

Design of Experiments Using Statgraphics Centurion

Neil W. Polhemus, CTO, StatPoint Technologies, Inc.

Copyright 2011 by StatPoint Technologies, Inc.

Web site: www.statgraphics.com



STATPOINT
TECHNOLOGIES, INC.

Design of Experiments Wizard

- Phase 1: Creating an experiment
- Phase 2: Analyzing the results
- Phase 3: Further experimentation



Phase 1: Creating an experiment

- Phase 1: Creating an experiment
 - Step 1: Define responses
 - Step 2: Define experimental factors
 - Step 3: Select design
 - Step 4: Specify model
 - Step 5: Select runs
 - Step 6: Evaluate design
 - Step 7: Save design
- Phase 2: Analyzing the results
- Phase 3: Further experimentation



Phase 2: Analyzing the results

- Phase 1: Creating an experiment
- Phase 2: Analyzing the results
 - Step 8: Analyze data
 - Step 9: Optimize responses
 - Step 10: Save results
- Phase 3: Further experimentation



Phase 3: Further experimentation

- Phase 1: Creating an experiment
- Phase 2: Analyzing the results
- Phase 3: Further experimentation
 - Step 11: Augment design
 - Step 12: Extrapolate

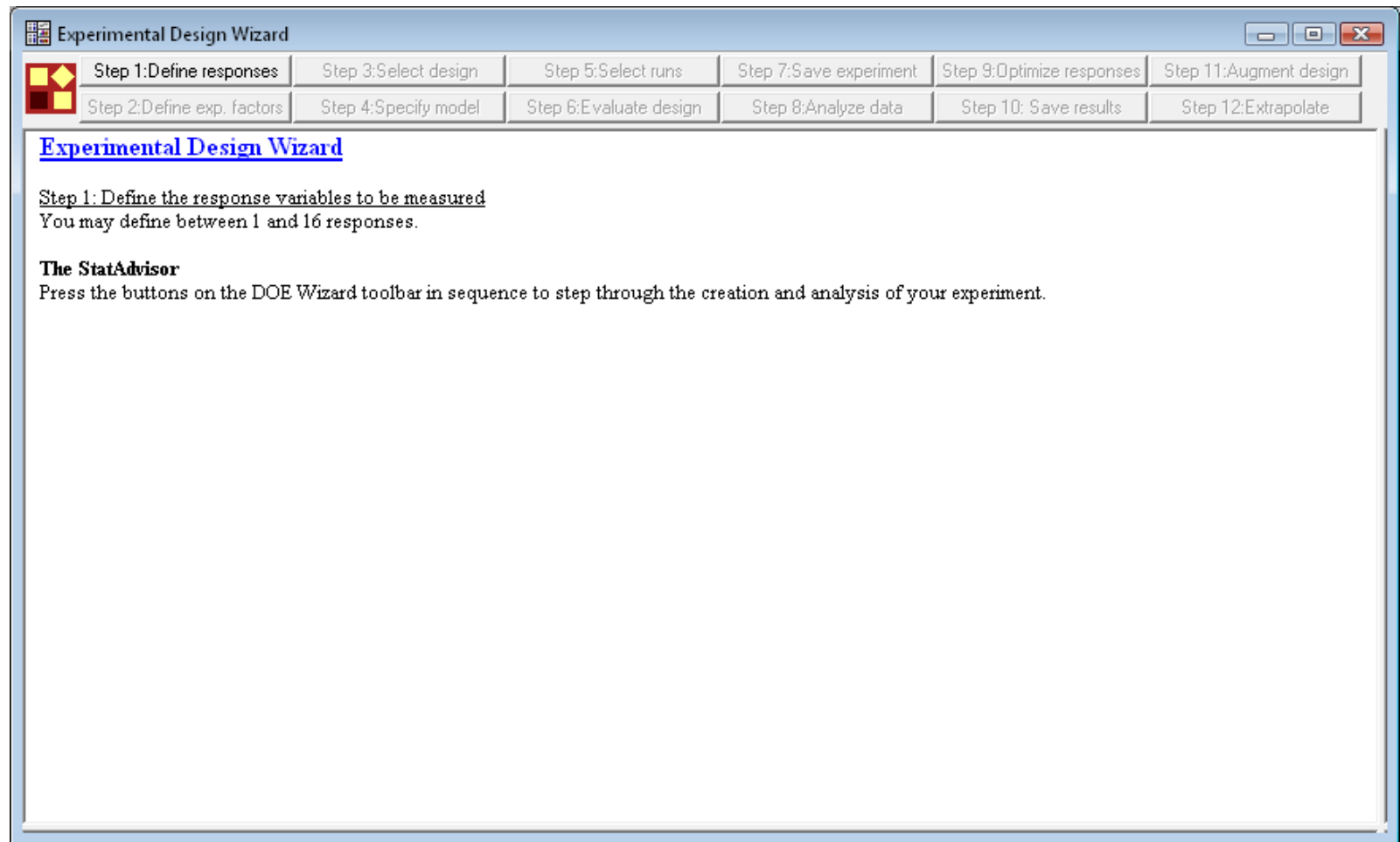


Example – from Response Surface Methodology by Myers and Montgomery

Find the settings of *time*, *temperature* and *catalyst* that maximize the *conversion percentage* of a chemical process while keeping the *thermal activity* as close as possible to 57.5.



DOE Wizard – Main Window



Step 1: Define responses

Design of Experiments Wizard - Define Responses

Design file: <untitled>

Comment: RSM Example

Number of responses: 2

Response	Name	Units	Analyze	Goal	Target	Impact (1-5)	Sensitivity	Minimum	Maximum
1	conversion	%	Mean	Maximize	0.5	3.0	Medium	80	100
2	thermal activity		Mean	Hit target	57.5	3.0	Medium	55	60
3	Var_3		Mean	Maximize	0.5	3.0	Medium		
4	Var_4		Mean	Maximize	0.5	3.0	Medium		
5	Var_5		Mean	Maximize	0.5	3.0	Medium		
6	Var_6		Mean	Maximize	0.5	3.0	Medium		
7	Var_7		Mean	Maximize	0.5	3.0	Medium		
8	Var_8		Mean	Maximize	0.5	3.0	Medium		
9	Var_9		Mean	Maximize	0.5	3.0	Medium		
10	Var_10		Mean	Maximize	0.5	3.0	Medium		
11	Var_11		Mean	Maximize	0.5	3.0	Medium		
12	Var_12		Mean	Maximize	0.5	3.0	Medium		
13	Var_13		Mean	Maximize	0.5	3.0	Medium		
14	Var_14		Mean	Maximize	0.5	3.0	Medium		
15	Var_15		Mean	Maximize	0.5	3.0	Medium		
16	Var_16		Mean	Maximize	0.5	3.0	Medium		

OK Cancel Help



Step 2: Define experimental factors

Design of Experiments Wizard - Define Factors

Design file: <untitled>

Comment: RSM Example

Number of controllable process factors: 3 Number of controllable mixture components: 0 Number of noise factors: 0

Factor	Name	Units	Type	Role	Low	High	Levels
A	time	minutes	Continuous	Controllable	10	15	1,2,3,4
B	temperature	degrees C	Continuous	Controllable	170	200	1,2,3,4
C	catalyst	%	Continuous	Controllable	2	3	1,2,3,4
D	Factor_D		Continuous		-1.0	1.0	1,2,3,4
E	Factor_E		Continuous		-1.0	1.0	1,2,3,4
F	Factor_F		Continuous		-1.0	1.0	1,2,3,4
G	Factor_G		Continuous		-1.0	1.0	1,2,3,4
H	Factor_H		Continuous		-1.0	1.0	1,2,3,4
I	Factor_I		Continuous		-1.0	1.0	1,2,3,4
J	Factor_J		Continuous		-1.0	1.0	1,2,3,4
K	Factor_K		Continuous		-1.0	1.0	1,2,3,4
L	Factor_L		Continuous		-1.0	1.0	1,2,3,4
M	Factor_M		Continuous		-1.0	1.0	1,2,3,4

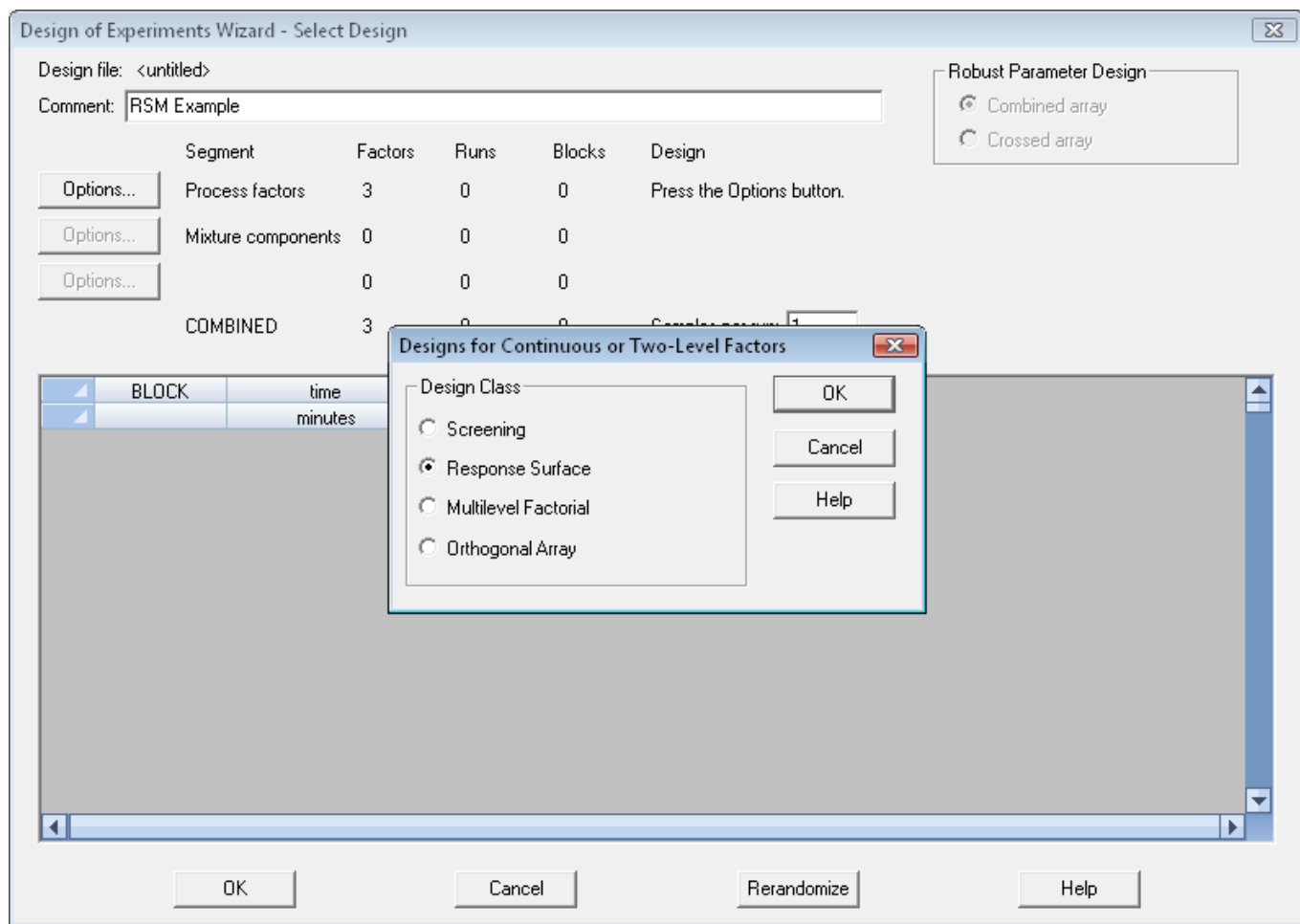
Total for controllable mixture components: 1.0

Factors A-M Factors N-Z

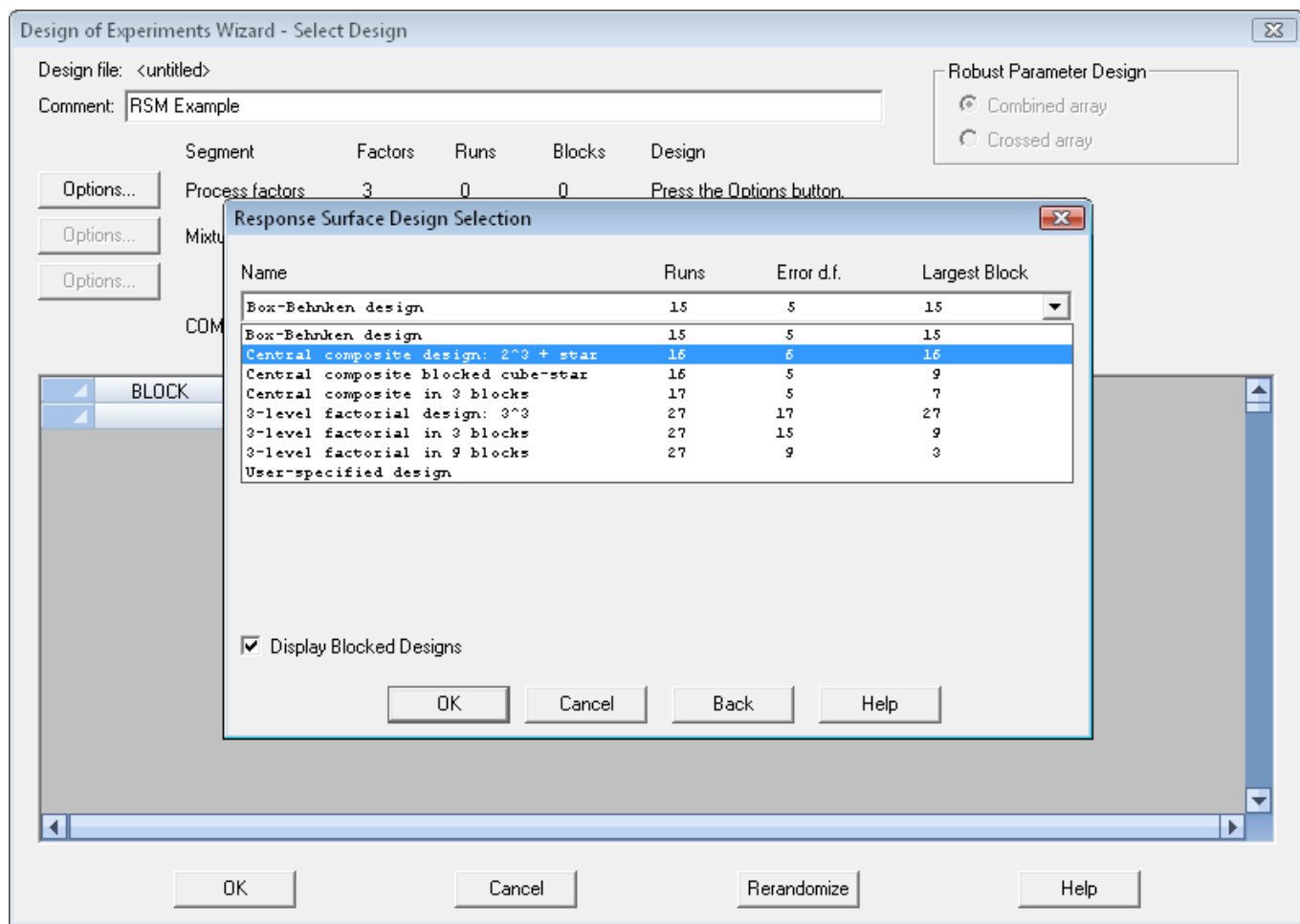
OK Back Cancel Help



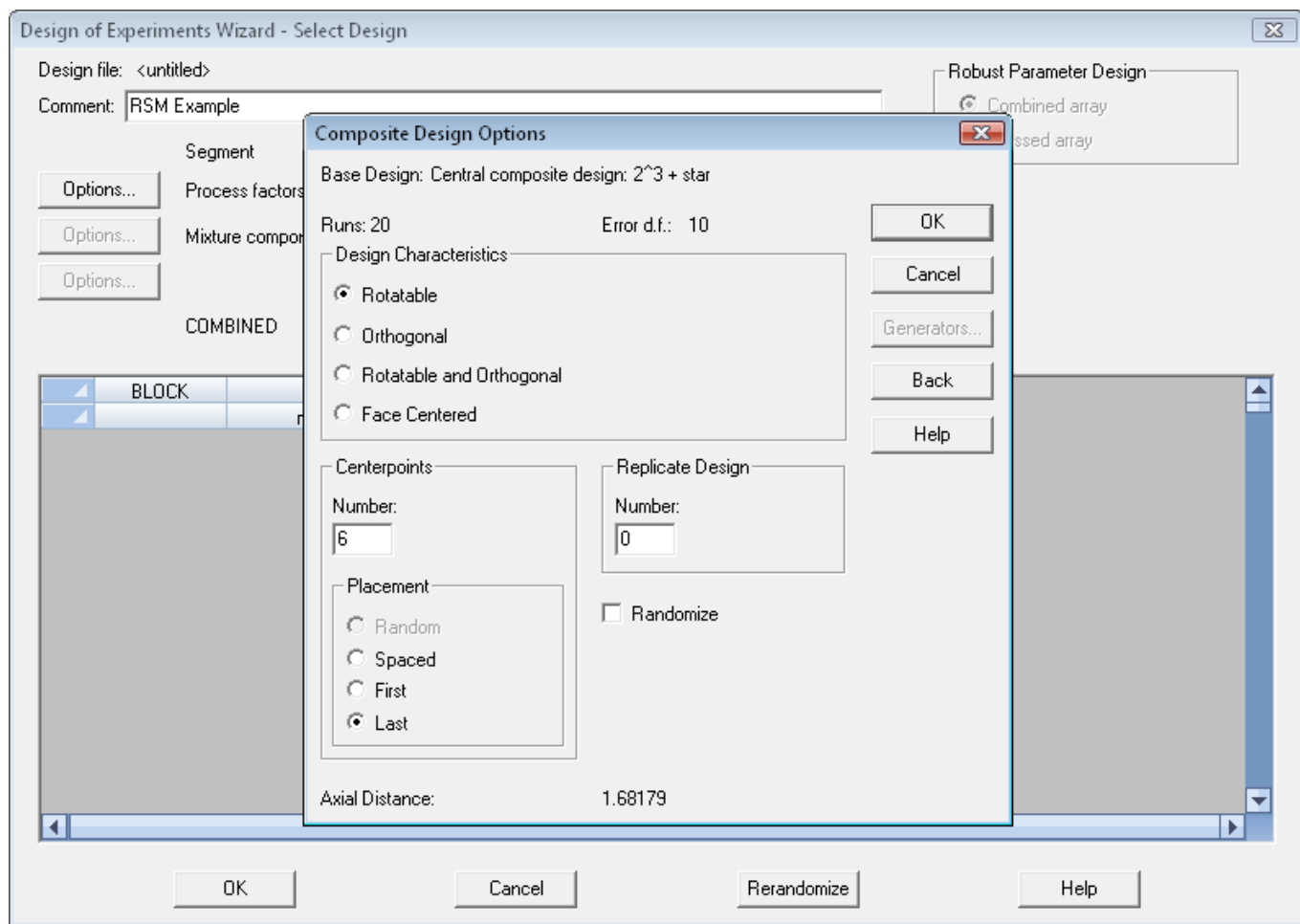
Step 3: Select design



Step 3: Select design (cont.)



Step 3: Select design (cont.)



Step 3: Select design (cont.)

Design of Experiments Wizard - Select Design

Design file: <untitled>

Comment: RSM Example

Robust Parameter Design

☒ Combined array

☐ Crossed array

	Segment	Factors	Runs	Blocks	Design
Options...	Process factors	3	20	1	Central composite design: 2 ³ + star
Options...	Mixture components	0	0	0	
Options...		0	0	0	
	COMBINED	3	20	1	Samples per run: 1

	BLOCK	time minutes	temperature degrees C	catalyst %
1	1	10.0	170.0	2.0
2	1	15.0	170.0	2.0
3	1	10.0	200.0	2.0
4	1	15.0	200.0	2.0
5	1	10.0	170.0	3.0
6	1	15.0	170.0	3.0
7	1	10.0	200.0	3.0
8	1	15.0	200.0	3.0
9	1	8.29552	185.0	2.5
10	1	16.7045	185.0	2.5
11	1	12.5	159.773	2.5
12	1	12.5	210.227	2.5
13	1	12.5	185.0	1.6591
14	1	12.5	185.0	3.3409
15	1	12.5	185.0	2.5

OK Cancel Rerandomize Help



Datasheet

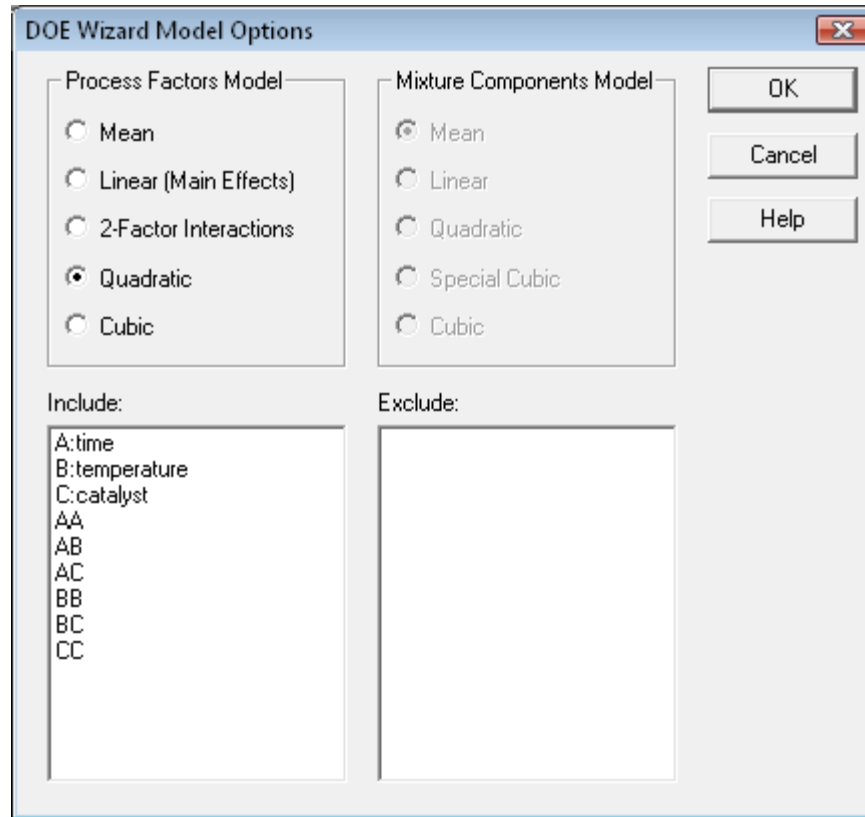
<untitled>

	BLOCK	time minutes	temperature degrees C	catalyst %	conversion %	thermal
1	1	10.0	170.0	2.0		
2	1	15.0	170.0	2.0		
3	1	10.0	200.0	2.0		
4	1	15.0	200.0	2.0		
5	1	10.0	170.0	3.0		
6	1	15.0	170.0	3.0		
7	1	10.0	200.0	3.0		
8	1	15.0	200.0	3.0		
9	1	8.3	185.0	2.5		
10	1	16.7	185.0	2.5		
11	1	12.5	160	2.5		
12	1	12.5	210	2.5		
13	1	12.5	185.0	1.66		
14	1	12.5	185.0	3.34		
15	1	12.5	185.0	2.5		
16	1	12.5	185.0	2.5		
17	1	12.5	185.0	2.5		
18	1	12.5	185.0	2.5		
19	1	12.5	185.0	2.5		
20	1	12.5	185.0	2.5		
21						

A B C



Step 4: Select model



The image shows a software dialog box titled "DOE Wizard Model Options". It is divided into two main sections: "Process Factors Model" and "Mixture Components Model".

Process Factors Model:

- ☐ Mean
- ☐ Linear (Main Effects)
- ☐ 2-Factor Interactions
- ☒ Quadratic
- ☐ Cubic

Mixture Components Model:

- ☒ Mean
- ☐ Linear
- ☐ Quadratic
- ☐ Special Cubic
- ☐ Cubic

On the right side of the dialog are three buttons: "OK", "Cancel", and "Help".

Below the model selection sections are two list boxes:

Include:

- A:time
- B:temperature
- C:catalyst
- AA
- AB
- AC
- BB
- BC
- CC

Exclude:

-



Step 5: Select runs (D-optimal design only)

Design of Experiments Wizard - Select Runs

	BLOCK	time minutes	temperature degrees C	catalyst %	conversion %	thermal activity
1	1	10.0	170.0	2.0		
2	1	15.0	170.0	2.0		
3	1	10.0	200.0	2.0		
4	1	15.0	200.0	2.0		
5	1	10.0	170.0	3.0		
6	1	15.0	170.0	3.0		
7	1	10.0	200.0	3.0		
8	1	15.0	200.0	3.0		
9	1	8.3	185.0	2.5		
10	1	16.7	185.0	2.5		
11	1	12.5	160.0	2.5		
12	1	12.5	210.0	2.5		
13	1	12.5	185.0	1.66		
14	1	12.5	185.0	3.34		
15	1	12.5	185.0	2.5		
16	1	12.5	185.0	2.5		
17	1	12.5	185.0	2.5		
18	1	12.5	185.0	2.5		
19	1	12.5	185.0	2.5		
20	1	12.5	185.0	2.5		

Number of runs desired:

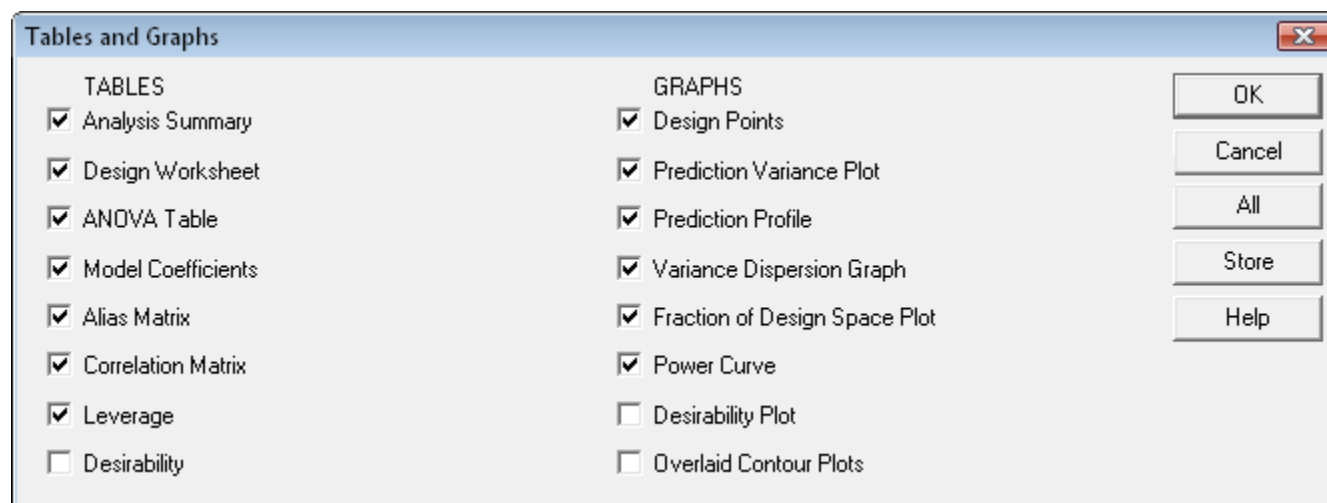
Model coefficients: 10

☒ Apply exchange algorithm at end

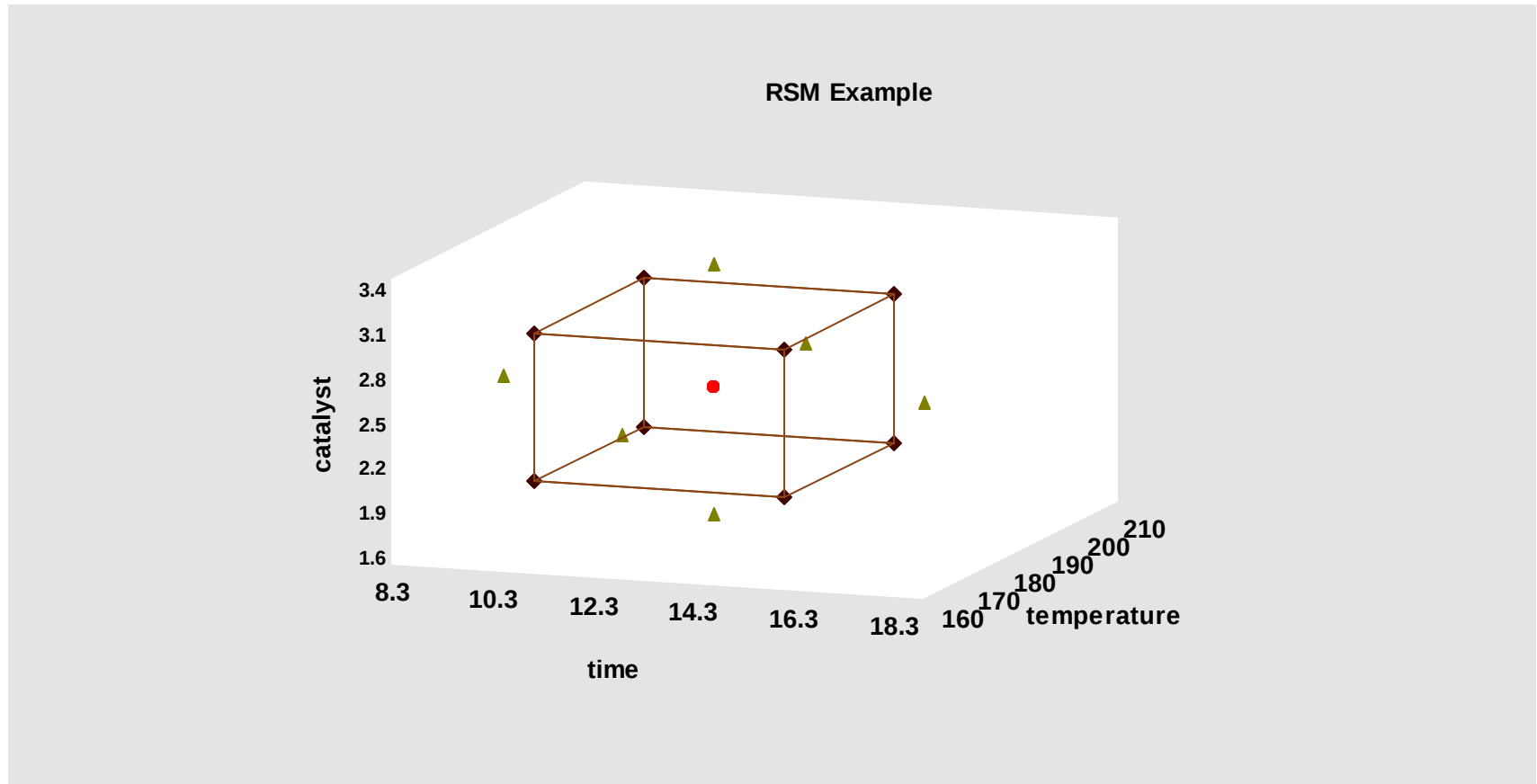
D-efficiency: 65.09%
A-efficiency: 33.47%
G-efficiency: 39.86%



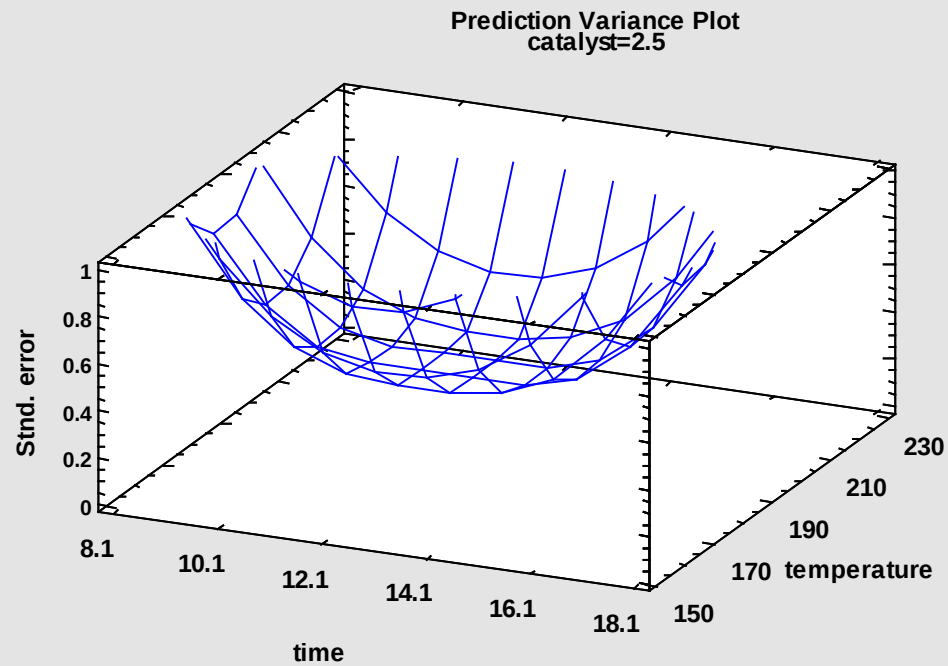
Step 6: Evaluate design



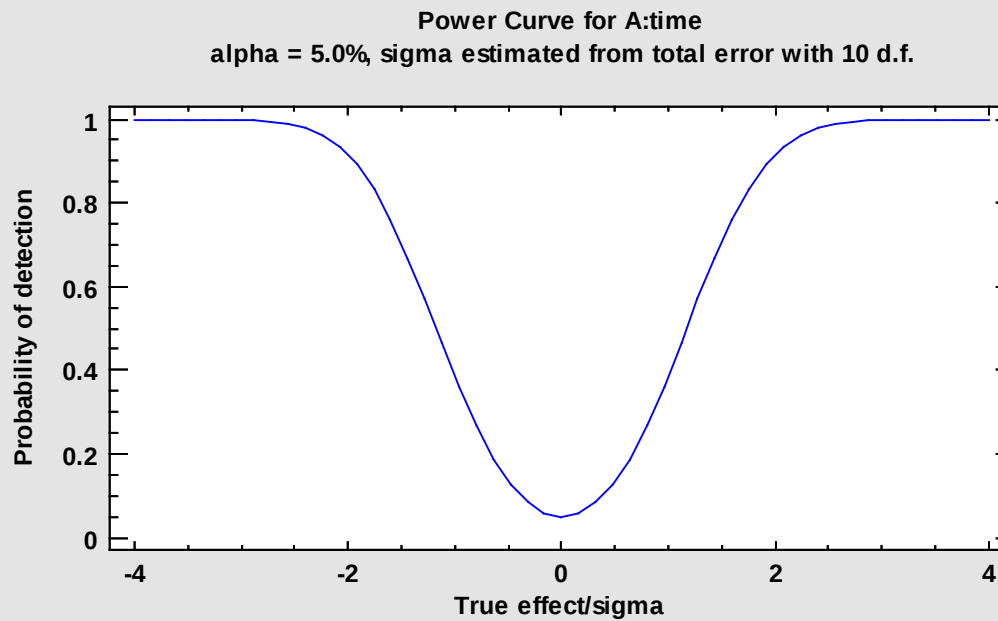
Plot of design space



Prediction variance plot



Power curve



Do the experiment!

Then enter the results:

Conversion & activity.sgx

	BLOCK	time	temperature	catalyst	conversion	thermal activity
		minutes	degrees C	%	%	
1	1	10.0	170.0	2.0	74	53.2
2	1	15.0	170.0	2.0	51	62.9
3	1	10.0	200.0	2.0	88	53.4
4	1	15.0	200.0	2.0	70	62.6
5	1	10.0	170.0	3.0	71	57.3
6	1	15.0	170.0	3.0	90	67.9
7	1	10.0	200.0	3.0	66	59.8
8	1	15.0	200.0	3.0	97	67.8
9	1	8.3	185.0	2.5	76	59.1
10	1	16.7	185.0	2.5	79	65.9
11	1	12.5	160	2.5	85	60
12	1	12.5	210	2.5	97	60.7
13	1	12.5	185.0	1.66	55	57.4
14	1	12.5	185.0	3.34	81	63.2
15	1	12.5	185.0	2.5	81	59.2
16	1	12.5	185.0	2.5	75	60.4
17	1	12.5	185.0	2.5	76	59.1
18	1	12.5	185.0	2.5	83	60.6
19	1	12.5	185.0	2.5	80	60.8
20	1	12.5	185.0	2.5	91	58.9

Conversion & activity B C



Step 8: Analyze data

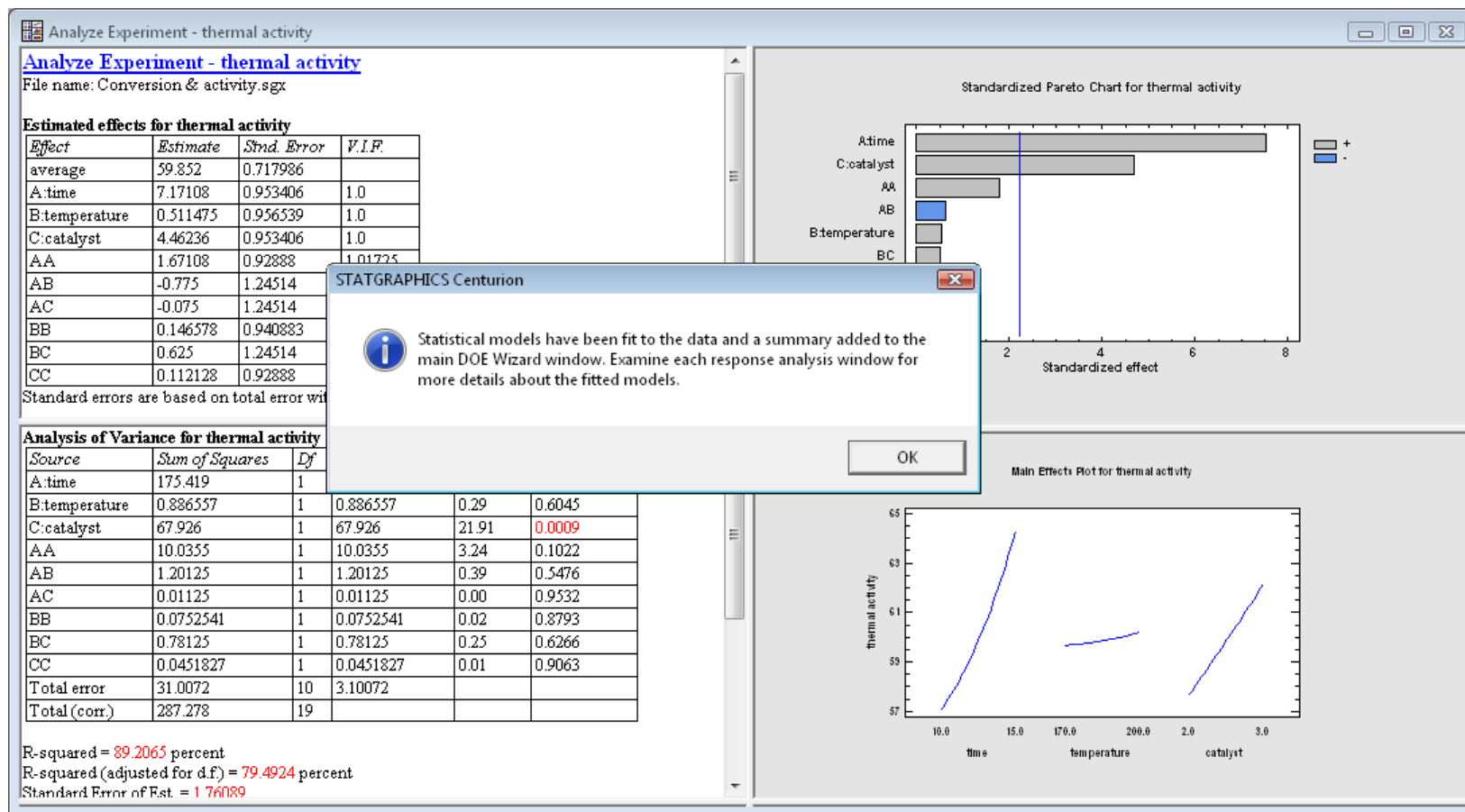
Design of Experiments Wizard - Analyze Data

Response	Transformation	Power	Addend
conversion	None	1.0	0
thermal activity	None	1.0	0

OK Cancel Help



Step 8: Analyze data (cont.)



ANOVA table

Analyze Experiment - thermal activity

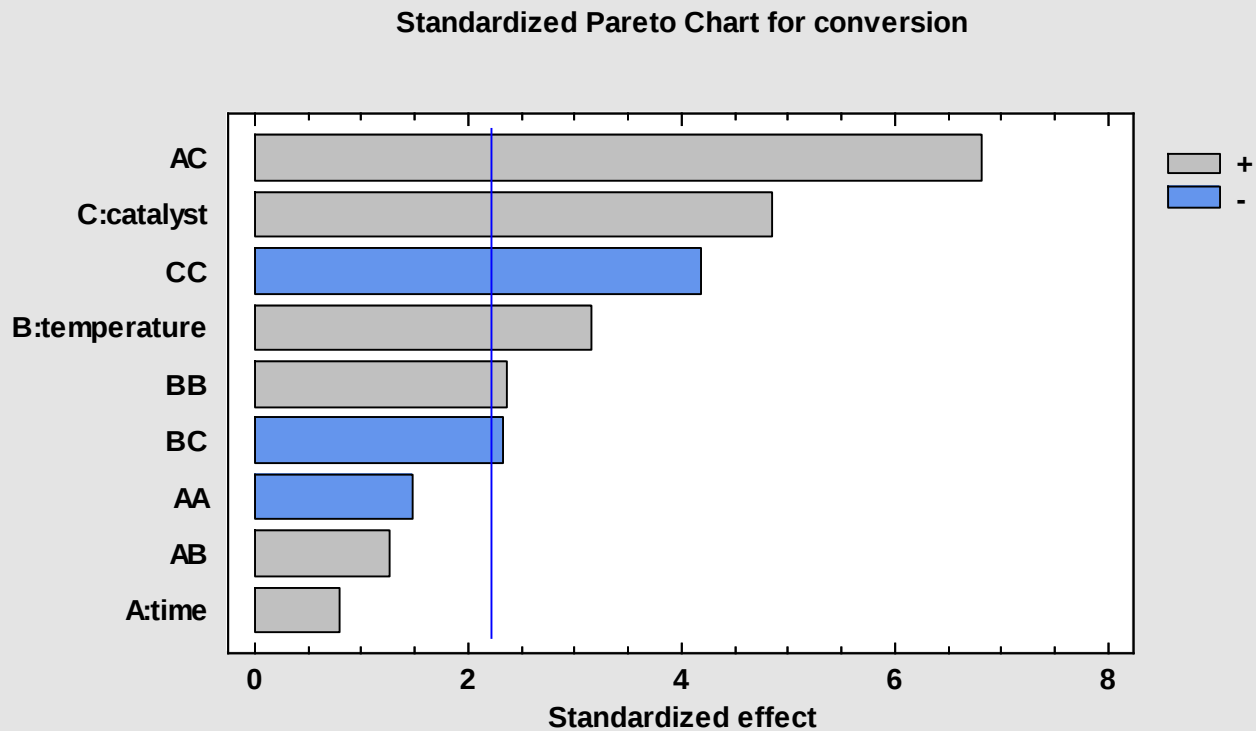
Analysis of Variance for thermal activity

Source	Sum of Squares	Df	Mean Square	F-Ratio	P-Value
A:time	175.419	1	175.419	56.57	0.0000
B:temperature	0.886557	1	0.886557	0.29	0.6045
C:catalyst	67.926	1	67.926	21.91	0.0009
AA	10.0355	1	10.0355	3.24	0.1022
AB	1.20125	1	1.20125	0.39	0.5476
AC	0.01125	1	0.01125	0.00	0.9532
BB	0.0752541	1	0.0752541	0.02	0.8793
BC	0.78125	1	0.78125	0.25	0.6266
CC	0.0451827	1	0.0451827	0.01	0.9063
Total error	31.0072	10	3.10072		
Total (corr.)	287.278	19			

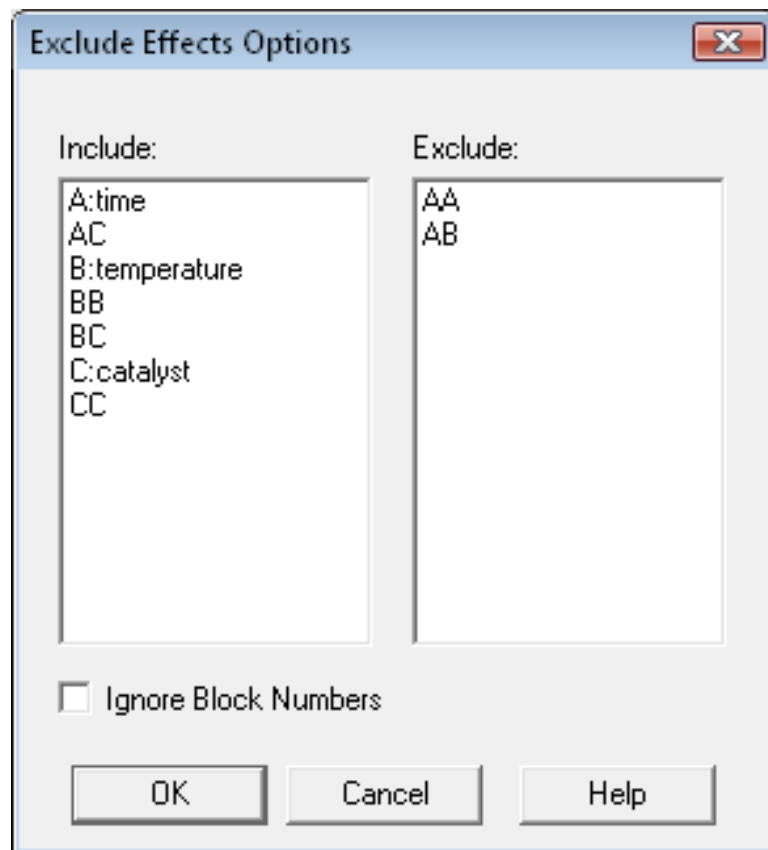
R-squared = 89.2065 percent
R-squared (adjusted for d.f.) = 79.4924 percent
Standard Error of Est. = 1.76089
Mean absolute error = 1.04743
Durbin-Watson statistic = 2.74873 (P=0.9013)
Lag 1 residual autocorrelation = -0.422046



Pareto chart

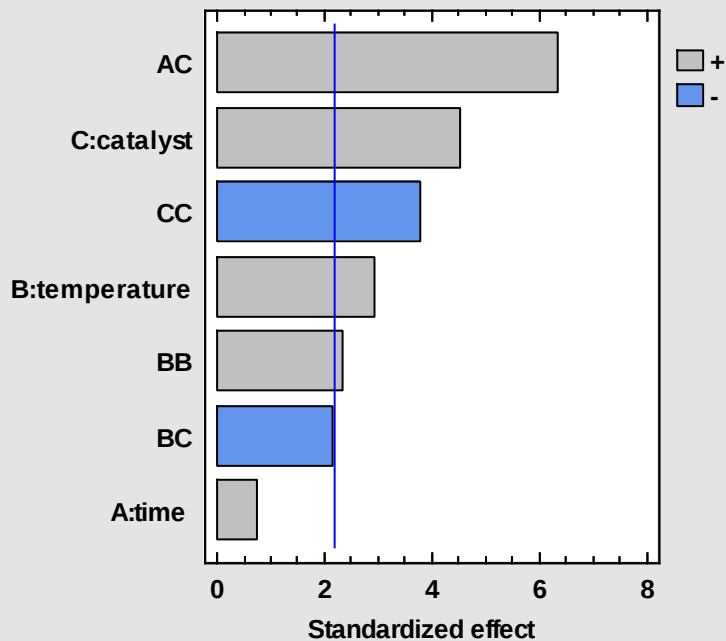


Exclude effects

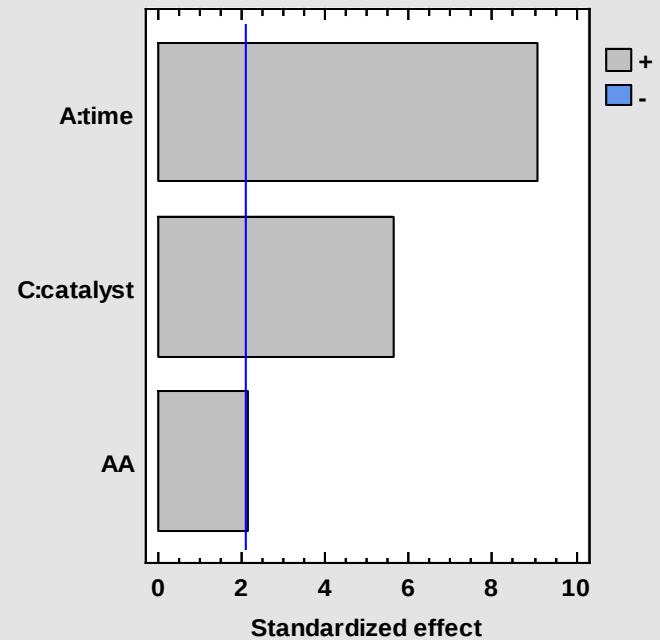


Final models

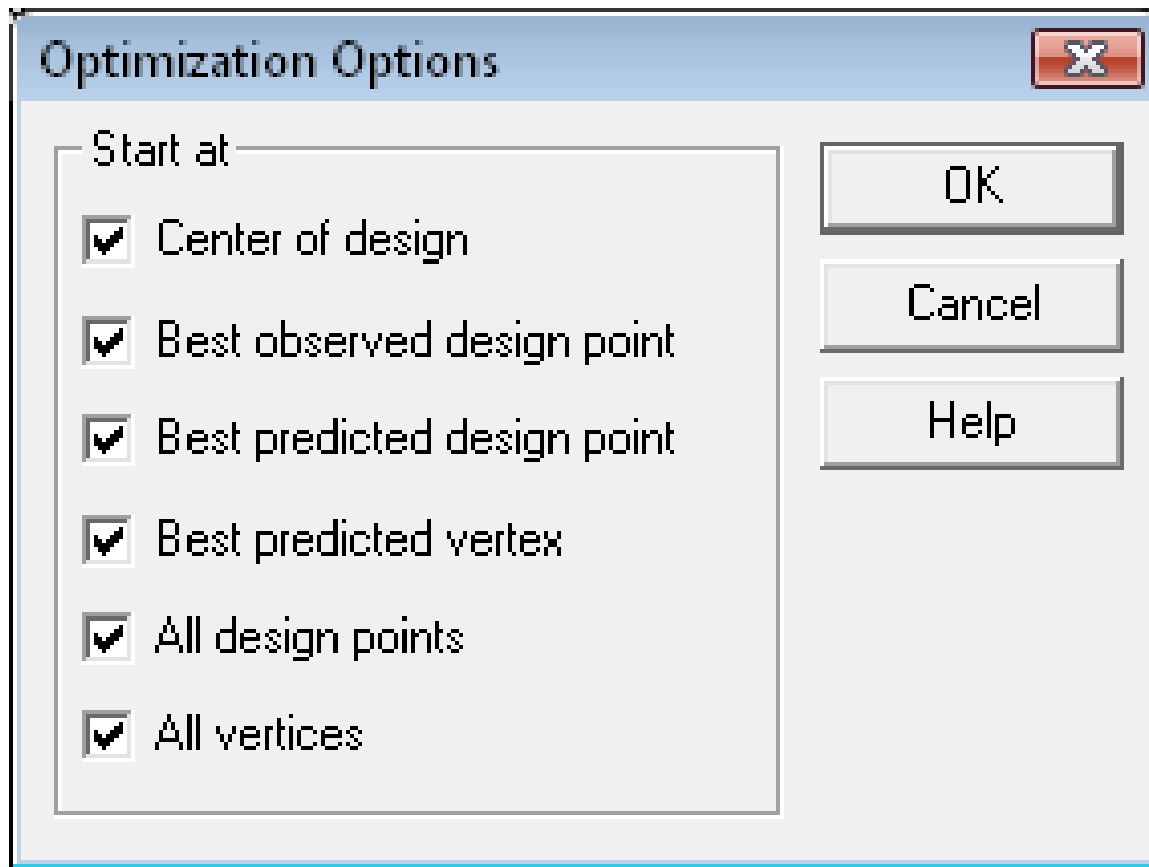
Standardized Pareto Chart for conversion



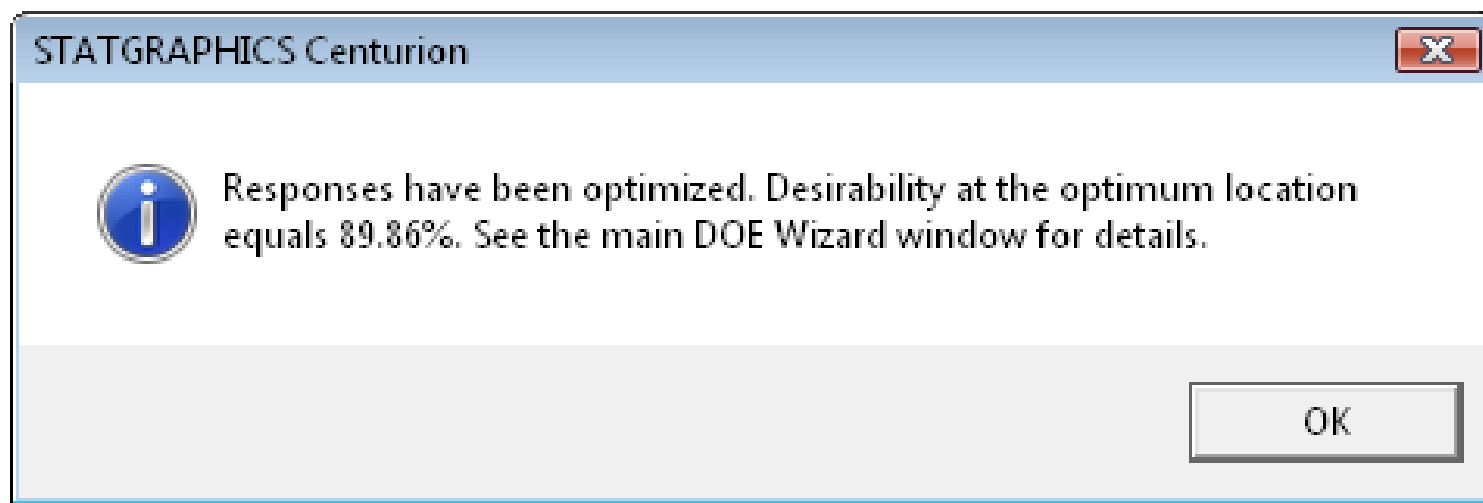
Standardized Pareto Chart for thermal activity



Step 9: Optimize responses



Step 9: Optimize responses (cont.)



Step 9: Optimize responses (cont.)

The screenshot shows the 'Experimental Design Wizard' window. At the top, a series of buttons represent the steps: Step 1: Define responses, Step 2: Define exp. factors, Step 3: Select design, Step 4: Specify model, Step 5: Select runs, Step 6: Evaluate design, Step 7: Save experiment, Step 8: Analyze data, Step 9: Optimize responses (highlighted), Step 10: Save results, Step 11: Augment design, and Step 12: Extrapolate.

Below the buttons, the main area is titled 'Step 9: Optimize the responses'. It contains the following information:

Response Values at Optimum

Response	Optimized	Prediction	Lower 95.0% Limit	Upper 95.0% Limit
conversion	yes	96.148	87.2221	105.074
thermal activity	yes	57.5	56.5677	58.4323

Desirability

0.807398
1.0

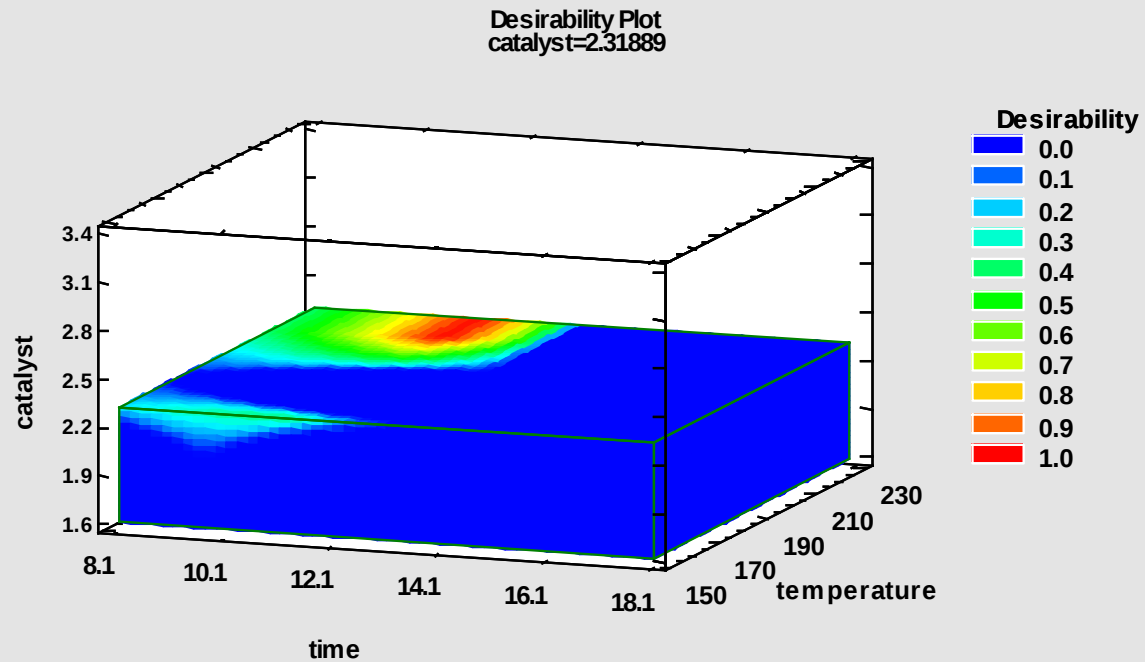
Optimized desirability = 0.898553

Factor Settings at Optimum

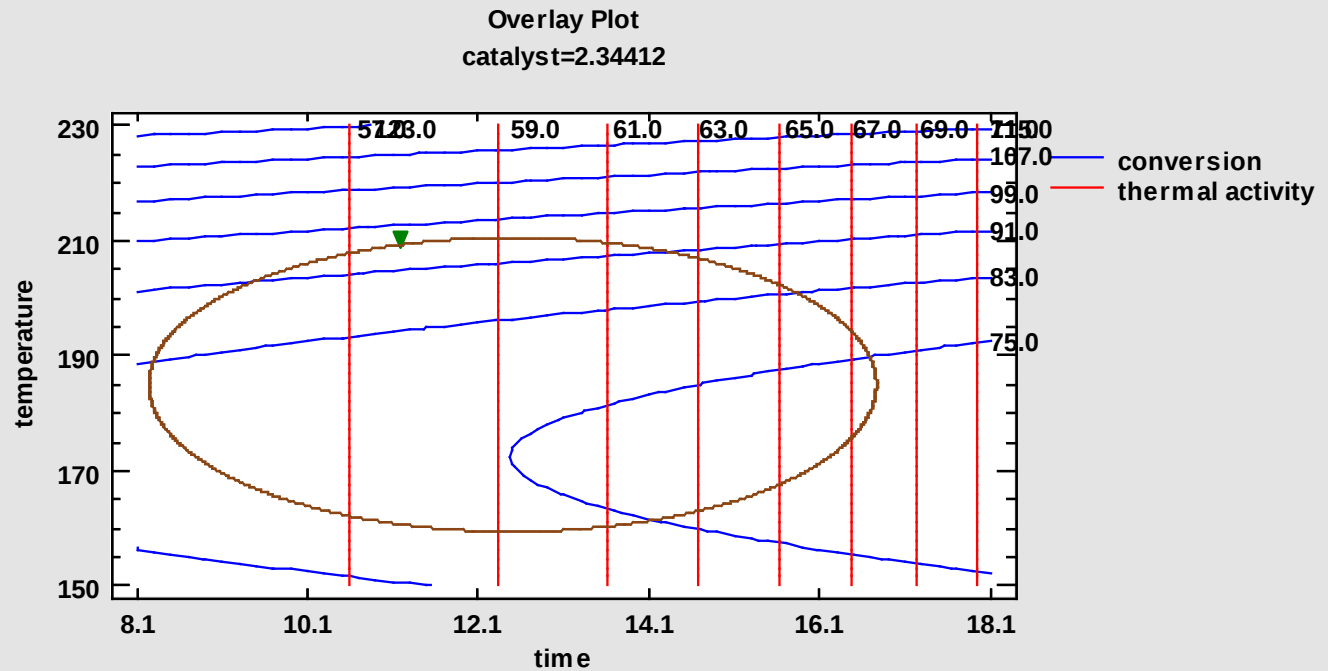
Factor	Setting
time	11.2019
temperature	210.0
catalyst	2.31889



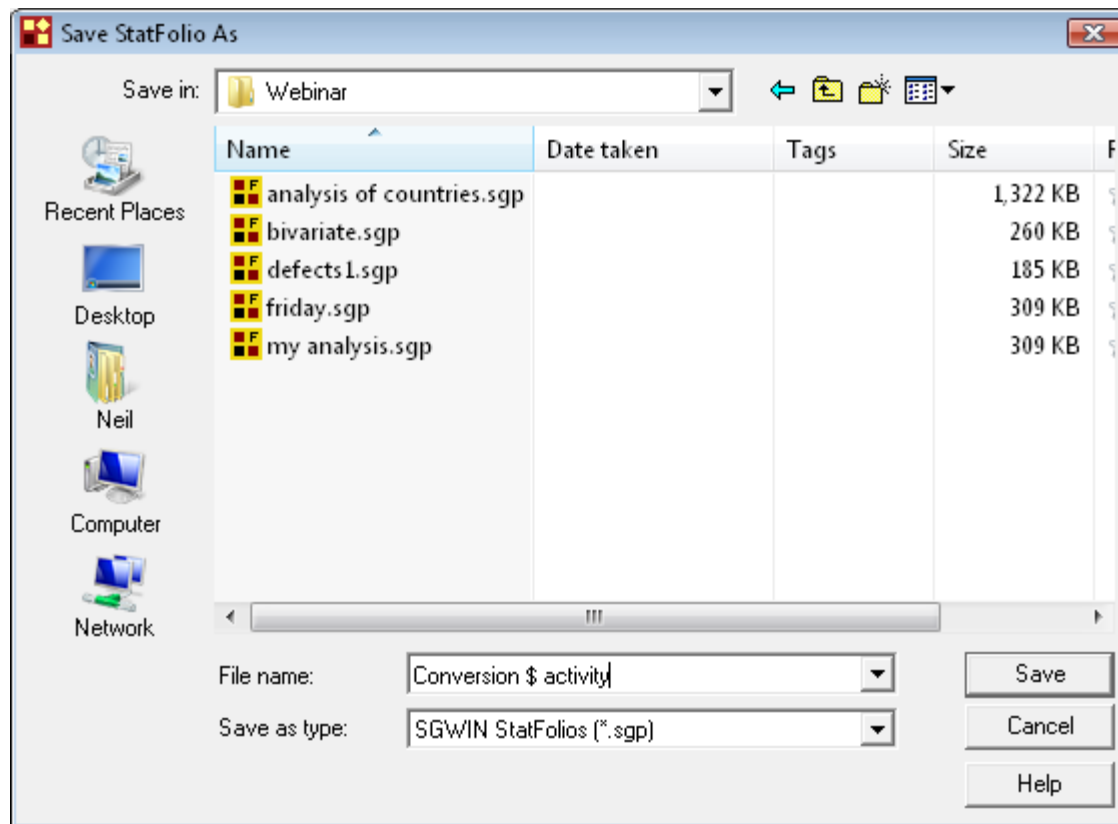
3-D contour plot



Overlaid contour plots



Step 10: Save results



Step 11: Augment design

Design of Experiments Wizard - Augment Design

	BLOCK	time minutes	temperature degrees C	catalyst %
1	1	10.0	170.0	2.0
2	1	15.0	170.0	2.0
3	1	10.0	200.0	2.0
4	1	15.0	200.0	2.0
5	1	10.0	170.0	3.0
6	1	15.0	170.0	3.0
7	1	10.0	200.0	3.0
8	1	15.0	200.0	3.0
9	1	8.3	185.0	2.5
10	1	16.7	185.0	2.5
11	1	12.5	160.0	2.5
12	1	12.5	210.0	2.5
13	1	12.5	185.0	1.66

Action

Add replicates: 1

Add a fraction

Clear main effects

Clear a factor: clear time

Add star points

Total runs: 20

Total blocks: 1

OK Cancel Reset Help



Step 12: Extrapolate

Extrapolation Options

Start at:

- ☒ Center of design
- ☐ Best observed design point
- ☐ Best predicted design point
- ☐ Best predicted vertex
- ☐ Derived optimum
- ☐ Other

Display steps of: %

OK

Cancel

Help

More...

Change	Start	Low	High
☒ time	11.2019	10.0	15.0
☒ temperature	210.0	170.0	300
☒ catalyst	2.31889	2.0	3.0
☐	0.0	0.0	1.0
☐	0.0	0.0	1.0
☐	0.0	0.0	1.0
☐	0.0	0.0	1.0
☐	0.0	0.0	1.0
☐	0.0	0.0	1.0
☐	0.0	0.0	1.0
☐	0.0	0.0	1.0
☐	0.0	0.0	1.0
☐	0.0	0.0	1.0



Step 12: Extrapolate (cont.)

The screenshot shows the 'Experimental Design Wizard' window. The top navigation bar includes steps from 1 to 12. Step 12, 'Extrapolate', is the active step. The main content area displays 'Step 12: Extrapolate model' and 'Extrapolated Response Values'.

Extrapolated Response Values

Step	Desirability	conversion	thermal activity
0	0.898546	96.148	57.4999
1	0.913903	96.7047	57.4999
2	0.929211	97.269	57.4999
3	0.94447	97.8408	57.4999
4	0.959683	98.4202	57.4999
5	0.974853	99.0072	57.4999
6	0.989981	99.6017	57.4999
7	0.99999	100.204	57.4999
8	0.99999	100.204	57.4999

Factor Settings for Extrapolation

Step	time	temperature	catalyst
0	11.2019	210.0	2.31889
1	11.2019	210.52	2.31889
2	11.2019	211.039	2.31889
3	11.2019	211.559	2.31889
4	11.2019	212.078	2.31889
5	11.2019	212.598	2.31889
6	11.2019	213.118	2.31889
7	11.2019	213.637	2.31889
8	11.2019	213.637	2.31889



More... (next webinar)

- Creating and using RPDs (Robust Parameter Designs)
- Analyzing designs with both process and mixture components
- Using D-optimal designs to fix a botched experiment



More Information

Go to www.statgraphics.com

Or send e-mail to info@statgraphics.com

