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Simplifying Progress

MODDE® 13 Release Letter

Henrik Widmark, March 2, 2021



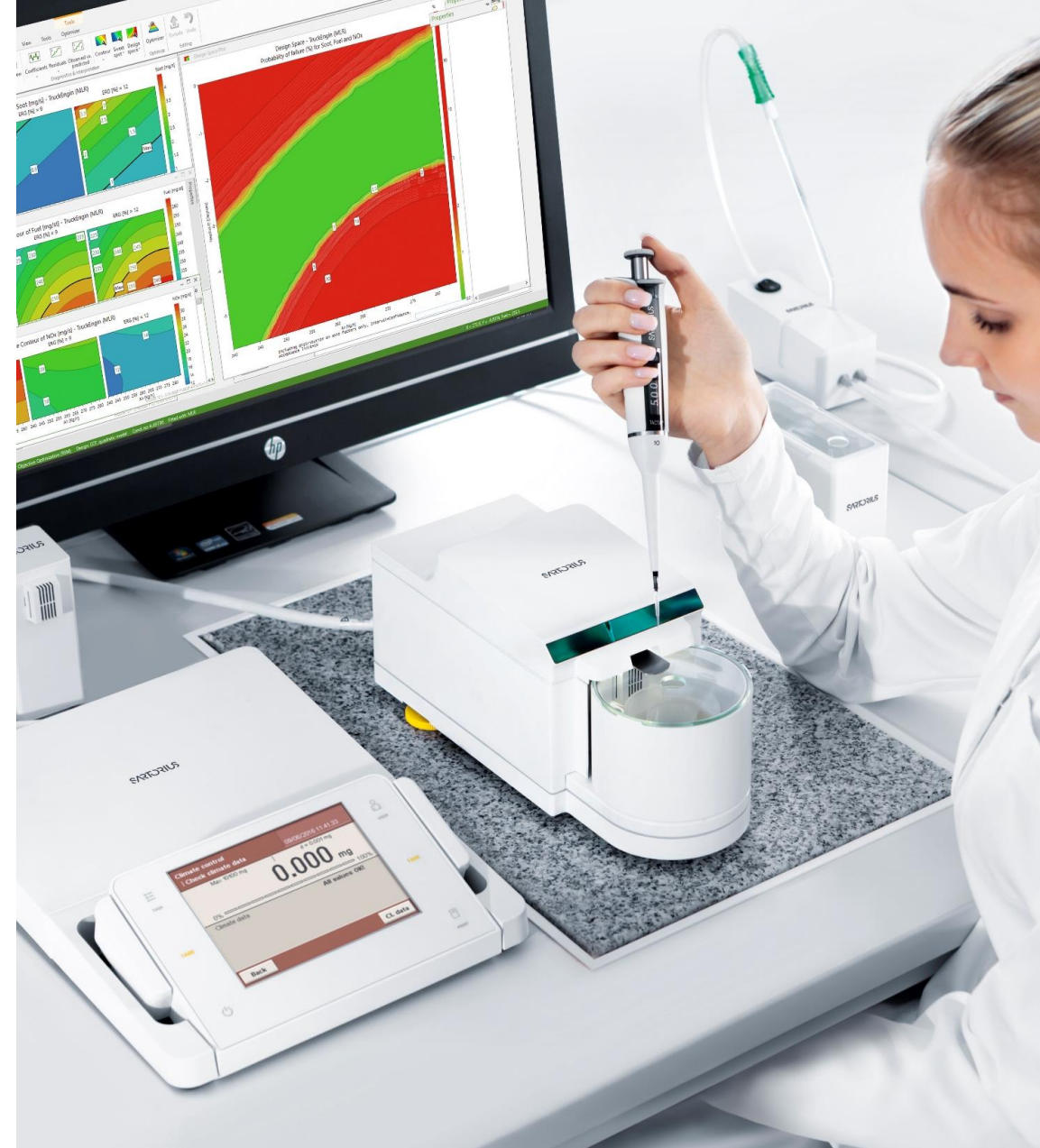
Content

MODDE 13 – Optimization in focus

Resources

Courses

What's New



MODDE® 13 targeting optimization

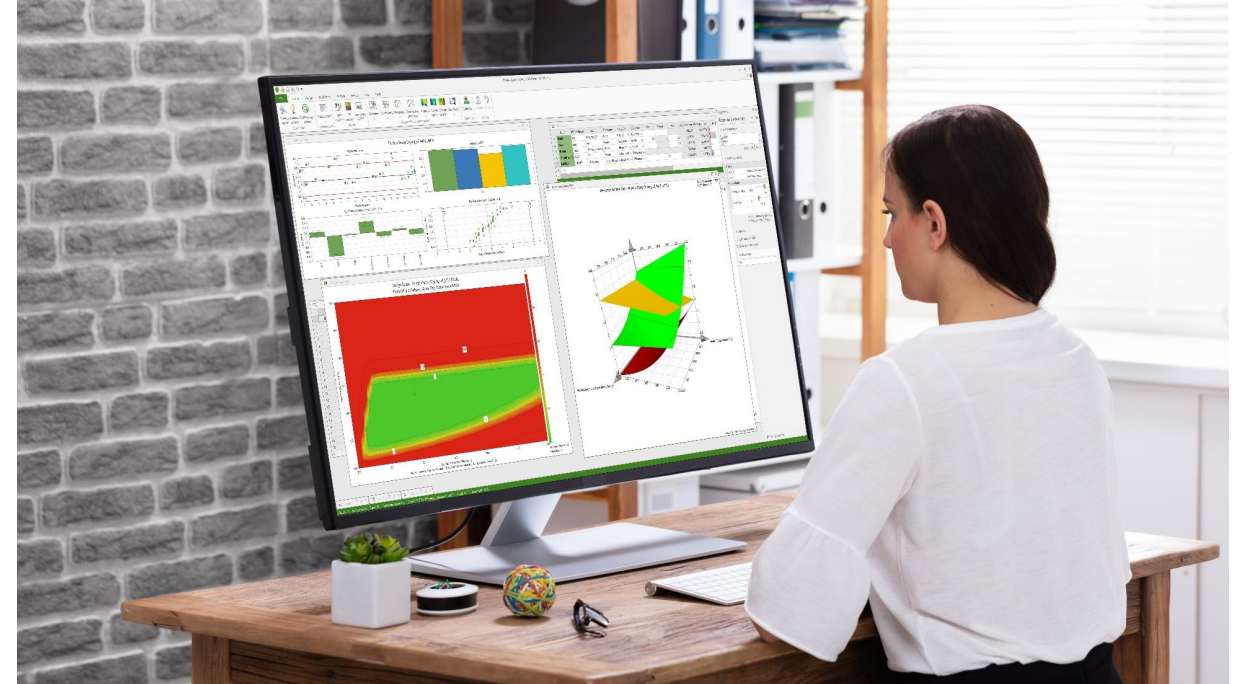
Why Optimization?

- Industry trend towards process intensification and continuous manufacturing
- Sustainability and waste minimization
- Production cost and product risk mitigation
- Empower new users to benefit from powerful optimization tools in a guided workflow



MODDE® 13 Optimization made easy

- A MODDE® made to equip all users with powerful optimization in a easy to use workflow
- Required and Desired response criteria's to identify best setpoint within a designs space
- Simulation and what if based on process parameter characteristics
- Visual comparison between setpoint alternatives including user defined reference setpoint



Product Sales Material



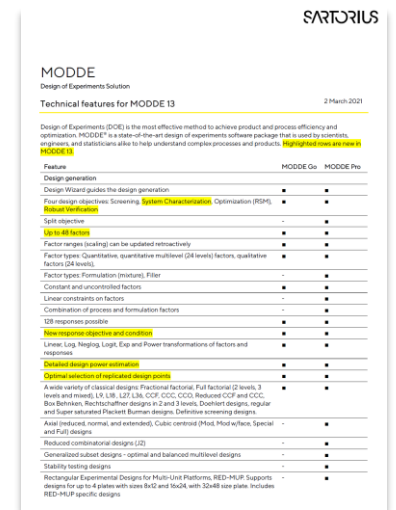
What's New?



Why DOE and what makes MODDE® unique



MODDE leaflet



MODDE Features

https://sartorius.sharepoint.com/:f:/r/sites/O365_SE_UmetricsMarketing/Shared%20Documents/Product%20sales%20material/MODDE?csf=1&web=1&e=dQfzok

SDA Sales Kit



The image shows a presentation slide for the Sartorius SDA Sales Kit. The slide is divided into three horizontal sections. The top section is yellow and features the Sartorius logo in black. The middle section is black and contains the text 'Simplifying Progress' in white. The bottom section is white and features the text 'MODDE®' and 'Get it right from the start!' in black. To the right of the text is a photograph of a scientist in a white lab coat using a pipette to transfer liquid into a small container on a Sartorius analytical balance. A computer monitor in the background displays a software interface with various graphs and data points.

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Simplifying Progress

MODDE®
Get it right from the start!

https://sartorius.sharepoint.com/:f:/r/sites/O365_SE_UmetricsMarketing/Shared%20Documents/Saleskit%20SSDA/1.Presentation?csf=1&web=1&e=S4xvla

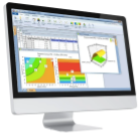
Webinars

- Webinar series highlighting new features in MODDE 13

	<p>STANDARD Design of Experiments (DOE) for the Beginner ⋮ TUE, JAN 26, 2021 03:00 PM - 04:00 PM CET</p>	<ul style="list-style-type: none">▪ Why DOE + Design Wizard
	<p>STANDARD Lean-and-clean DOE using One-click analysis ⋮ TUE, FEB 16, 2021 03:00 PM - 04:00 PM CET</p>	<ul style="list-style-type: none">▪ Analysis Wizard
	<p>STANDARD Robust optimization made easy ⋮ TUE, MAR 2, 2021 03:00 PM - 04:00 PM CET</p>	<ul style="list-style-type: none">▪ Optimization Wizard
	<p>STANDARD From Design of Experiments to Design Space Estimation ⋮ TUE, MAR 23, 2021 03:00 PM - 04:00 PM CET</p>	<ul style="list-style-type: none">▪ Design space estimation and setpoint analysis

<https://www.sartorius.com/en/products/process-analytical-technology/data-analytics-software/education-training/webinars>

New Courses material



Design of Experiments (DOE) – Web Course

\$2,000.00

Date /Location/ Language

- 8 March 2021 - Web Course (CET) - English
- 8 March 2021 - Web Course (CET) - English**
- 23 March 2021 - Web Course US (EST) - English
- 18 May 2021 - Web course Tokyo - English



Quality by Design (QBD) and Design Space – Web Course

\$2,700.00

Date /Location/ Language

- 8 March 2021 - Web Course (CET)- English

- 2 day (4 web sessions)
- Visit <https://webshop.umetrics.com>

- 2 + 1 day (4 + 2 web sessions)

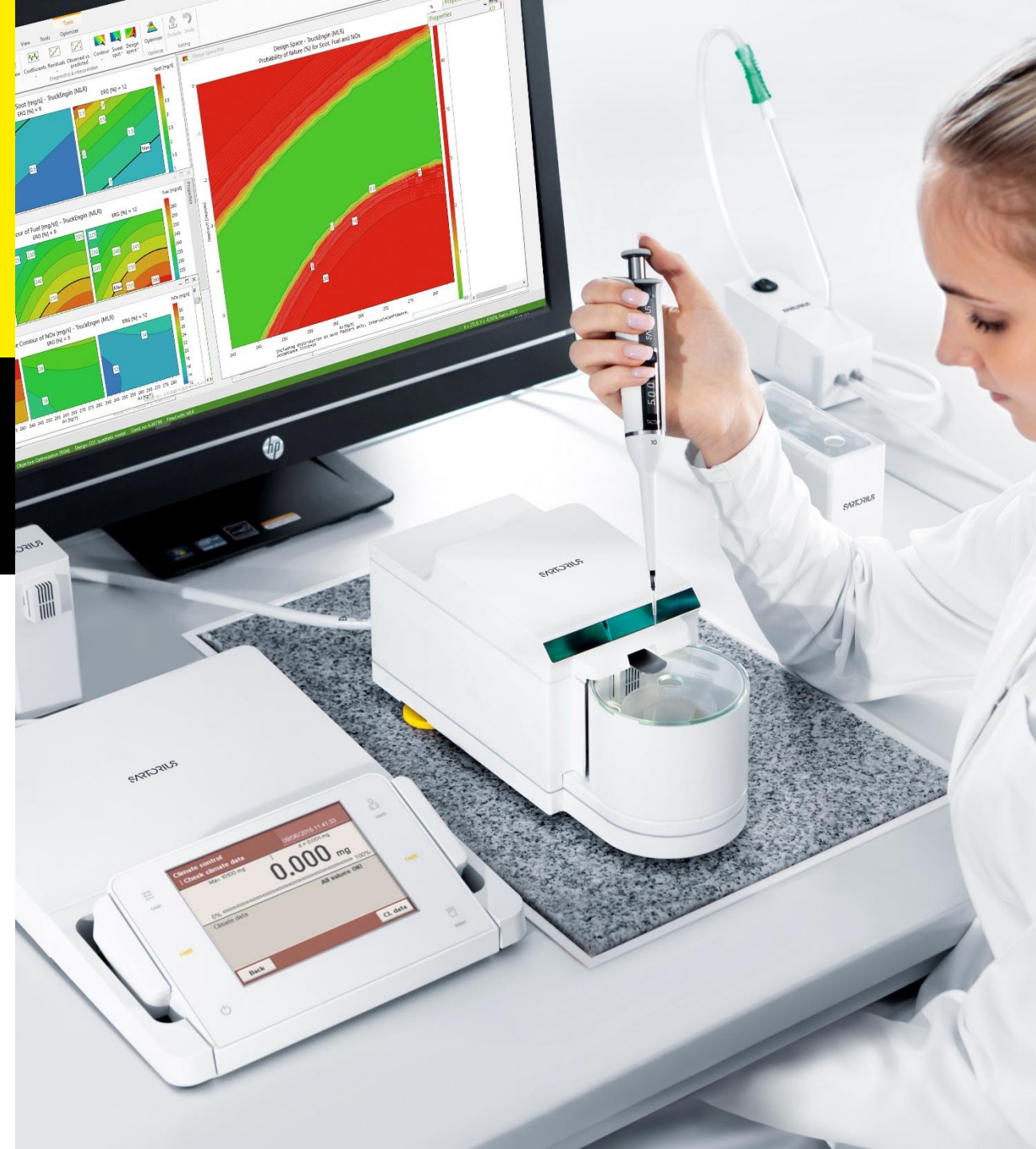
<https://webshop.umetrics.com/collections/courses>

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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 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



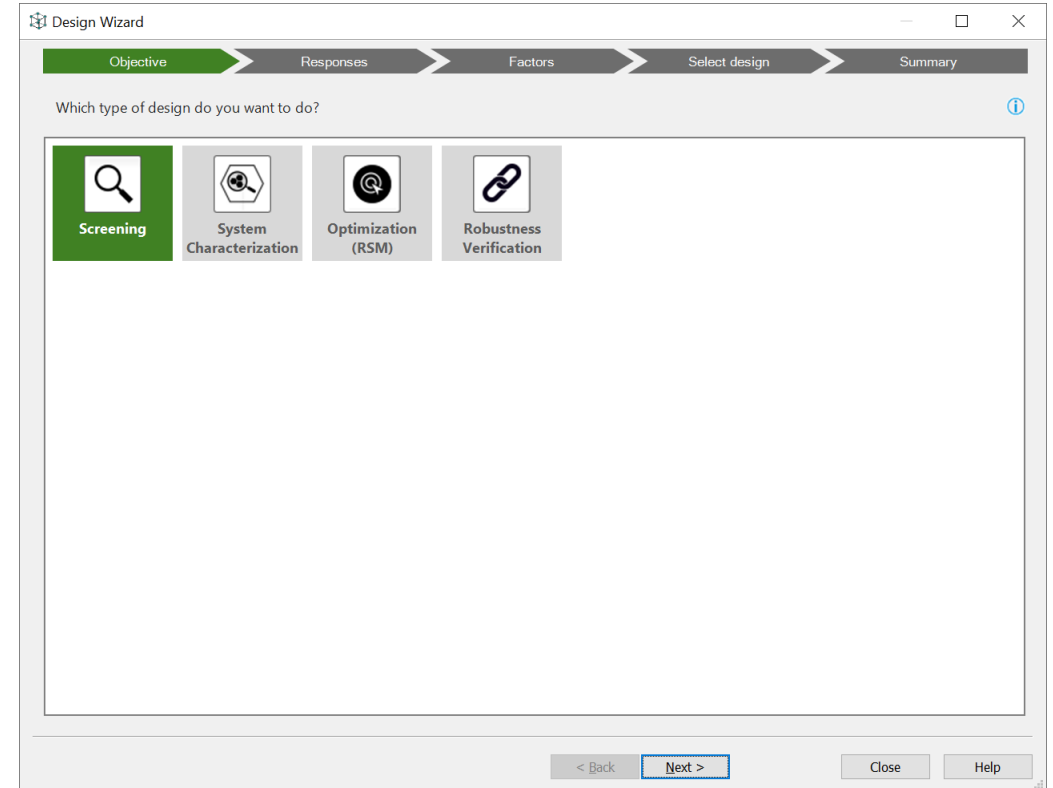
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MODDE® 13 What's New
Design Selection

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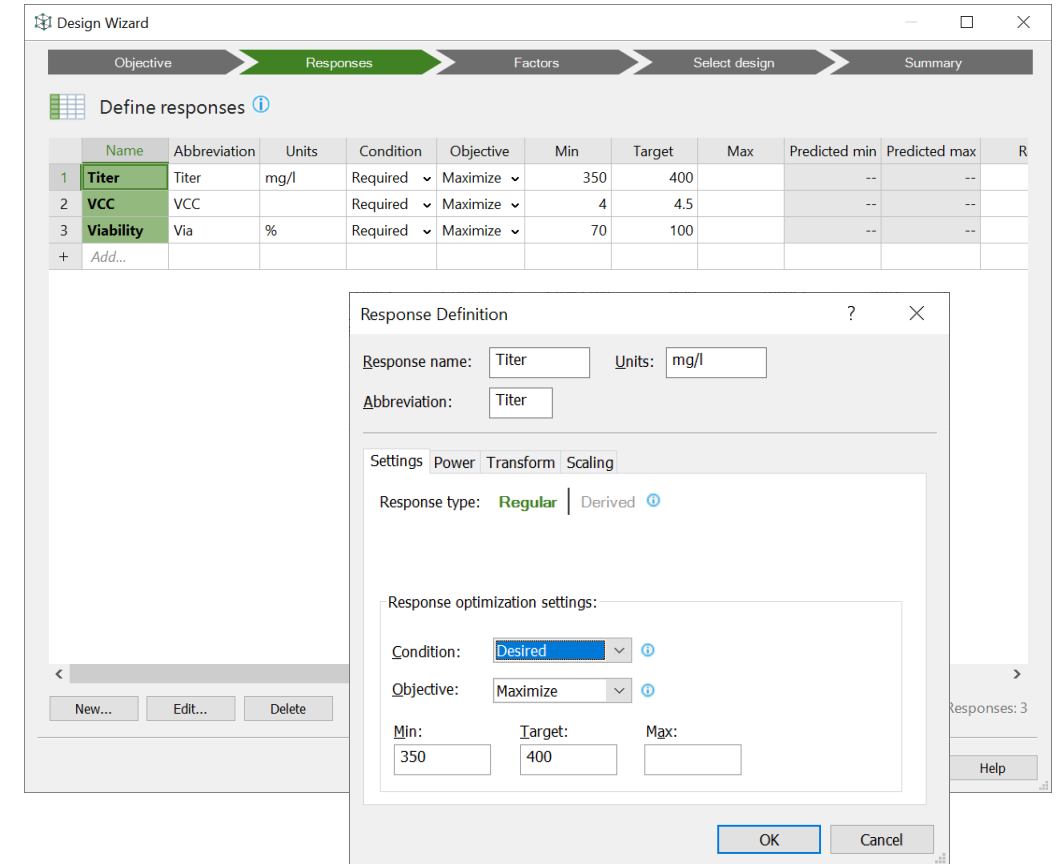
Design Wizard – Investigation Objective

- **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



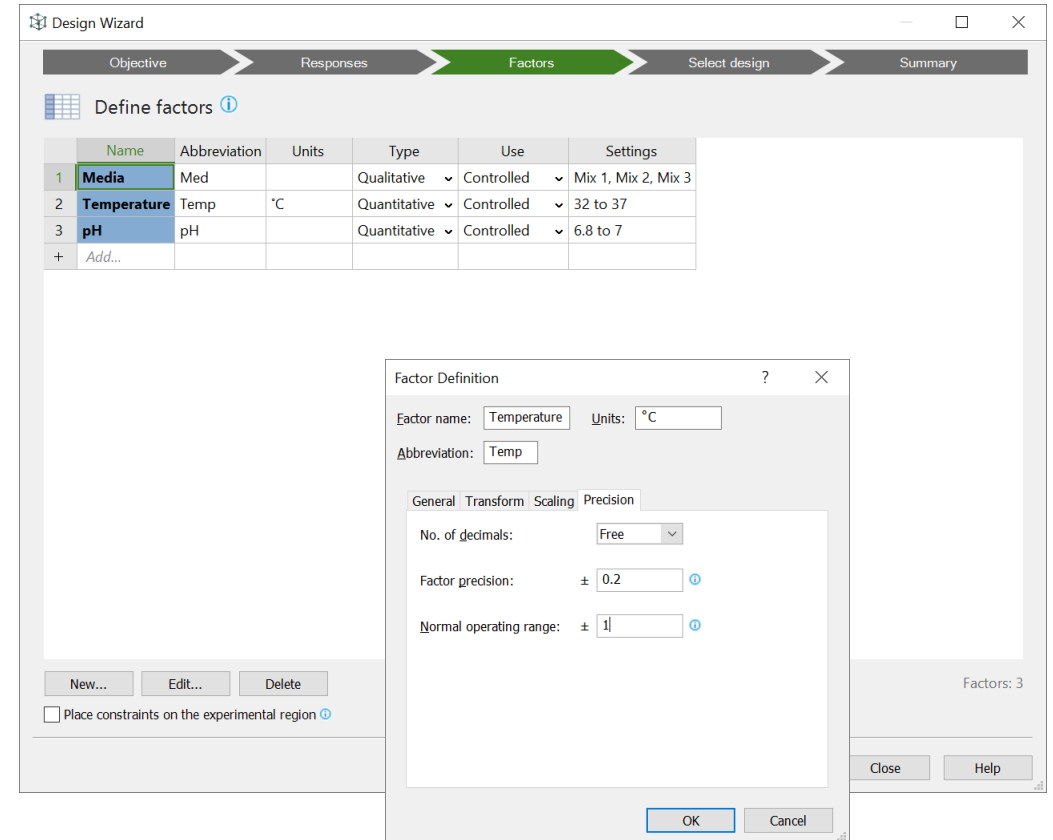
Design Wizard – Responses definition dialog

- 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



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
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

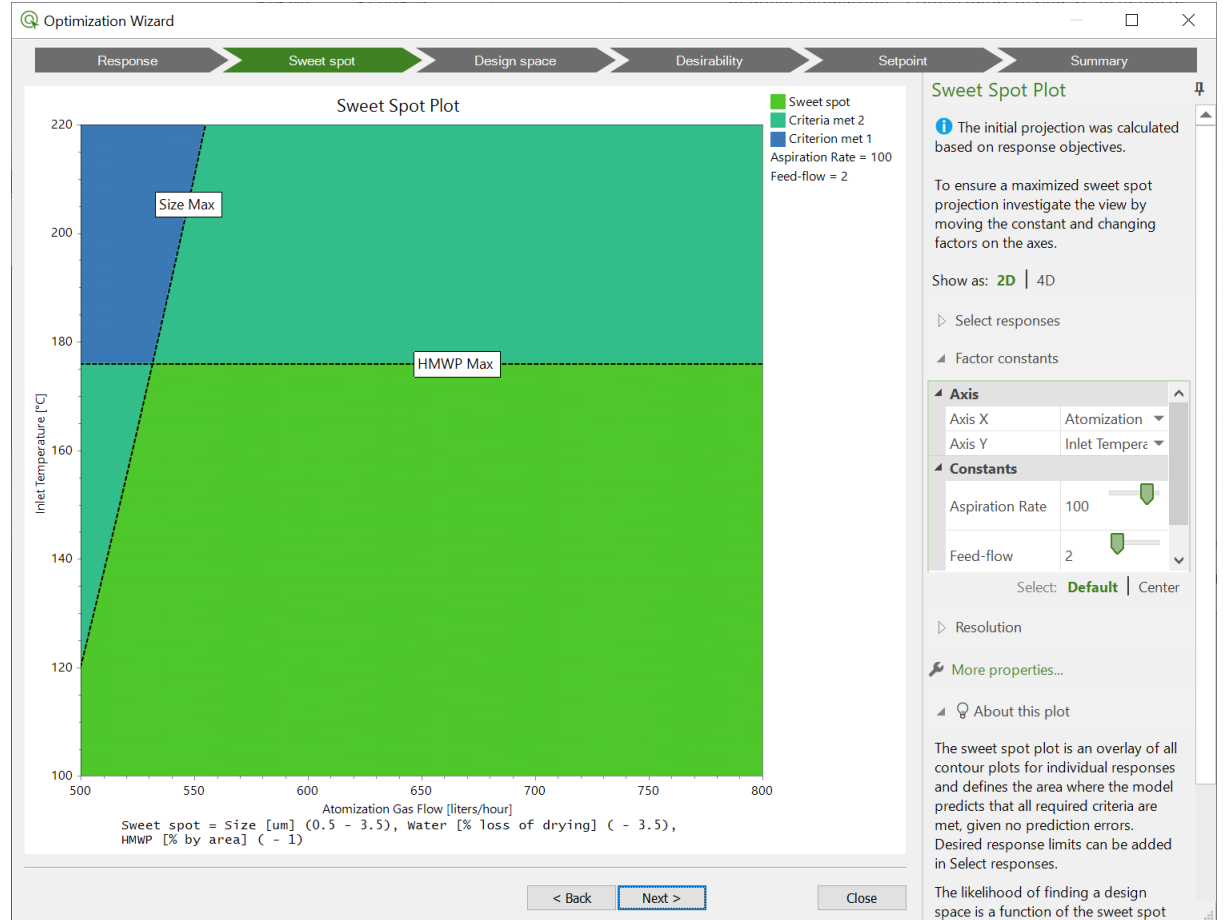
- Required responses are hard conditions. Only required responses are considered in the Sweet spot and Design space plots.
- Desired responses are wishes. Desired and required responses are used in the desirability calculations, and in calculation of optimal setpoints.
- Observed responses are predicted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

Objective

- Minimize, Maximize and Target

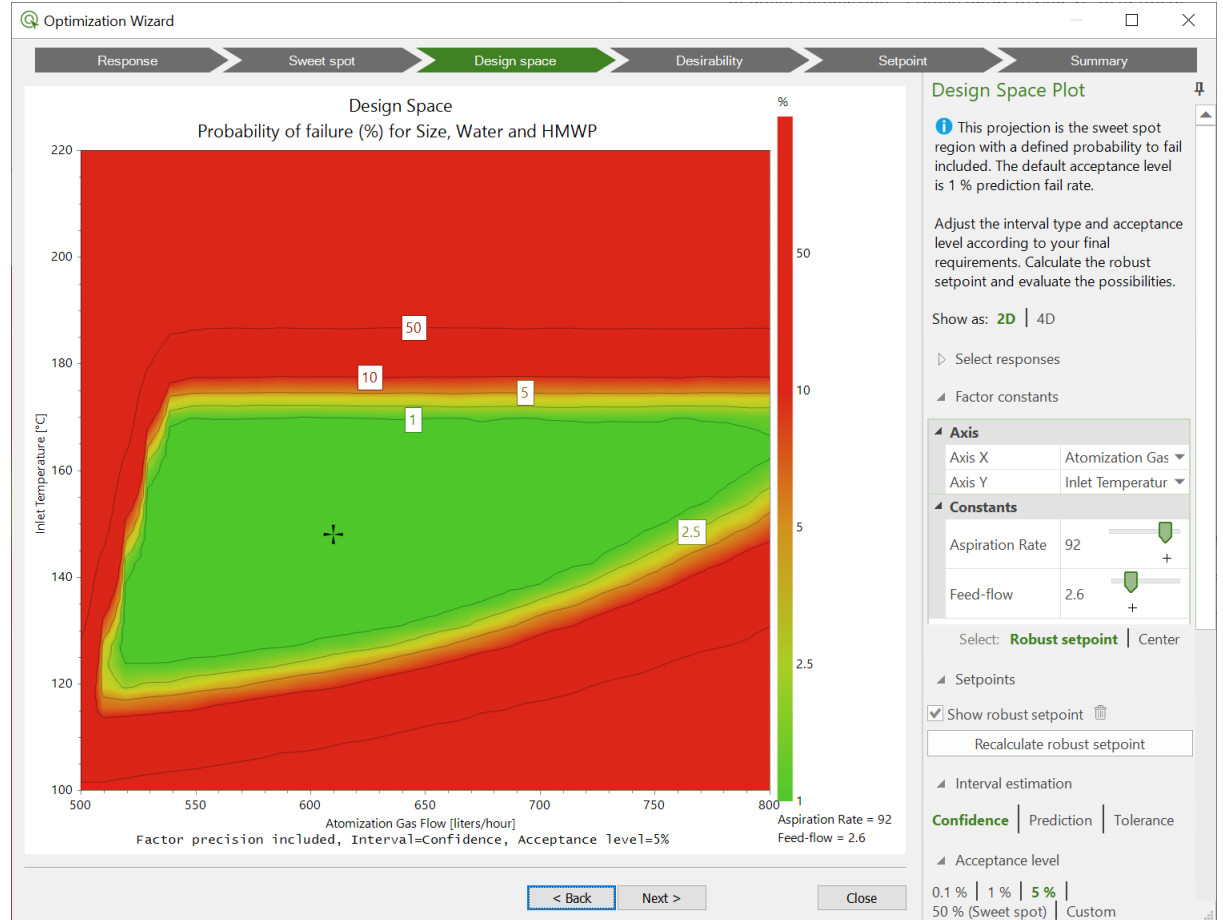
Optimization Wizard – Sweet spot

- 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



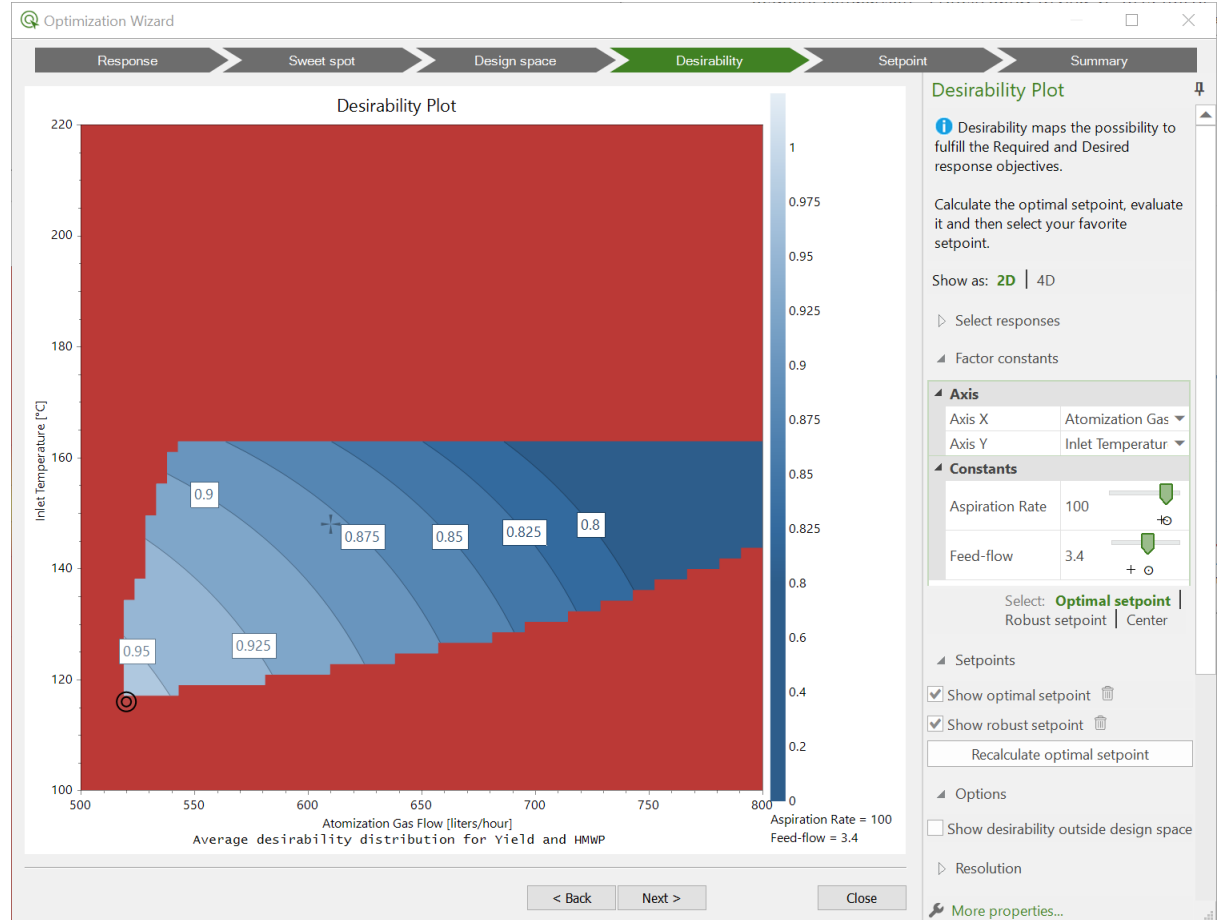
Optimization Wizard – Design Space

- 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



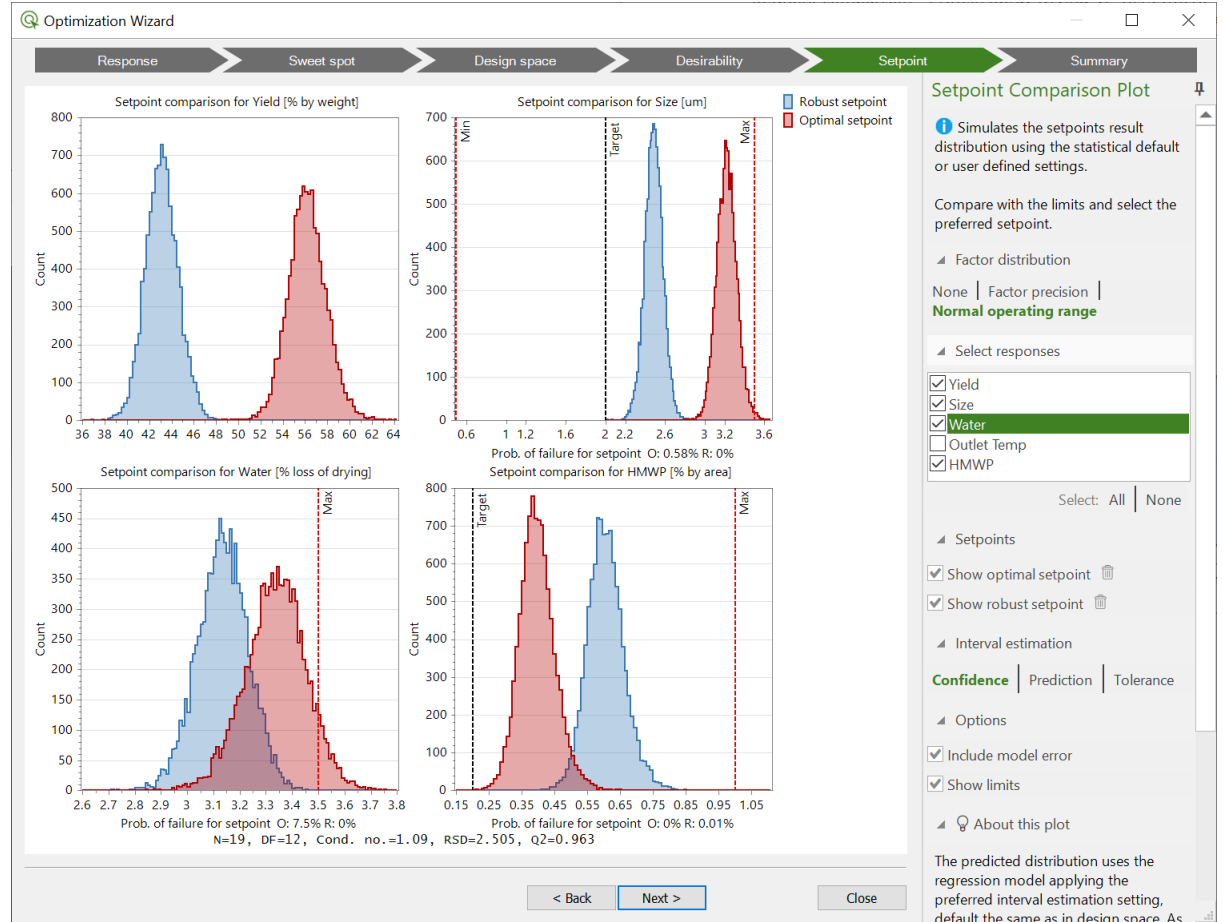
Optimization Wizard – Desirability

- 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 with a table of response characteristics and a table of factor settings.

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

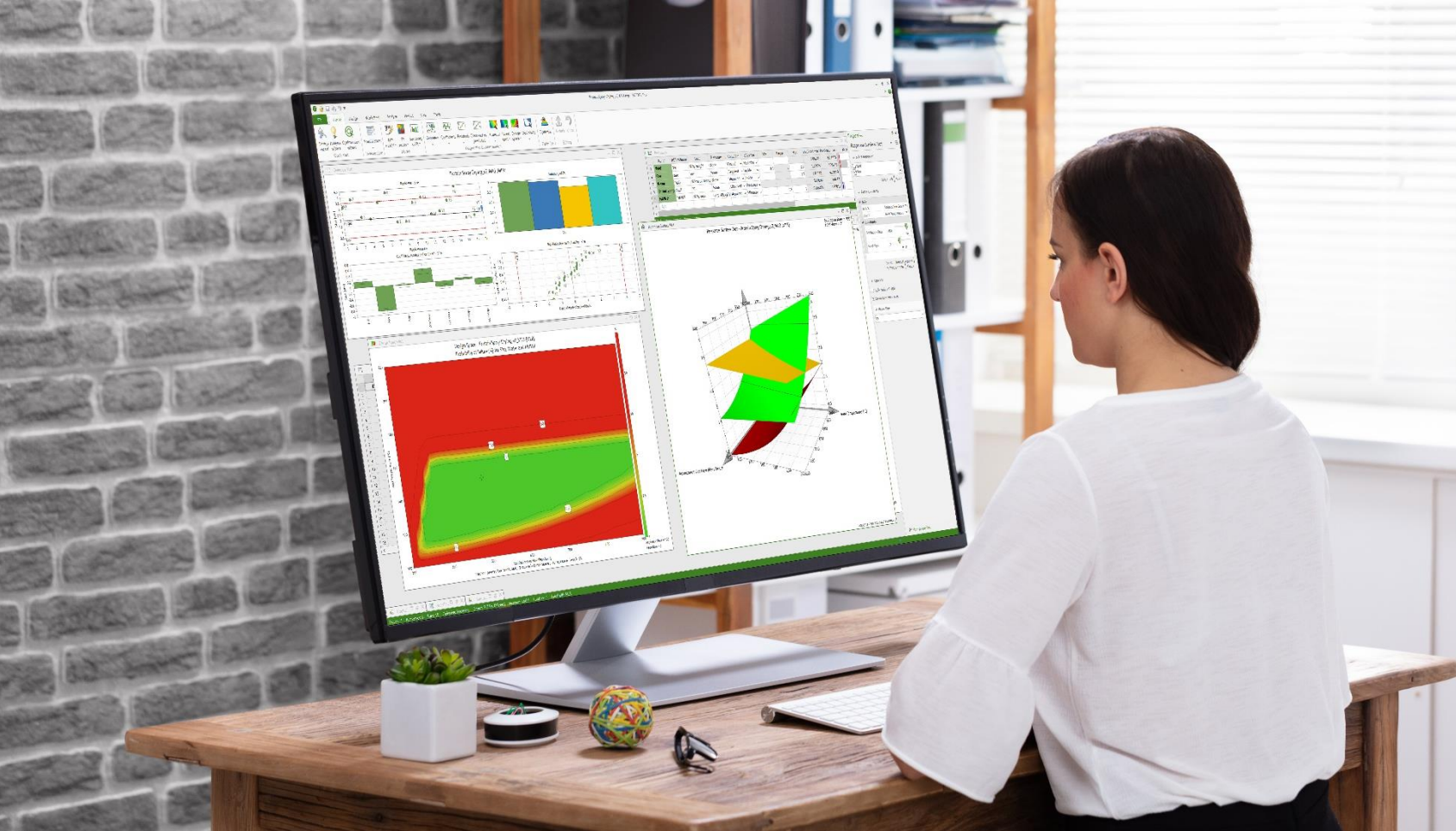
Robust setpoint
 Probability of failure: 0.005% (interval: Confidence)

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

Navigation buttons at the bottom: < Back, Next >, Finish, Close.

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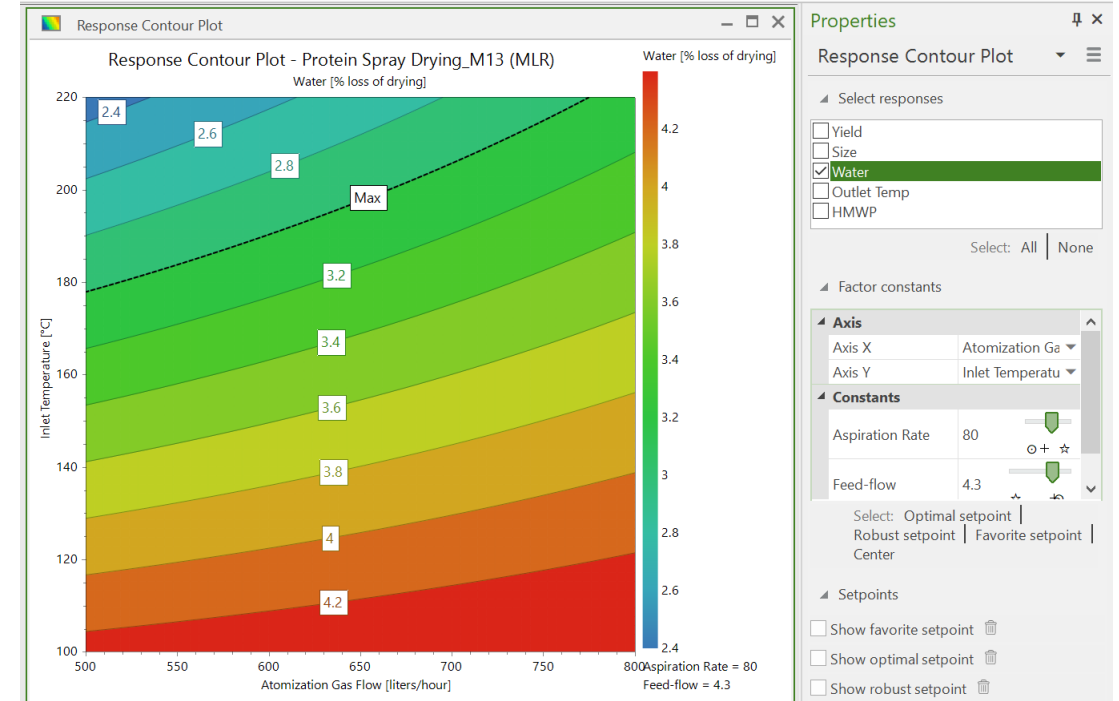


MODDE® 13 What's New
Features and improvements

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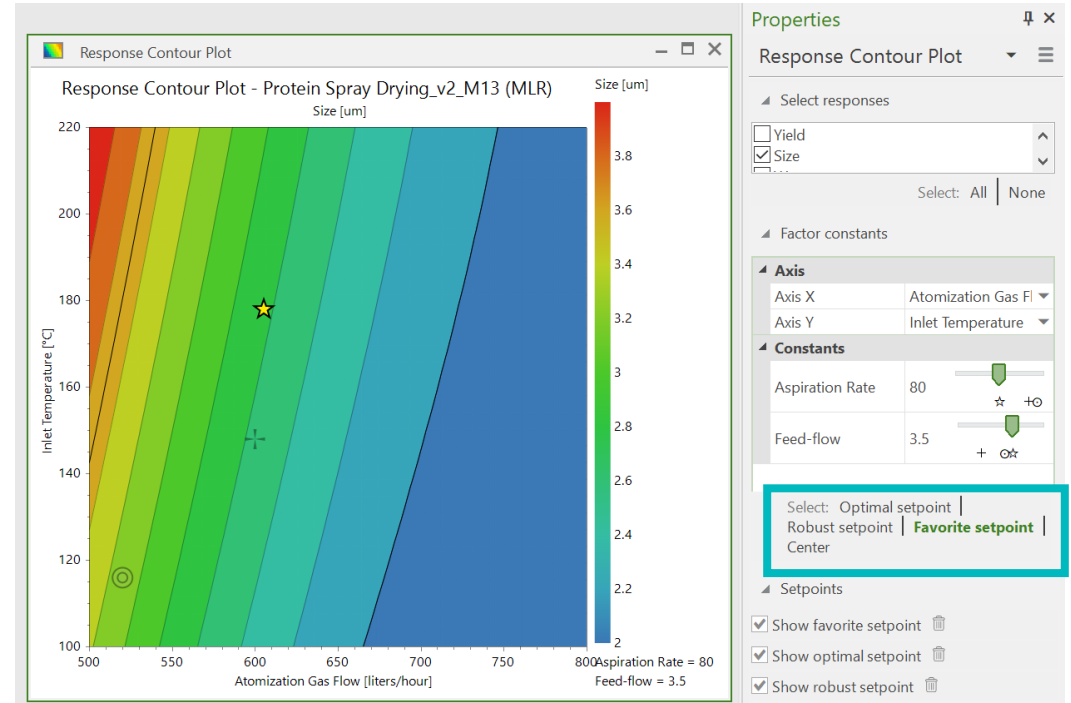
User interface

- 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



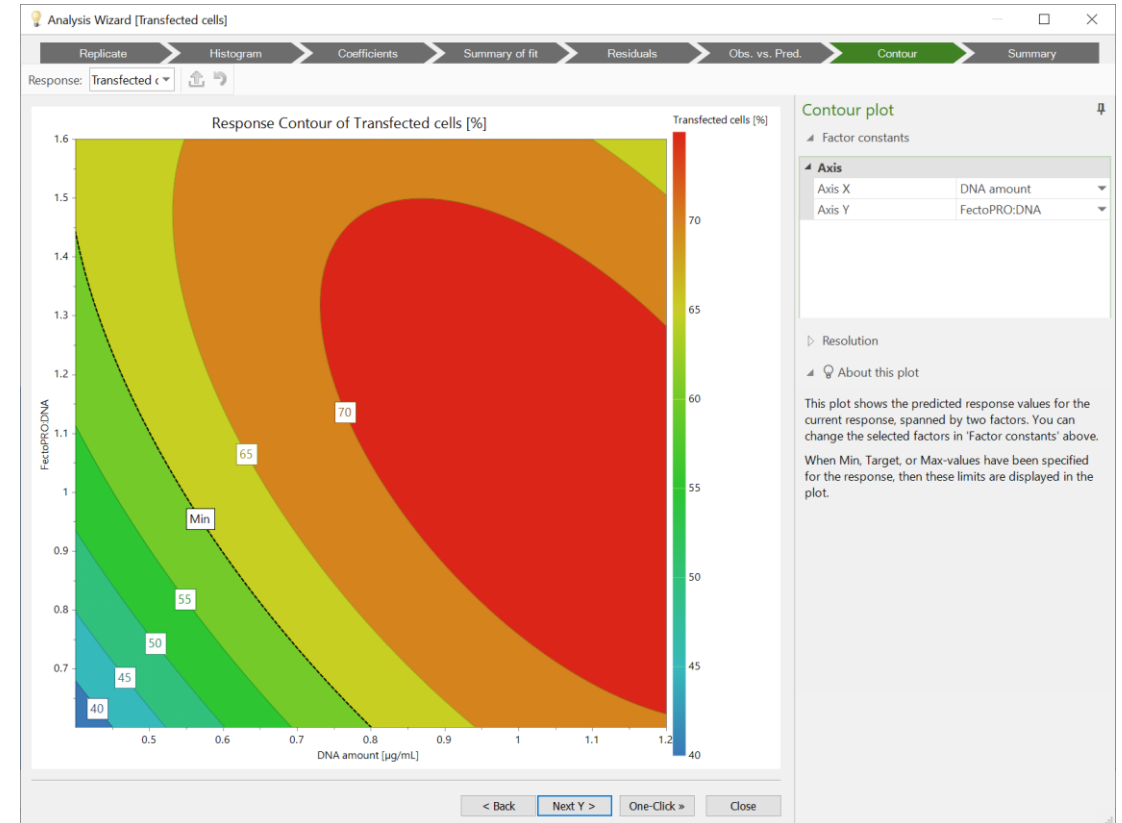
Robust, Optimal, and Favorite setpoint

- 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



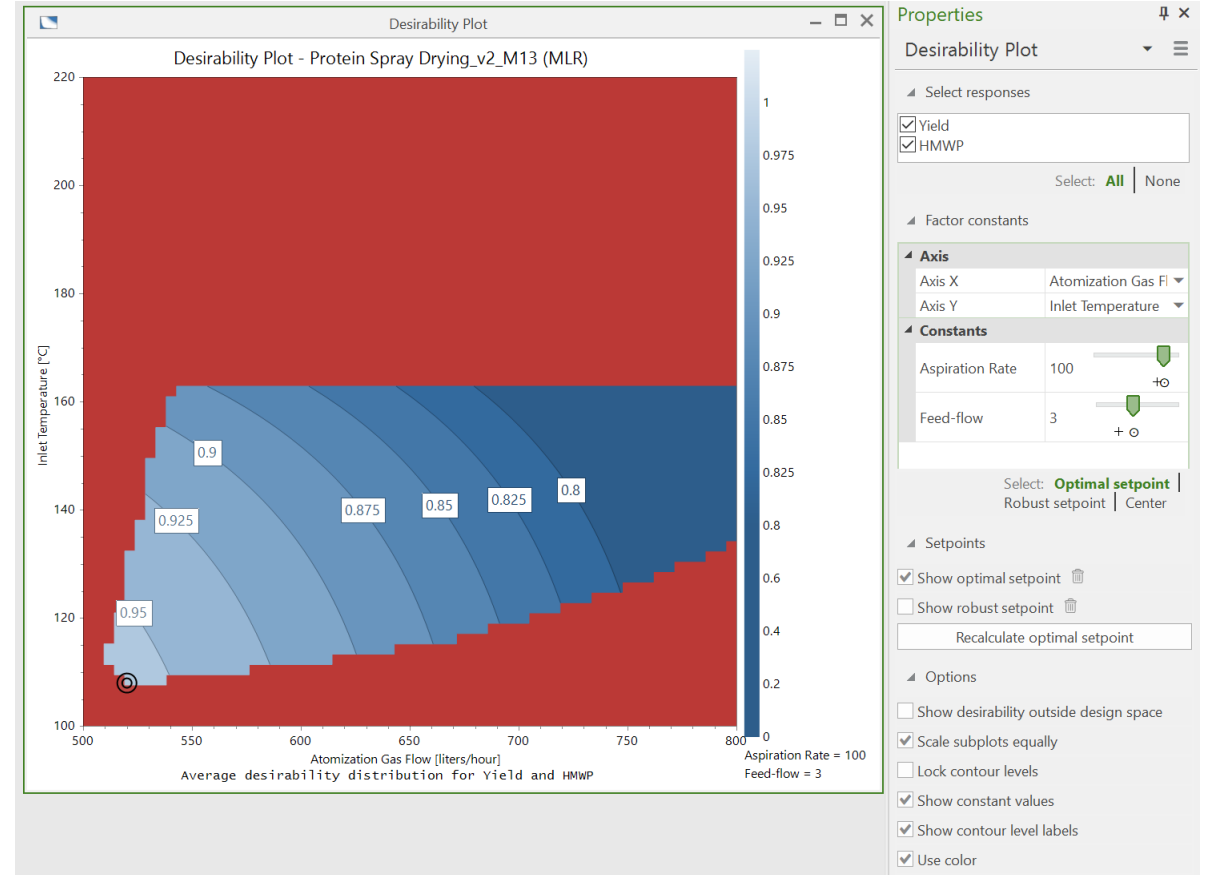
Analysis Wizard

- 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



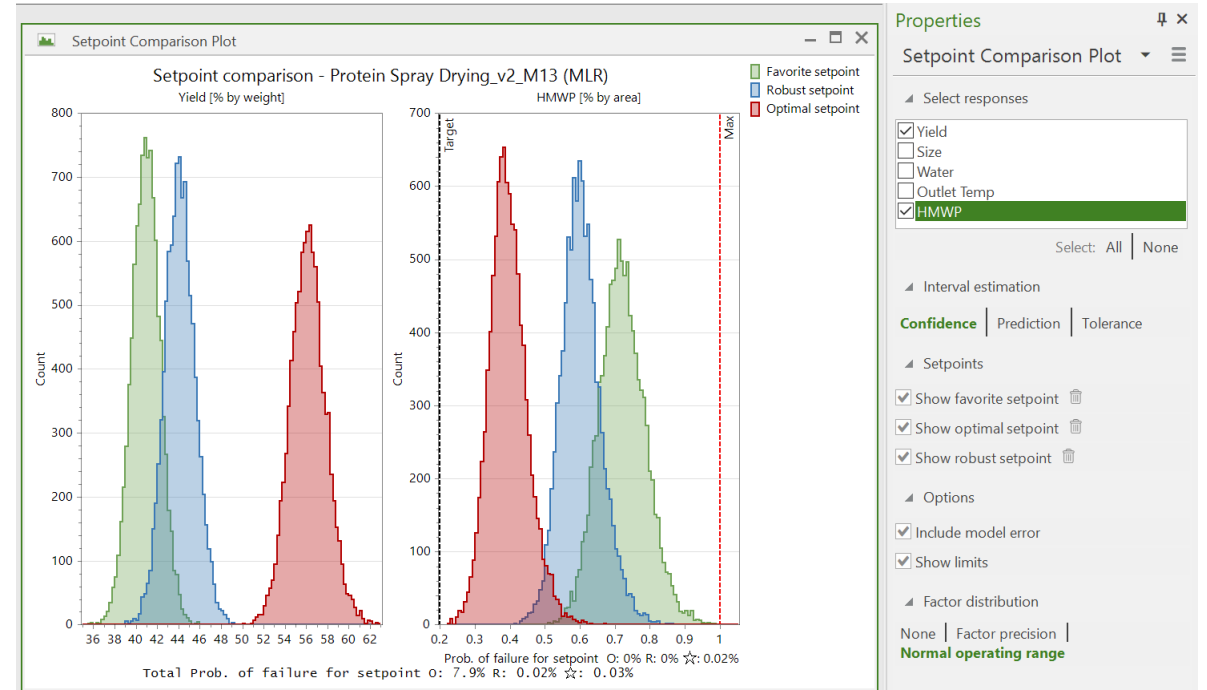
Optimization within design space

- 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.



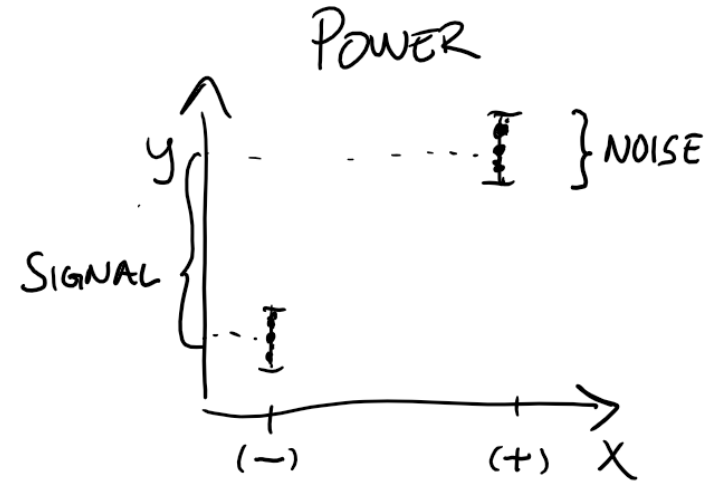
Setpoint comparison

- 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	Yield	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

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

Orthogonal (balanced) design with all combinations of the factor levels. Main effects and all interactions are clear of each other (not confounded).

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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