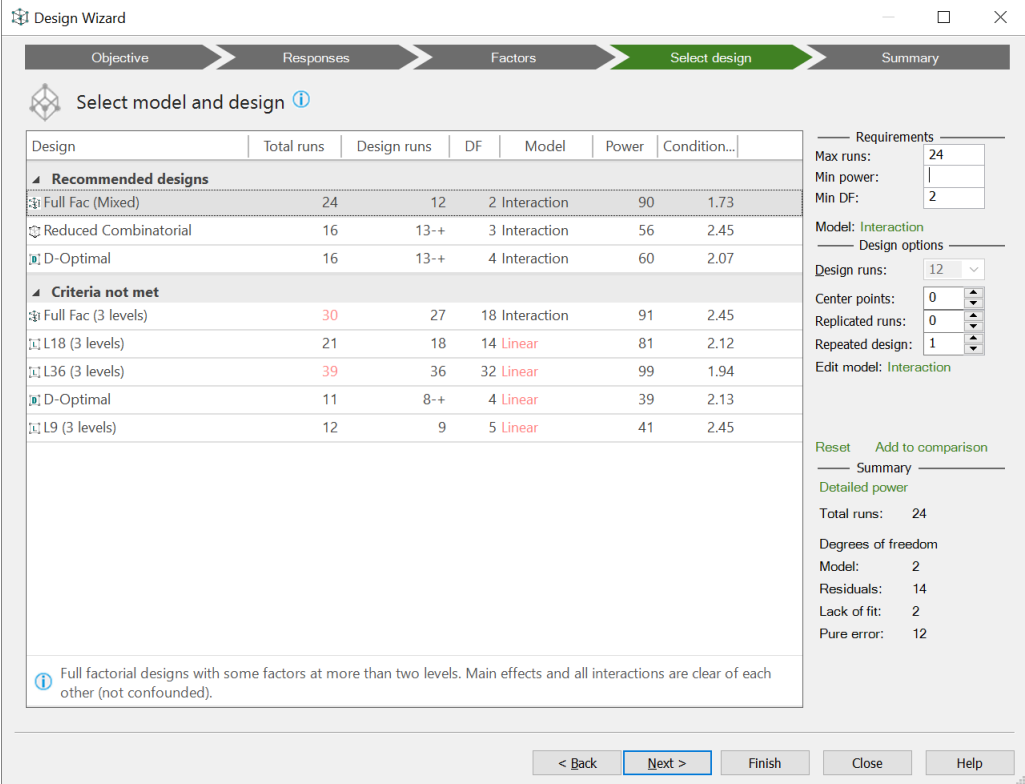
Design Wizard – Factor definition dialog

- 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



Design Wizard

Objective → Responses → Factors → **Select design** → Summary

Select model and design ⓘ

Design	Total runs	Design runs	DF	Model	Power	Condition...
Recommended designs						
Full Fac (Mixed)	24	12	2	Interaction	90	1.73
Reduced Combinatorial	16	13+	3	Interaction	56	2.45
D-Optimal	16	13+	4	Interaction	60	2.07
Criteria not met						
Full Fac (3 levels)	30	27	18	Interaction	91	2.45
L18 (3 levels)	21	18	14	Linear	81	2.12
L36 (3 levels)	39	36	32	Linear	99	1.94
D-Optimal	11	8+	4	Linear	39	2.13
L9 (3 levels)	12	9	5	Linear	41	2.45

Requirements

Max runs: 24
Min power: 1
Min DF: 2

Model: Interaction

Design options

Design runs: 12
Center points: 0
Replicated runs: 0
Repeated design: 1

Edit model: Interaction

Reset Add to comparison

Summary

Detailed power

Total runs: 24
Degrees of freedom: 2
Model: 2
Residuals: 14
Lack of fit: 2
Pure error: 12

Full factorial designs with some factors at more than two levels. Main effects and all interactions are clear of each other (not confounded).

< Back Next > Finish Close Help



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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.

	Name	Condition	Objective	Min	Target	Max	Predicted min	Predicted max	Response range	Desirability type	Desirability weight
1	Yield	Desired	Maximize	6.06249	62.1875		6.06249	62.1875		Target	1
2	Size	Required	Inside	0.5	2	3.5	1.55024	4.25312		Limit	1
3	Water	Required	Inside			3.5	2.01118	4.98619		Limit	1
4	Outlet Temp	Observed	Predicted				50.7698	146.27		Limit	1
5	HMWP	Required	Minimize		0.2	1	0.306471	1.98813		Target	1

Review response settings

The optimization wizard result depends on how well the Condition and Objective specifications match the predicted min and max ranges for each response.

About this list

Compare your specified Min and Max with the predicted min and predicted max. The predicted values are the minimal and maximum values that can be achieved by the respective models.

The likelihood of finding a design space increases when there is a big overlap of the desired range (difference Max - Min) and the achievable values (difference Predicted max - Predicted min).

The response range column is the graphical representation of the relation between specified Min, Max and Predicted min, Predicted max. The white area represents the overlap, the larger the better.

Condition

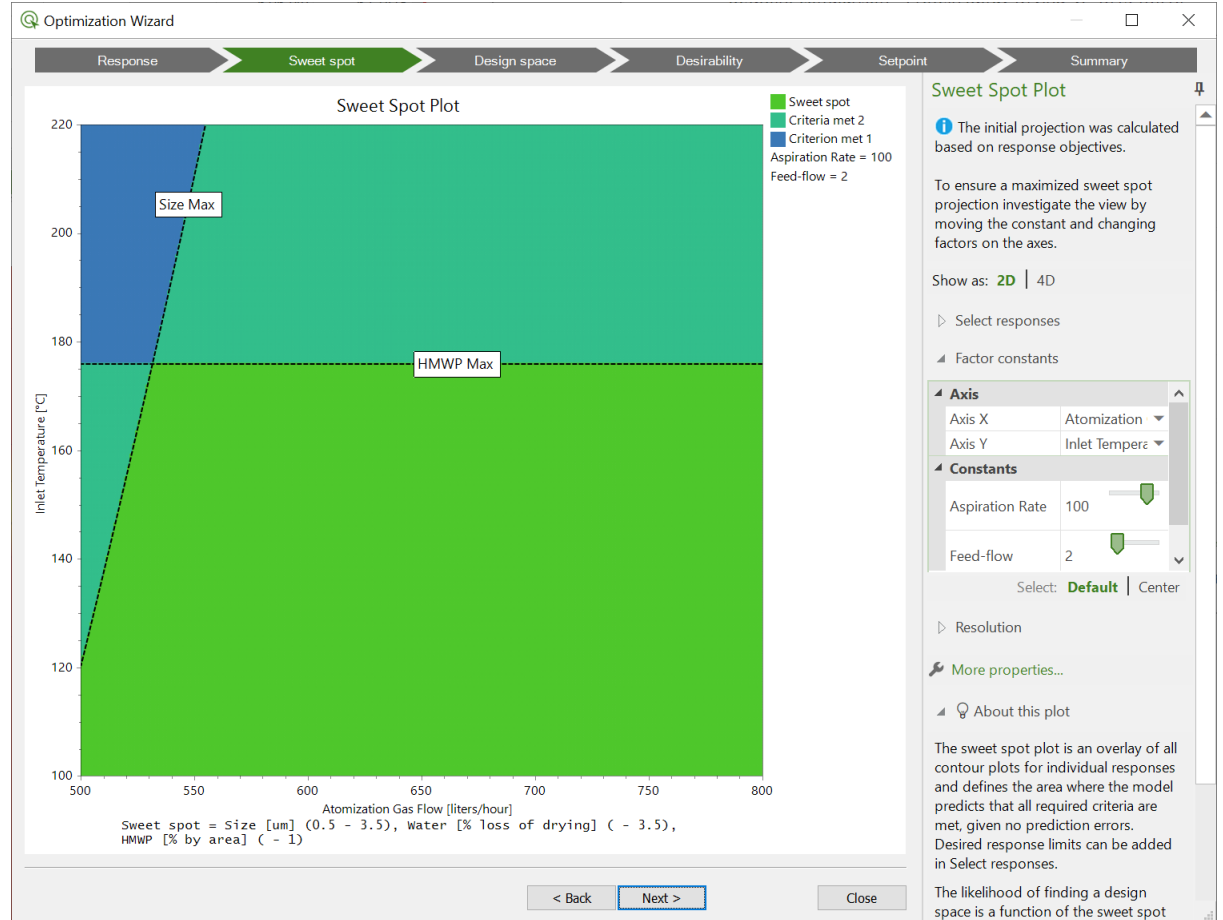
- Required responses are hard conditions. Only required responses are considered in the Sweet spot and Design space plots.
- Desired responses are wishes. Desired and required responses are used in the desirability calculations, and in calculation of optimal setpoints.
- Observed responses are predicted but do not influence desirability, design space or optimization calculations.

Objective

- Minimize, Maximize and Target

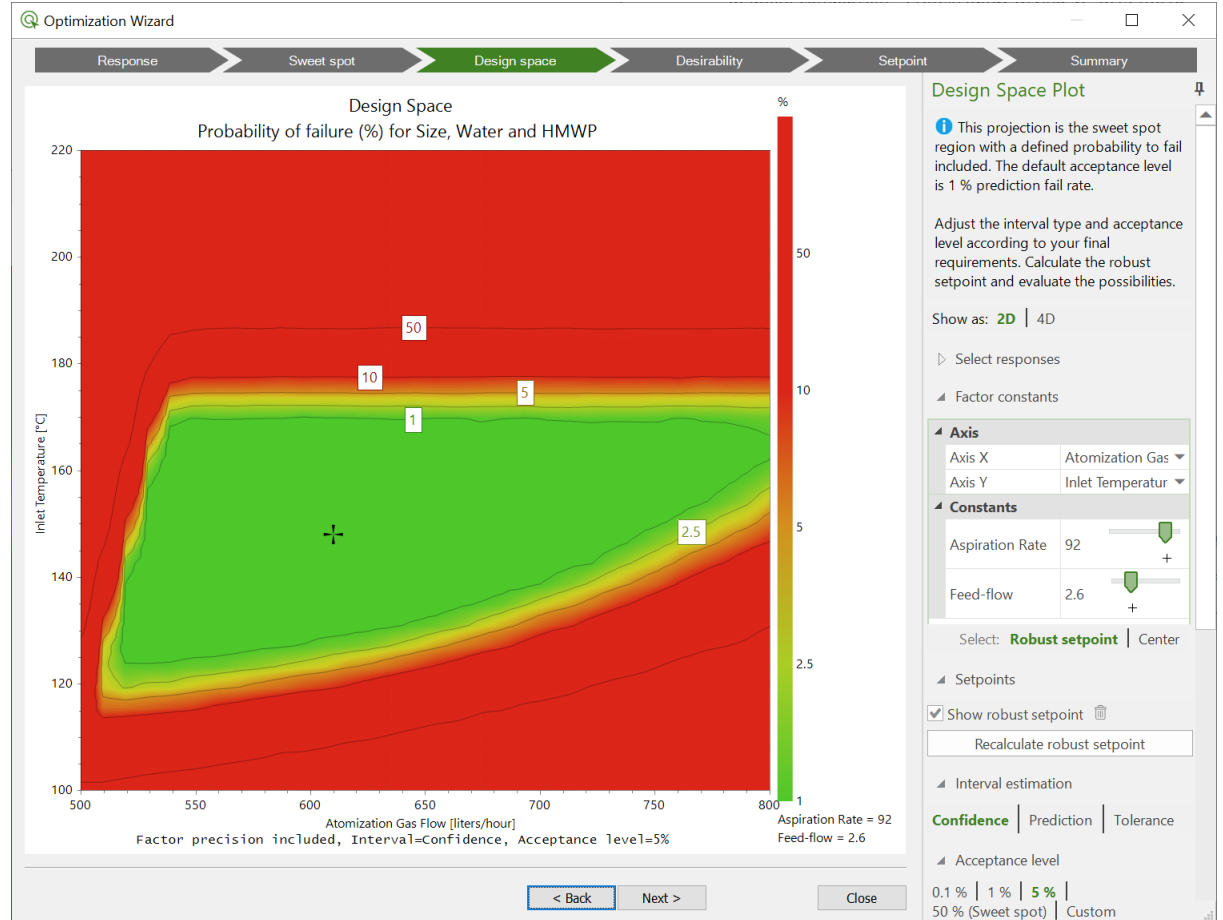
Optimization Wizard – Sweet spot

- 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



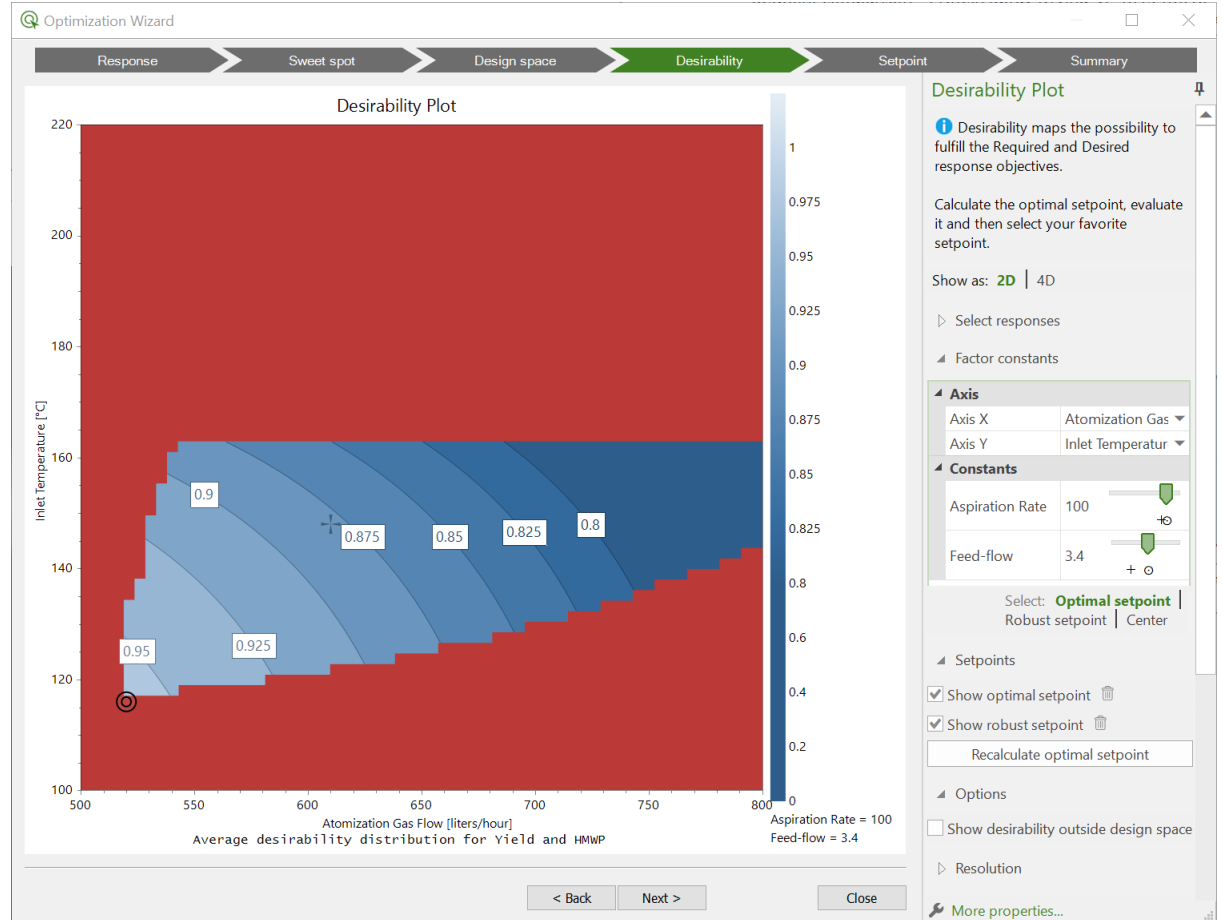
Optimization Wizard – Design Space

- 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



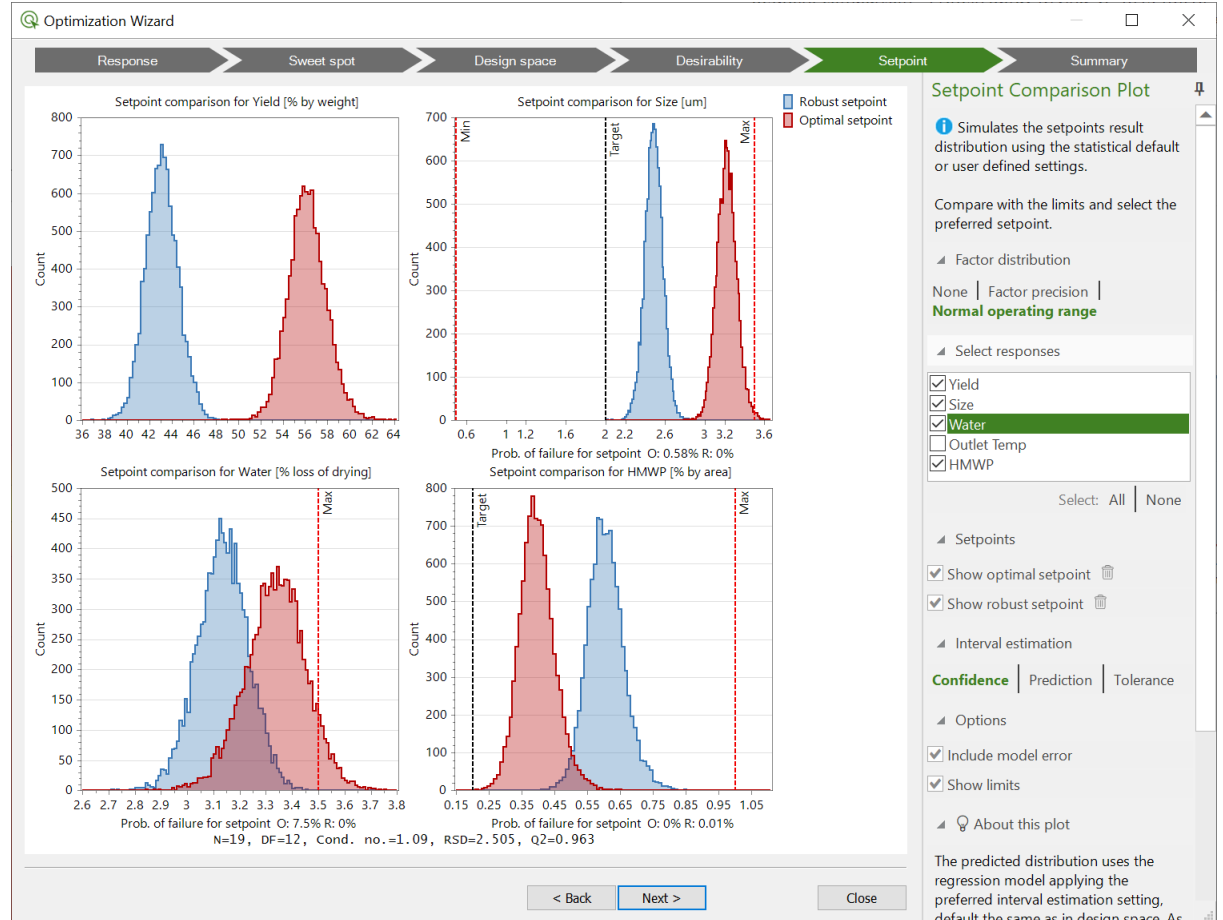
Optimization Wizard – Desirability

- 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



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

The screenshot shows the 'Summary' step of the Optimization Wizard. It displays two main sections: 'Optimal setpoint' and 'Robust setpoint'. Each section includes a table of response characteristics and a table of factor settings. The 'Optimal setpoint' section shows a 4.8% probability of failure, while the 'Robust setpoint' section shows a 0.005% probability of failure. The bottom of the window features navigation buttons: '< Back', 'Next >', 'Finish', and 'Close'.

Optimal setpoint
Probability of failure: 4.8% (interval: Confidence)

Response	Value	Unit	Prob.of failure	Cpk
Yield	56.196	% by weight		--
Size	3.220	um	0.16%	1.081
Water	3.338	% loss of drying	4.7%	0.550
Outlet Temp	79.170	°C		--
HMWP	0.393	% by area	0%	3.689

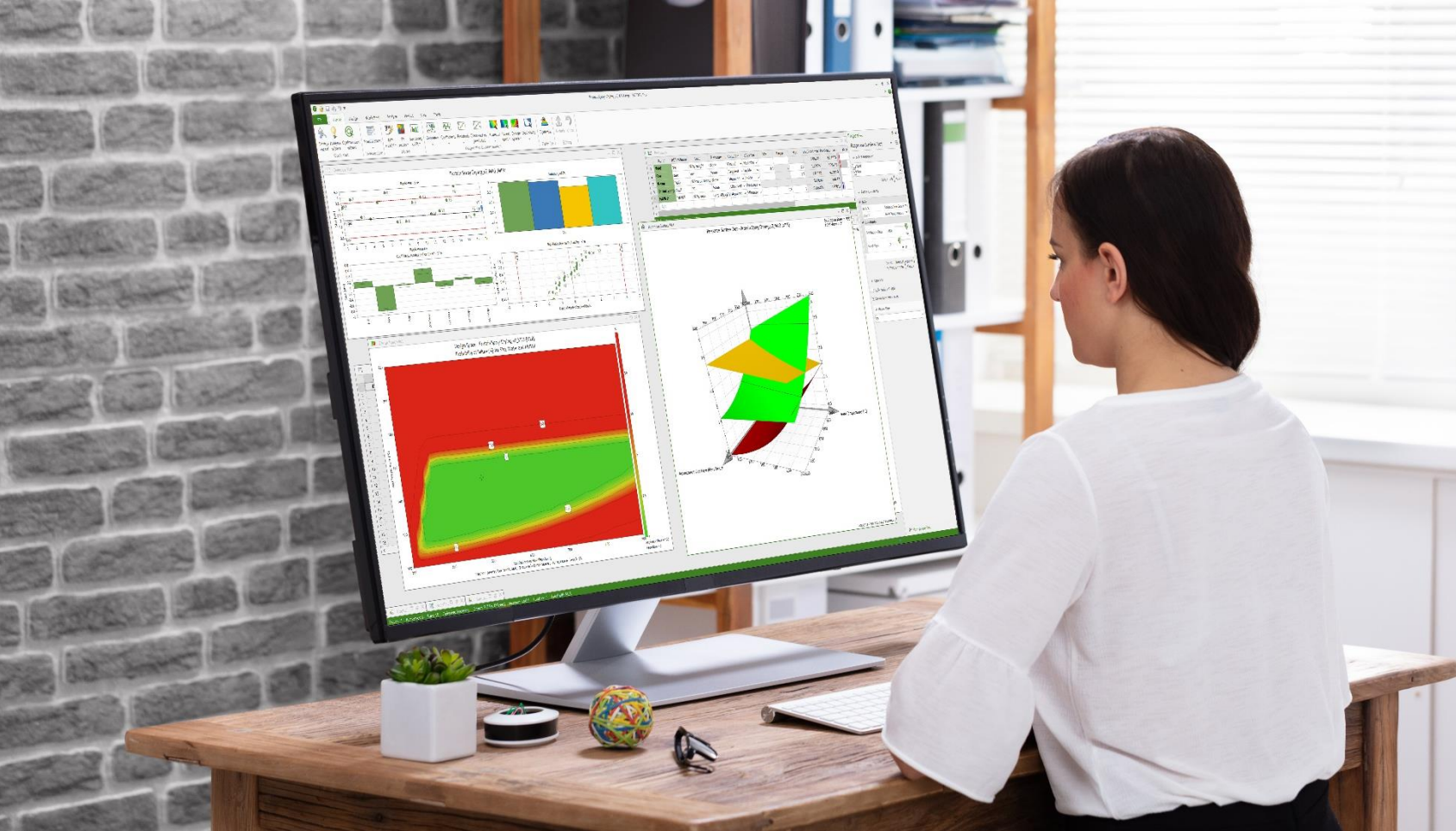
Factor	Value	Unit
Inlet Temperature	116.000	°C
Atomization Gas Flow	520.000	liters/hour
Aspiration Rate	100.000	%
Feed-flow	3.400	ml/min

Robust setpoint
Probability of failure: 0.005% (interval: Confidence)

Response	Value	Unit	Prob.of failure	Cpk
Yield	43.146	% by weight		--
Size	2.487	um	0%	4.008
Water	3.136	% loss of drying	0.005%	1.740
Outlet Temp	97.540	°C		--
HMWP	0.603	% by area	0%	2.401

Factor	Value	Unit	Robust low edge	Robust high edge	Hypercube low edge	Hypercube high edge
Inlet Temperature	148.000	°C	124.000	172.000	140.000	164.000
Atomization Gas Flow	610.000	liters/hour	540.000	780.000	540.000	640.000
Aspiration Rate	92.000	%	84.000	100.000	89.333	97.333
Feed-flow	2.600	ml/min	2.000	4.000	2.000	3.000

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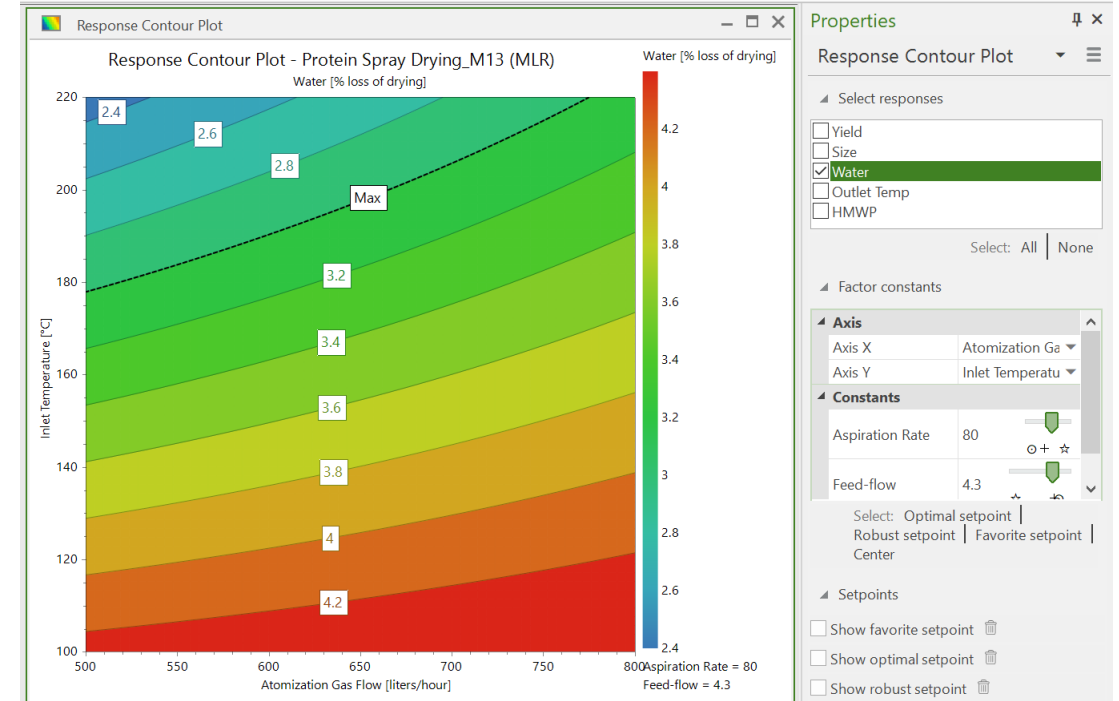


MODDE® 13 What's New
Features and improvements

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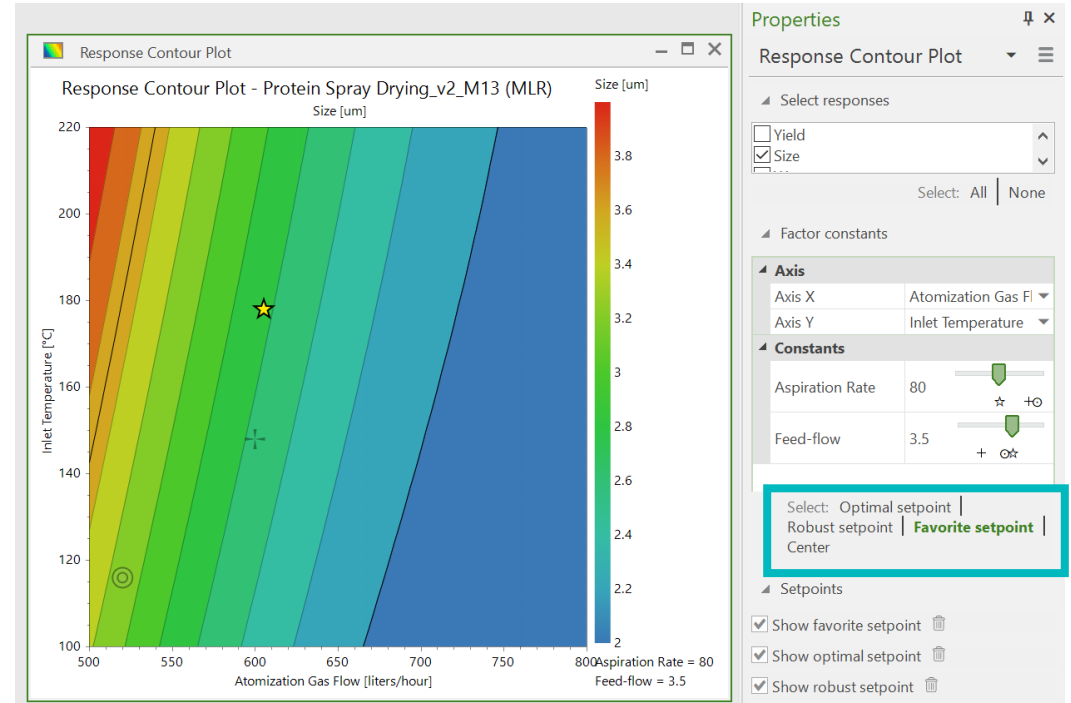
User interface

- 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



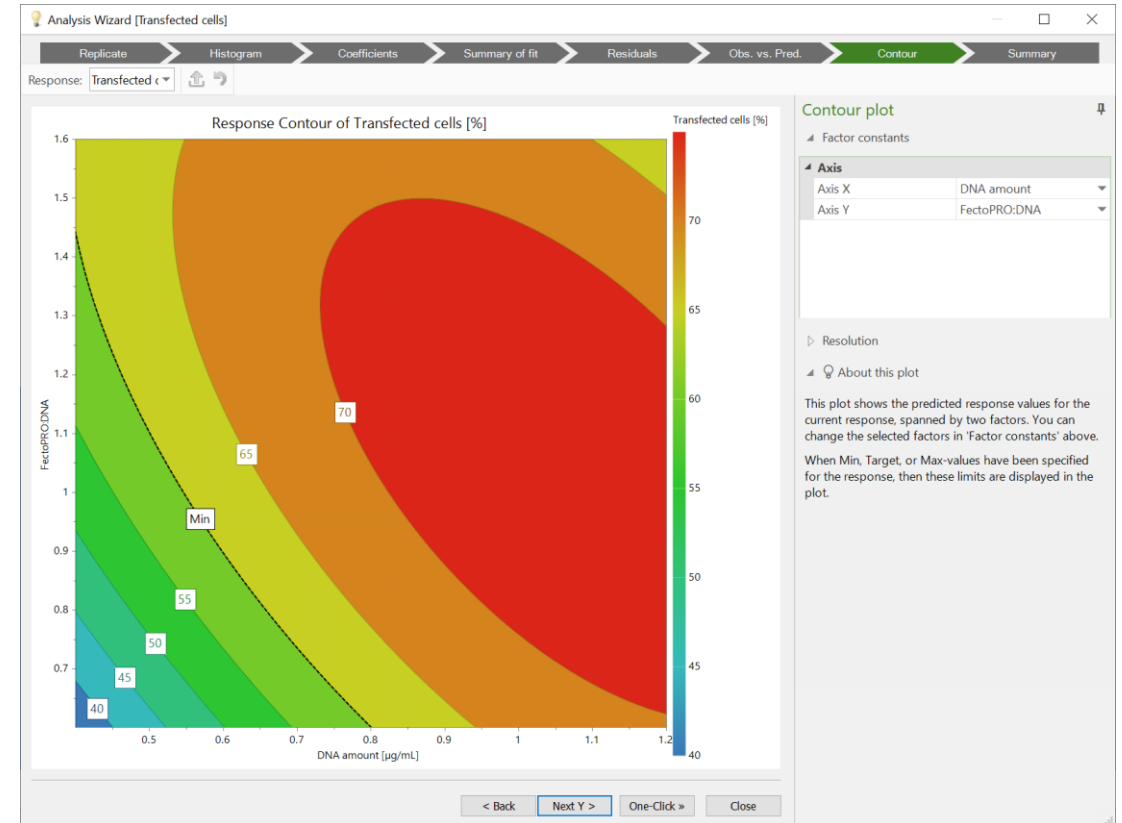
Robust, Optimal, and Favorite setpoint

- 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



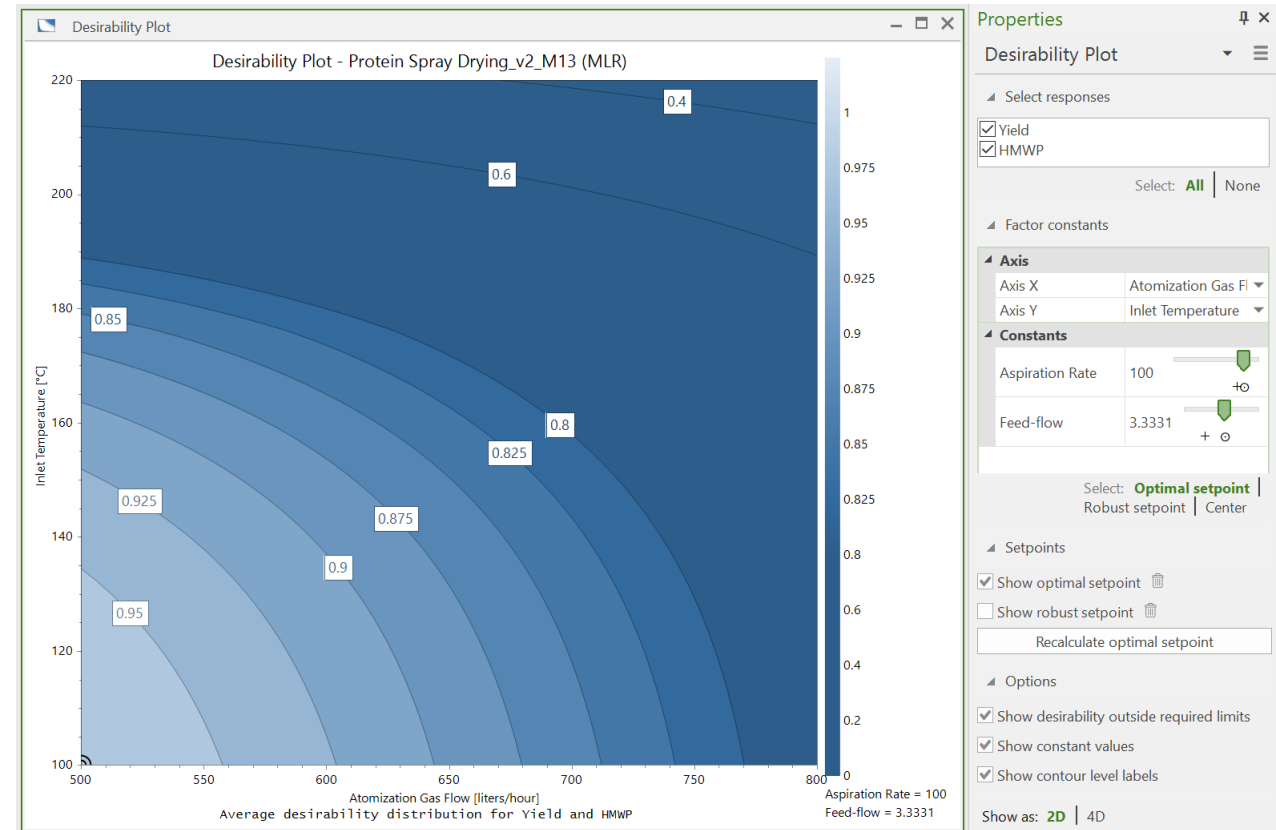
Analysis Wizard

- 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



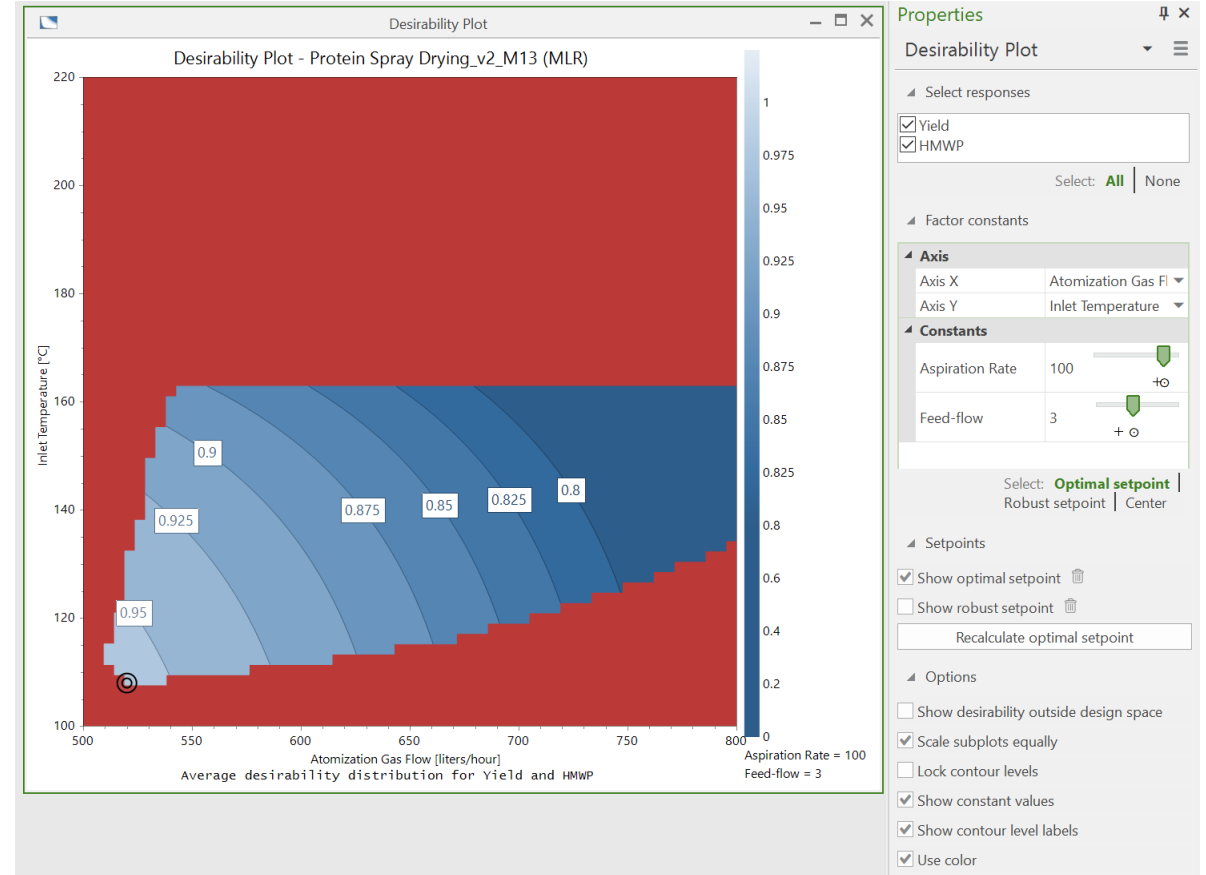
Desirability plot

- 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



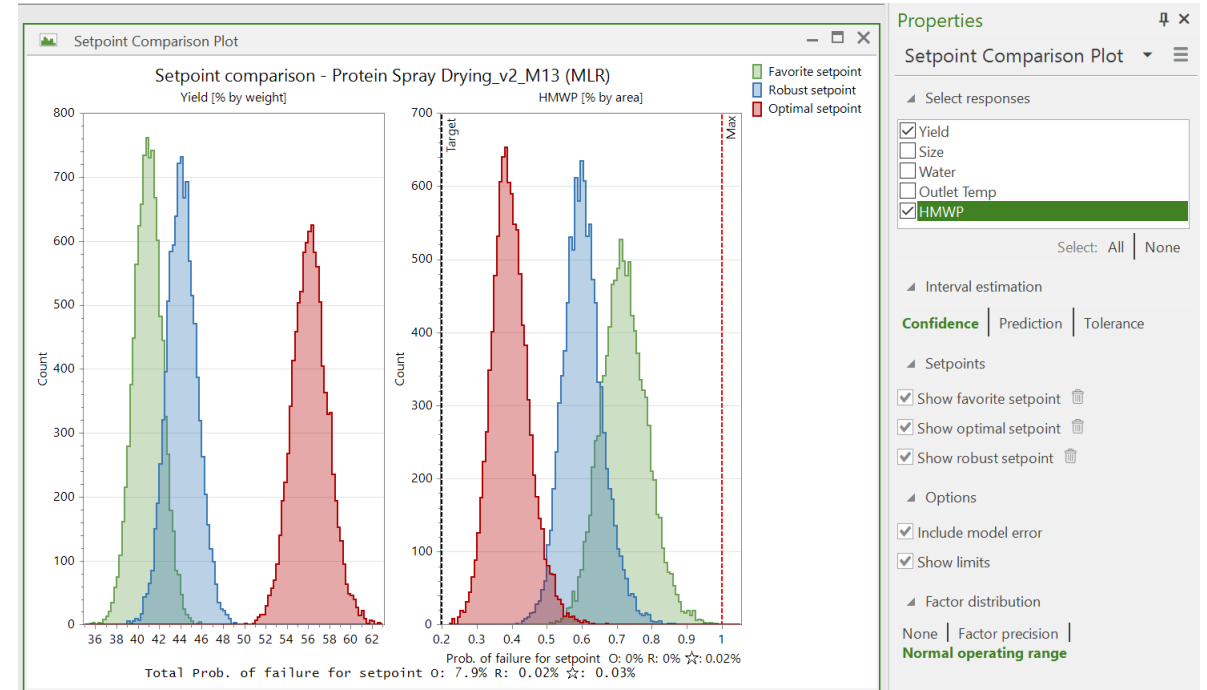
Optimization within design space

- 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.



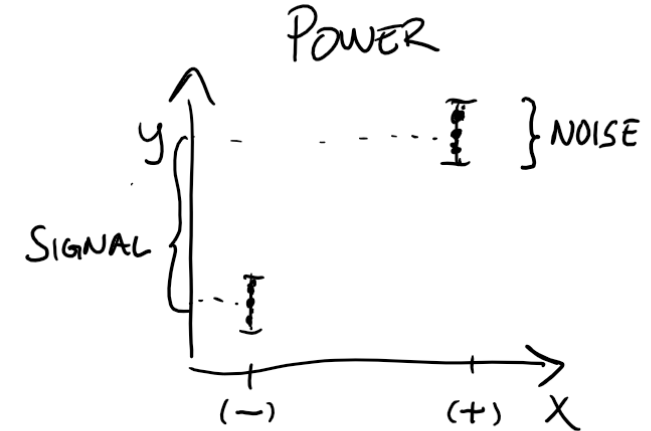
Setpoint comparison

- 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



	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

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

The screenshot shows the 'Design Wizard' software interface. The main window is titled 'Design Wizard' and has a progress bar at the top with steps: Objective, Responses, Factors, Select design (highlighted), and Summary. Below the progress bar is a 'Select model and design' section. A table lists various design options with columns for Design, Total runs, Design runs, DF, Model, Power, and Condition num... The table is divided into 'Compare designs' and 'Criteria not met' sections. The 'Compare designs' section includes 'Full Fac (2 levels)' designs with 22, 15, and 11 total runs. The 'Criteria not met' section includes designs like 'L18 (3 levels)', 'Plackett Burman', 'D-Optimal', 'L9 (3 levels)', 'Full Fac (2 levels)', 'D-Optimal', 'Rechtschaffner Res V', 'Frac Fac Res III', and 'L36 (3 levels)'. The 'Power' column shows values ranging from 29 to 100. On the right side, there are 'Requirements' and 'Design options' panels. The 'Requirements' panel shows 'Max runs: 80' and 'Min DF: 1'. The 'Design options' panel shows 'Design runs: 8', 'Center points: 3', 'Replicated runs: 4', and 'Repeated design: 0'. At the bottom, there are navigation buttons: '< Back', 'Next >', 'Finish', 'Close', and 'Help'.

Design	Total runs	Design runs	DF	Model	Power	Condition num...
Compare designs						
Full Fac (2 levels)	22	8	2	Interaction	96	1.17 Remove
Full Fac (2 levels)	15	8	2	Interaction	82	1.41 Remove
Full Fac (2 levels)	11	8	2	Interaction	57	1.17 Remove
Criteria not met						
L18 (3 levels)	21	18	15	Linear	90	1.32
Plackett Burman	11	8+	5	Linear	68	1.17
D-Optimal	13	10+	4	Interaction	66	1.32
L9 (3 levels)	12	9	6	Linear	58	1.41
Full Fac (2 levels)	11	8	2	Interaction	57	1.17
D-Optimal	10	7+	4	Linear	57	1.54
Rechtschaffner Res V	10	7	1	Interaction	32	2.86
Frac Fac Res III	7	4	1	Linear	29	1.32
L36 (3 levels)	39	36	33	Linear	100	1.27

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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