Definitive Screening Designs

Presented by
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Definitive Screening Designs

- A class of statistically designed experiments that may be used for both screening and optimization.
- Handle both quantitative and categorical factors.
- Quantitative factors are run at 3 levels, which allows the estimation of both linear and quadratic effects.
- First described by Bradley Jones and Christopher Nachtsheim in a 2011 article in the Journal of Quality Technology.

Properties

1. The required number of runs is very small, usually between 1 and 3 more than twice the number of factors.

2. Main effects are independent of two-factor interactions.

3. Two-factor interactions are not perfectly confounded with other two-factor interactions, although they are correlated.

4. For continuous factors, all of the quadratic effects can be estimated.

5. Quadratic effects are orthogonal to linear main effects and only partially confounded with two-factor interactions.

6. For designs involving 6 through 12 factors, the full second-order model can be estimated for any 3 or less factors.

DOE Wizard

- The Statgraphics DOE Wizard provides DSDs for any combination of 4 to 16 factors.

- Both blocked and unblocked designs are available.

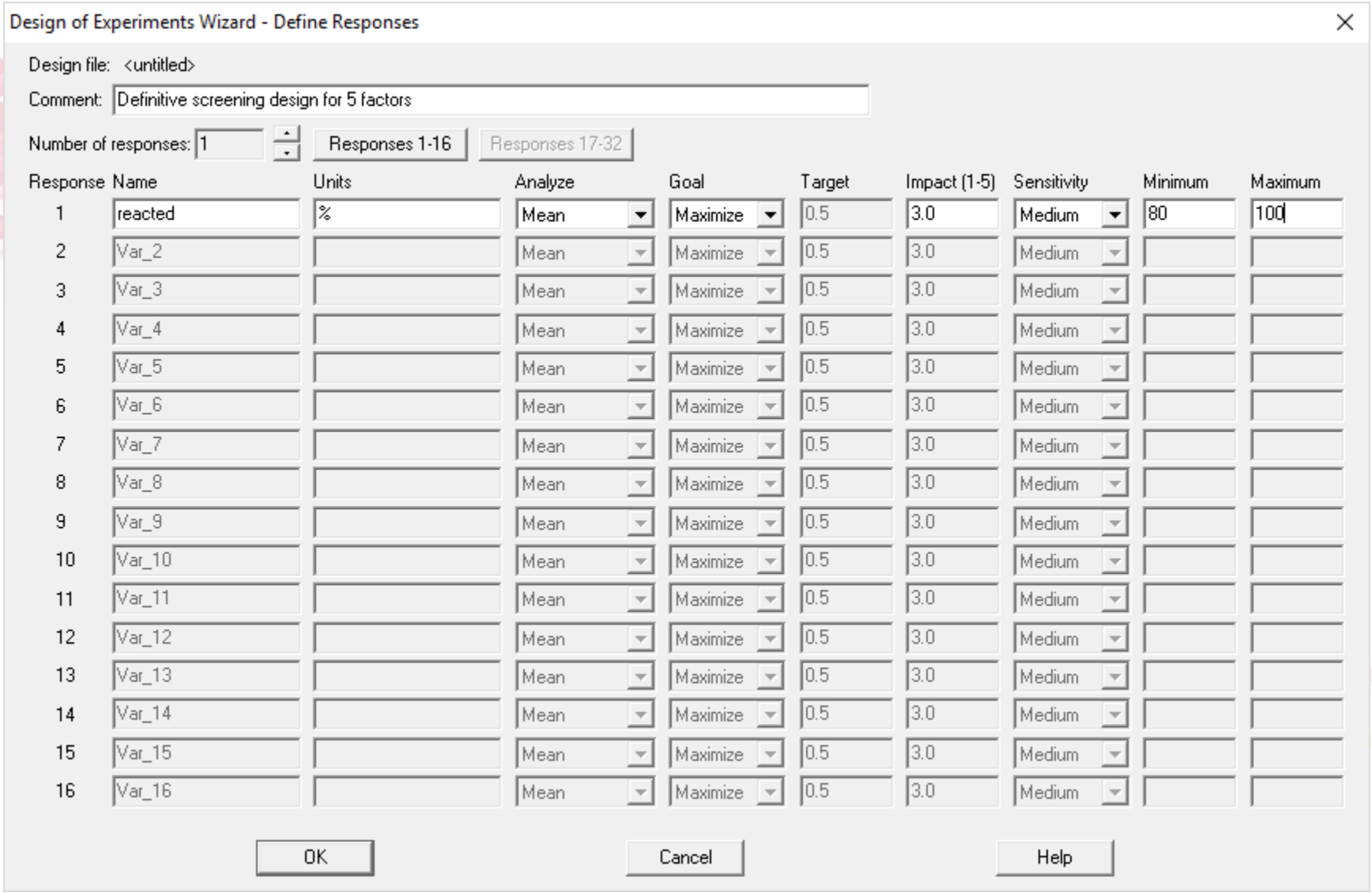
Example #1

- Optimization of a chemical reaction from Statistics for Experimenters by Box, Hunter and Hunter (2005).

- Response variable Y: *percent reacted*

- Experimental factors:
  - X1: *feed rate*
  - X2: *amount of catalyst*
  - X3: *agitation rate*
  - X4: *temperature*
  - X5: *concentration*

Step 1: Define Responses



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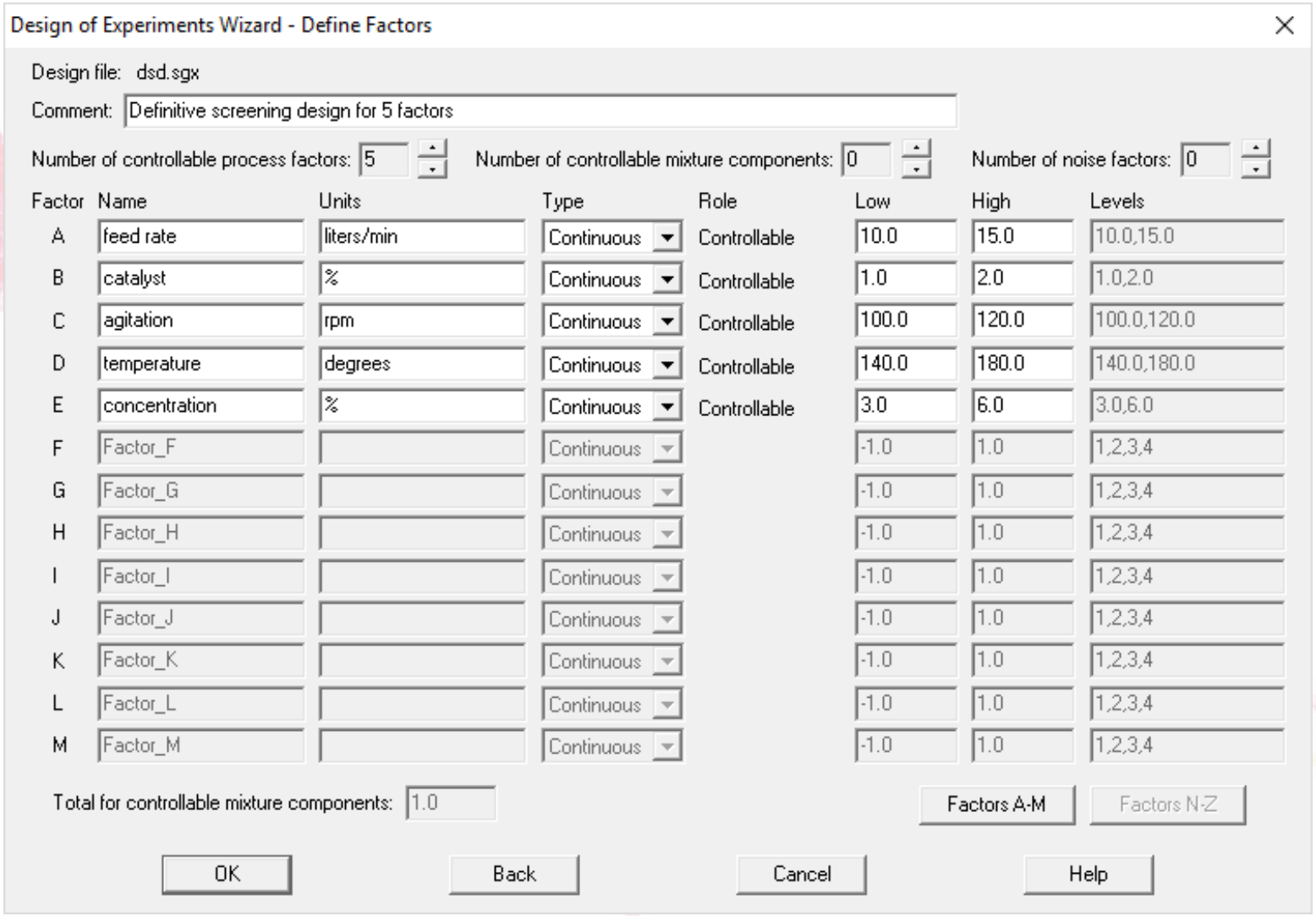
Step 2: Define Experimental Factors



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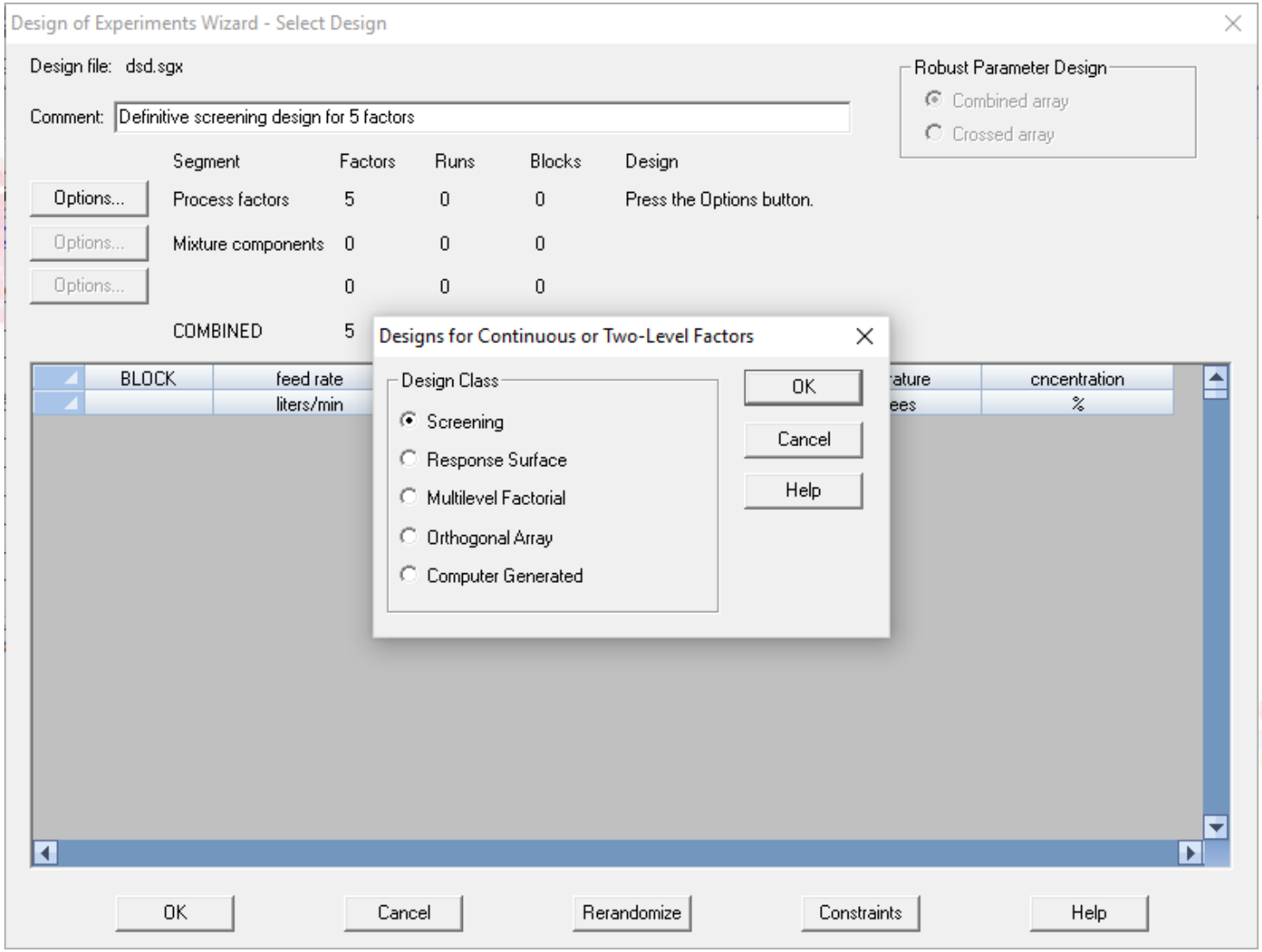
Step 3: Select Design



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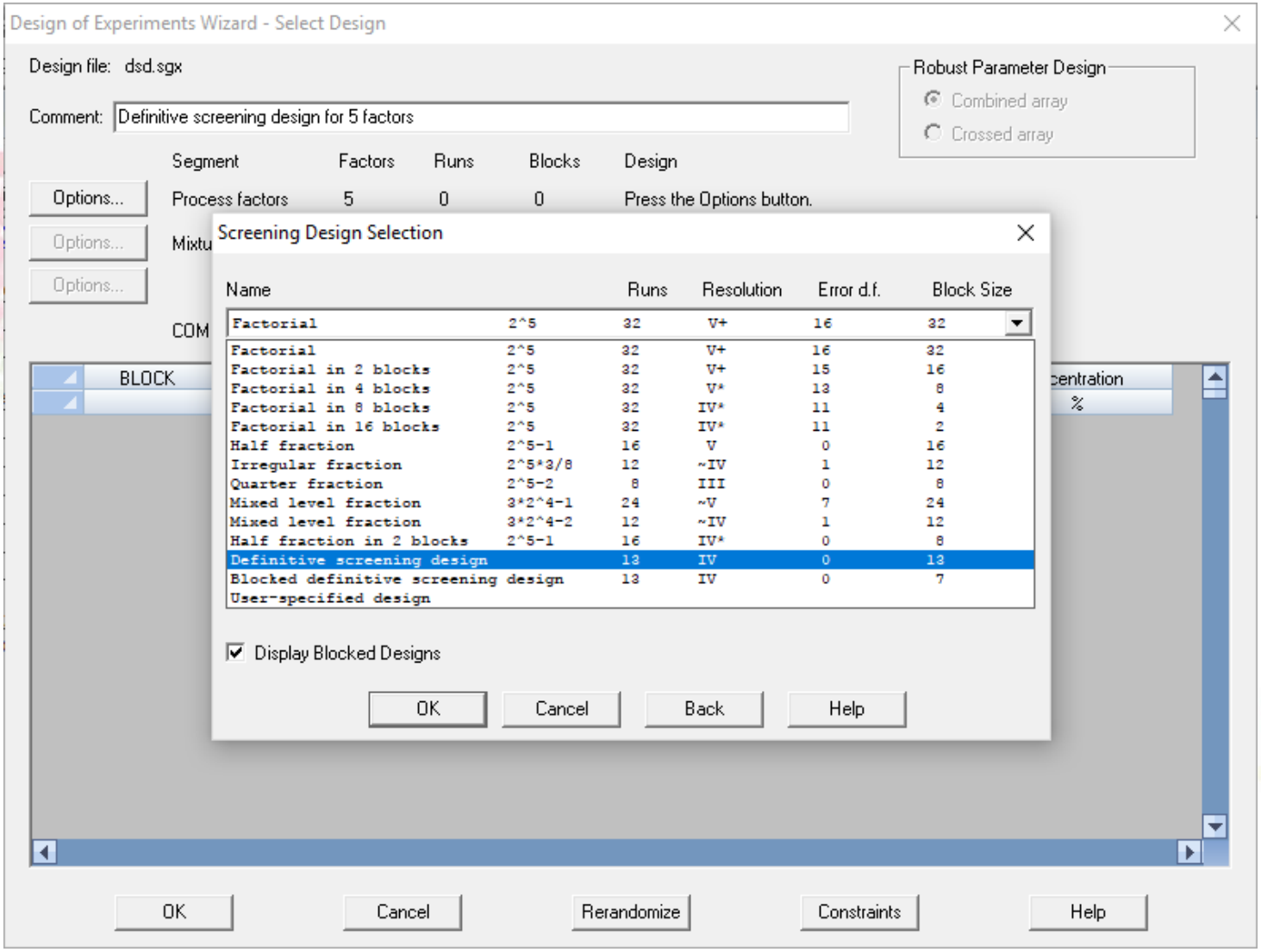
Step 3: Select Design (cont.)



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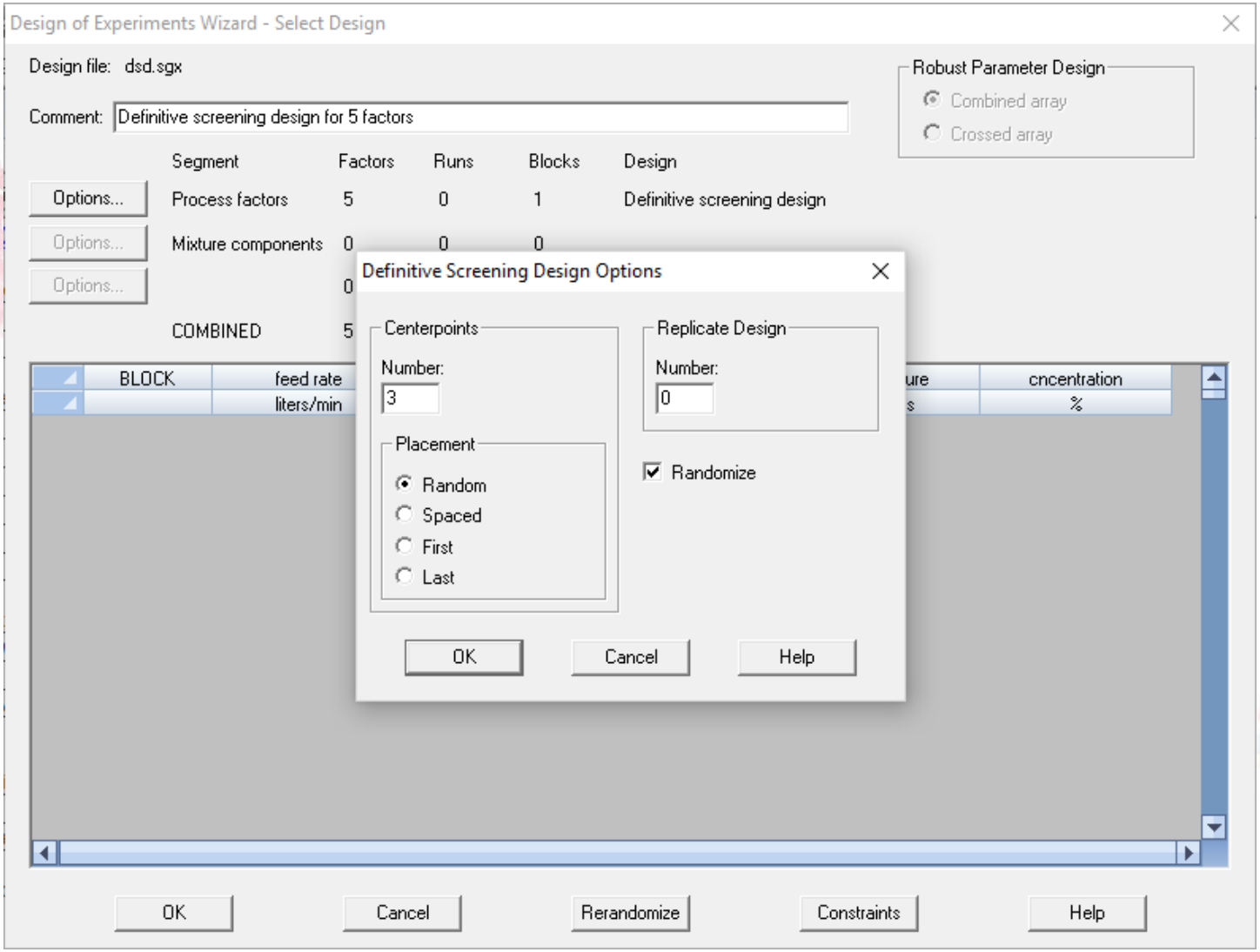
Step 3: Select Design (cont.)



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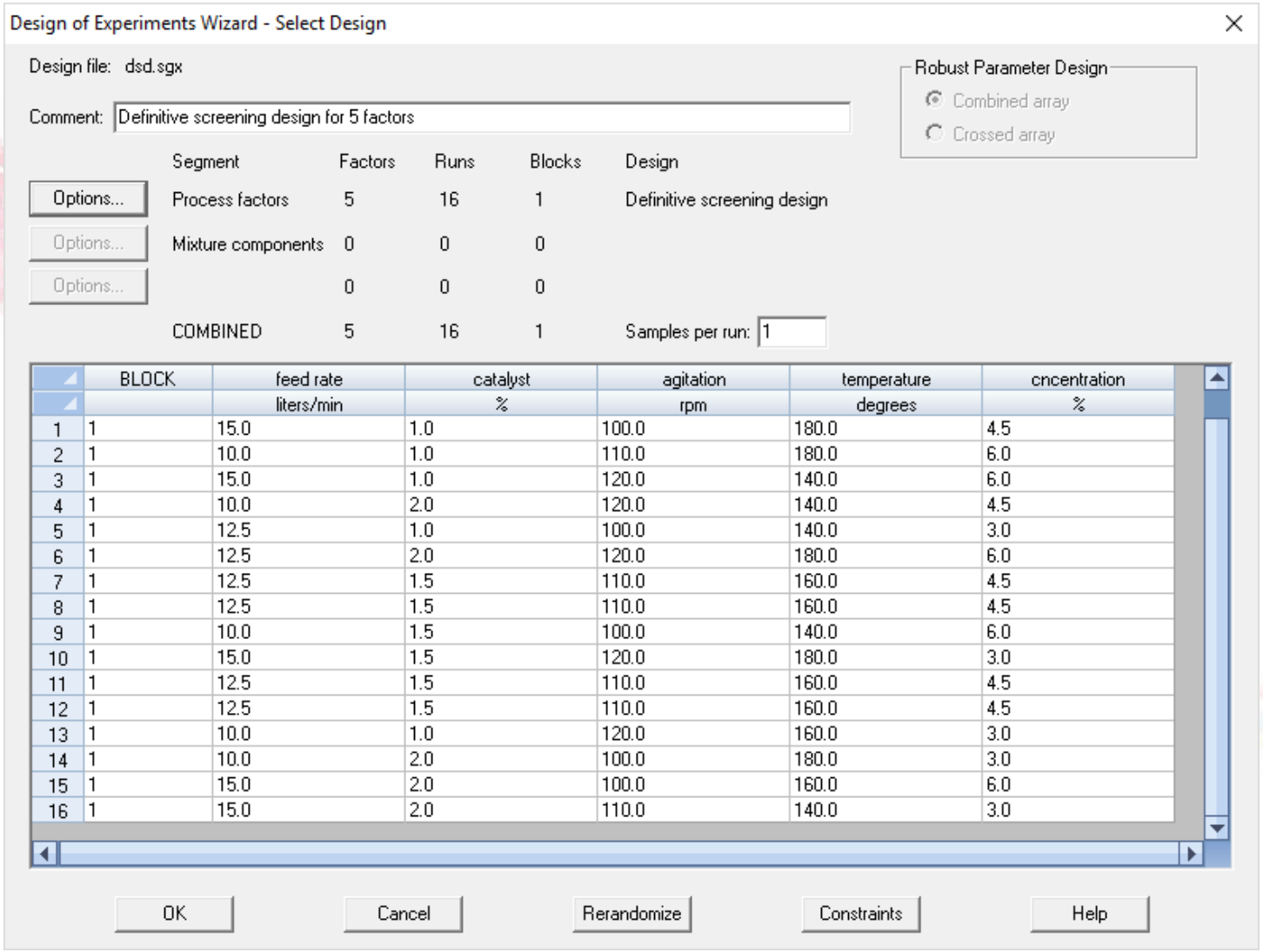
Step 3: Select Design (cont.)



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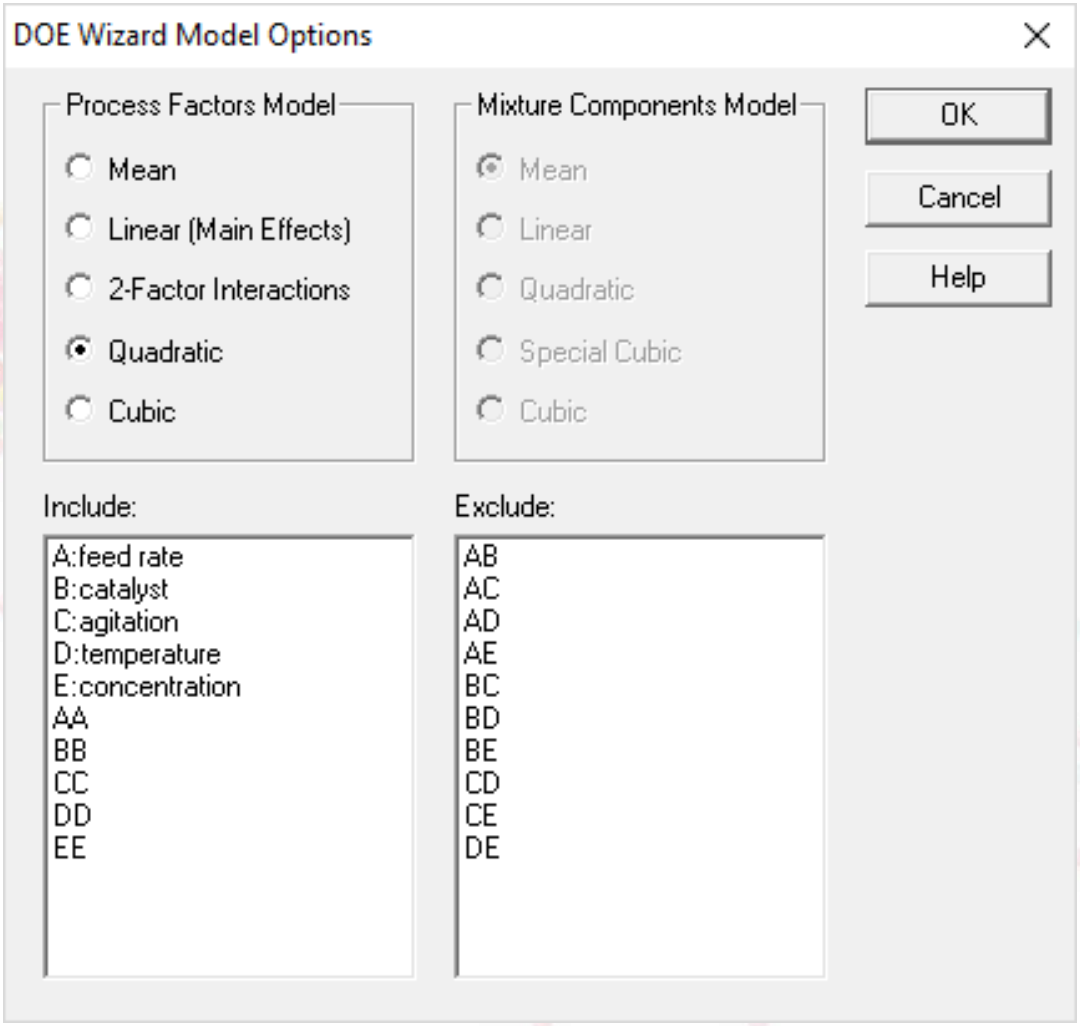
Step 4: Specify Model



Step 5: Select Runs

- Not required since the design already has the desired number of runs. This step is used for a computer generated design (such as a D-optimal design) when a subset of a large set of candidate runs needs to be selected.

Step 6: Evaluate Design

ANOVA Table

Source	D.F.
Model	10
Total Error	5
Lack-of-fit	2
Pure error	3
Total (corr.)	15

Step 6: Evaluate Design (cont.)

Model Coefficients

				Power at	*Power at*	*Power at*
Coefficient	*Standard Error*	*VIF*	*Ri-Squared*	*SN = 0.5*	*SN = 1.0*	*SN = 2.0*
constant	0.494152			7.01%	13.19%	37.52%
A	0.316228	1.0	0.0	9.96%	25.18%	71.61%
B	0.316228	1.0	0.0	9.96%	25.18%	71.61%
C	0.316228	1.0	0.0	9.96%	25.18%	71.61%
D	0.316228	1.0	0.0	9.96%	25.18%	71.61%
E	0.316228	1.0	0.0	9.96%	25.18%	71.61%
AA	0.646997	1.56977	0.362963	6.17%	9.74%	24.28%
BB	0.646997	1.56977	0.362963	6.17%	9.74%	24.28%
CC	0.646997	1.56977	0.362963	6.17%	9.74%	24.28%
DD	0.646997	1.56977	0.362963	6.17%	9.74%	24.28%
EE	0.646997	1.56977	0.362963	6.17%	9.74%	24.28%

alpha = 5.0%, sigma estimated from total error with 5 d.f.

Step 6: Evaluate Design (cont.)

Alias Matrix

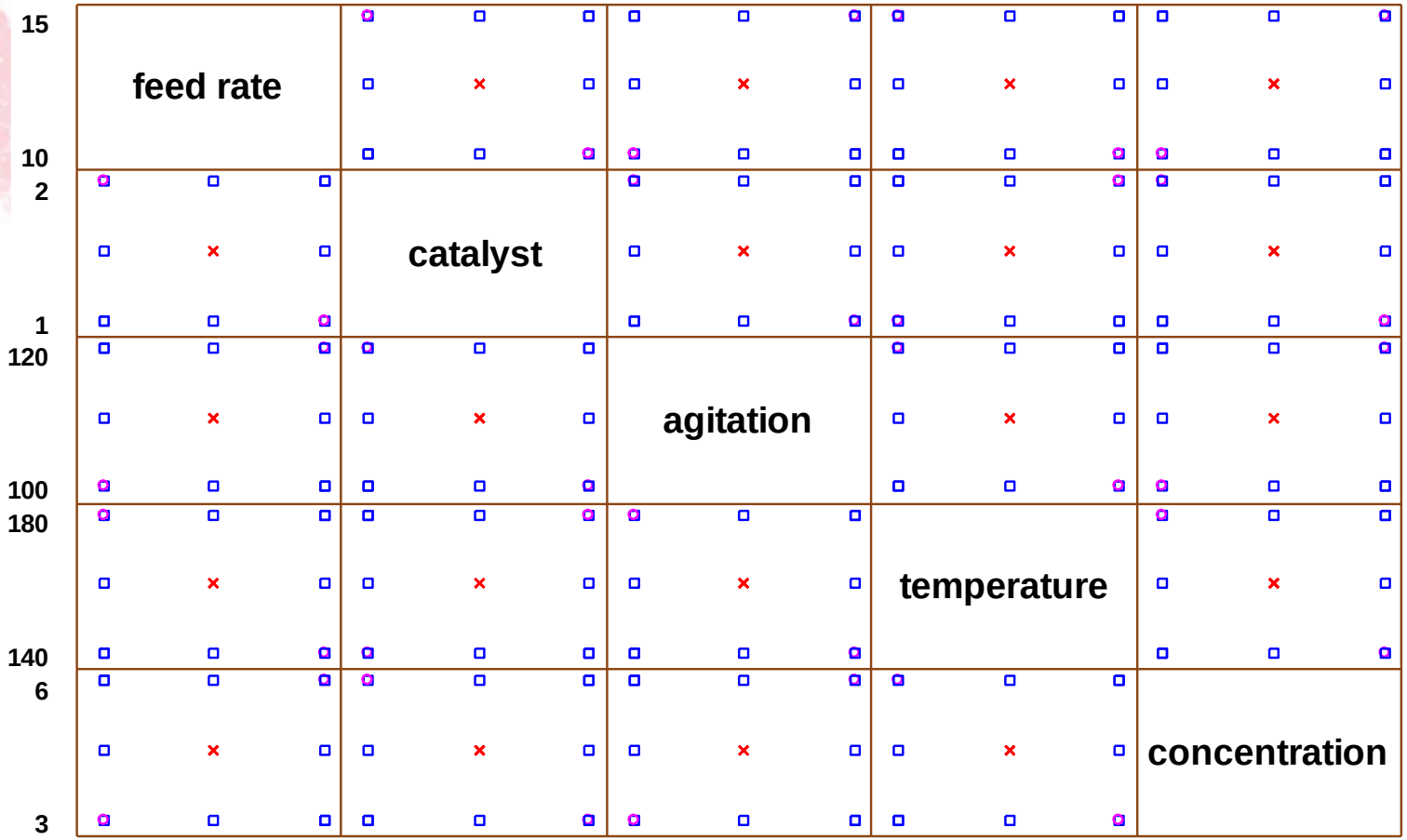
Effect	AB	AC	AD	AE	BC	BD	BE	CD	CE	DE
constant	0.1163	-0.1163	0.1163	-0.1163	0.1163	-0.1163	0.1163	0.1163	-0.1163	0.1163
A										
B										
C										
D										
E										
AA	0.1628	-0.1628	0.1628	-0.1628	-0.8372	-1.1628	-0.8372	-0.8372	-1.1628	-0.8372
BB	0.1628	-1.1628	-0.8372	0.8372	0.1628	-0.1628	0.1628	-0.8372	0.8372	1.1628
CC	-0.8372	-0.1628	1.1628	0.8372	0.1628	0.8372	1.1628	0.1628	-0.1628	-0.8372
DD	-0.8372	0.8372	0.1628	-1.1628	1.1628	-0.1628	-0.8372	0.1628	0.8372	0.1628
EE	1.1628	0.8372	-0.8372	-0.1628	-0.8372	0.8372	0.1628	1.1628	-0.1628	0.1628

Step 6: Evaluate Design (cont.)

Correlation Matrix

	A	B	C	D	E	AA	BB	CC	DD	EE
A	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
B	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
C	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
D	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
E	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AA	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.4667	0.4667	0.4667	0.4667
BB	0.0000	0.0000	0.0000	0.0000	0.0000	0.4667	1.0000	0.4667	0.4667	0.4667
CC	0.0000	0.0000	0.0000	0.0000	0.0000	0.4667	0.4667	1.0000	0.4667	0.4667
DD	0.0000	0.0000	0.0000	0.0000	0.0000	0.4667	0.4667	0.4667	1.0000	0.4667
EE	0.0000	0.0000	0.0000	0.0000	0.0000	0.4667	0.4667	0.4667	0.4667	1.0000

Step 6: Evaluate Design (cont.)



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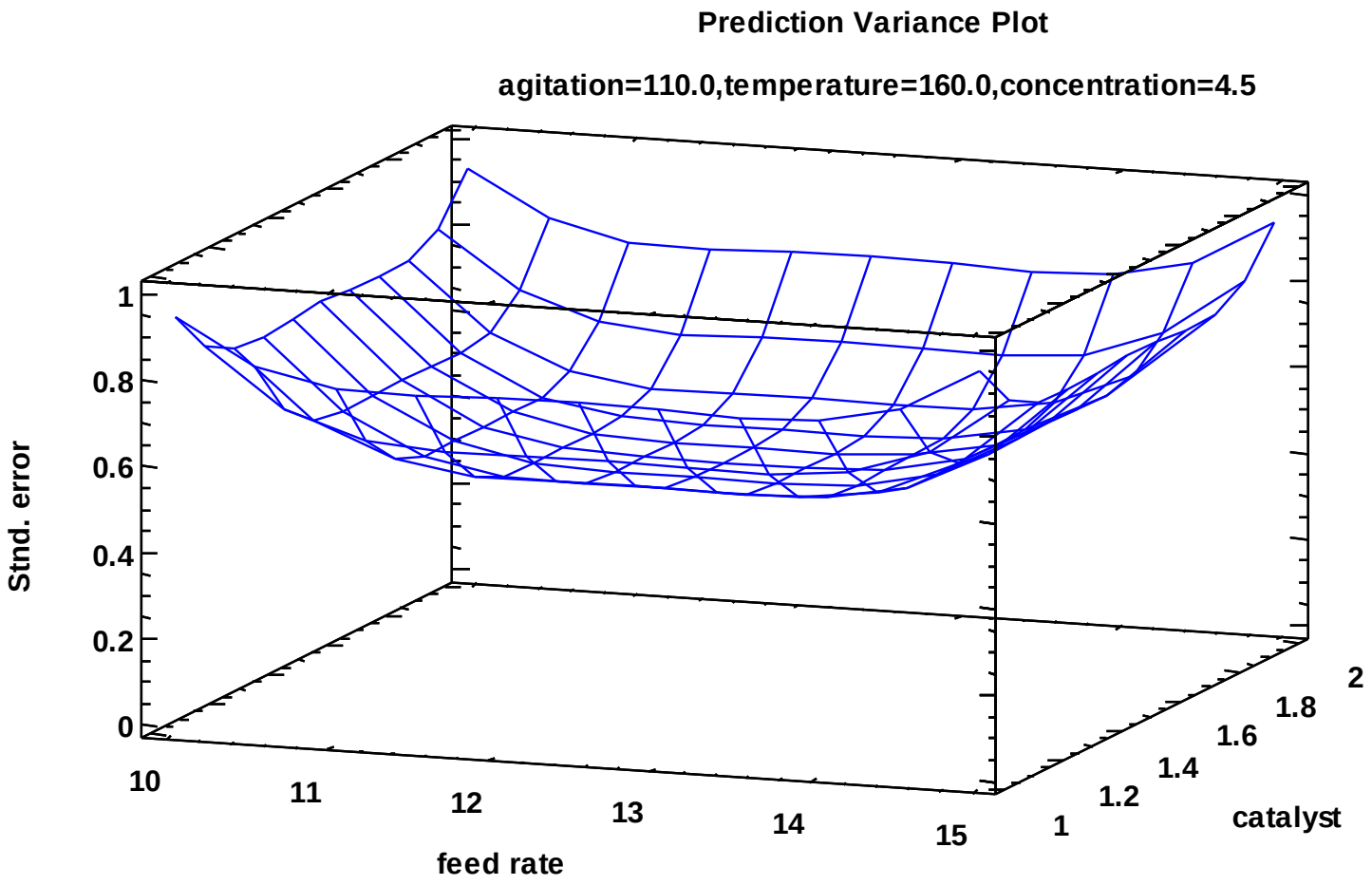
Step 6: Evaluate Design (cont.)



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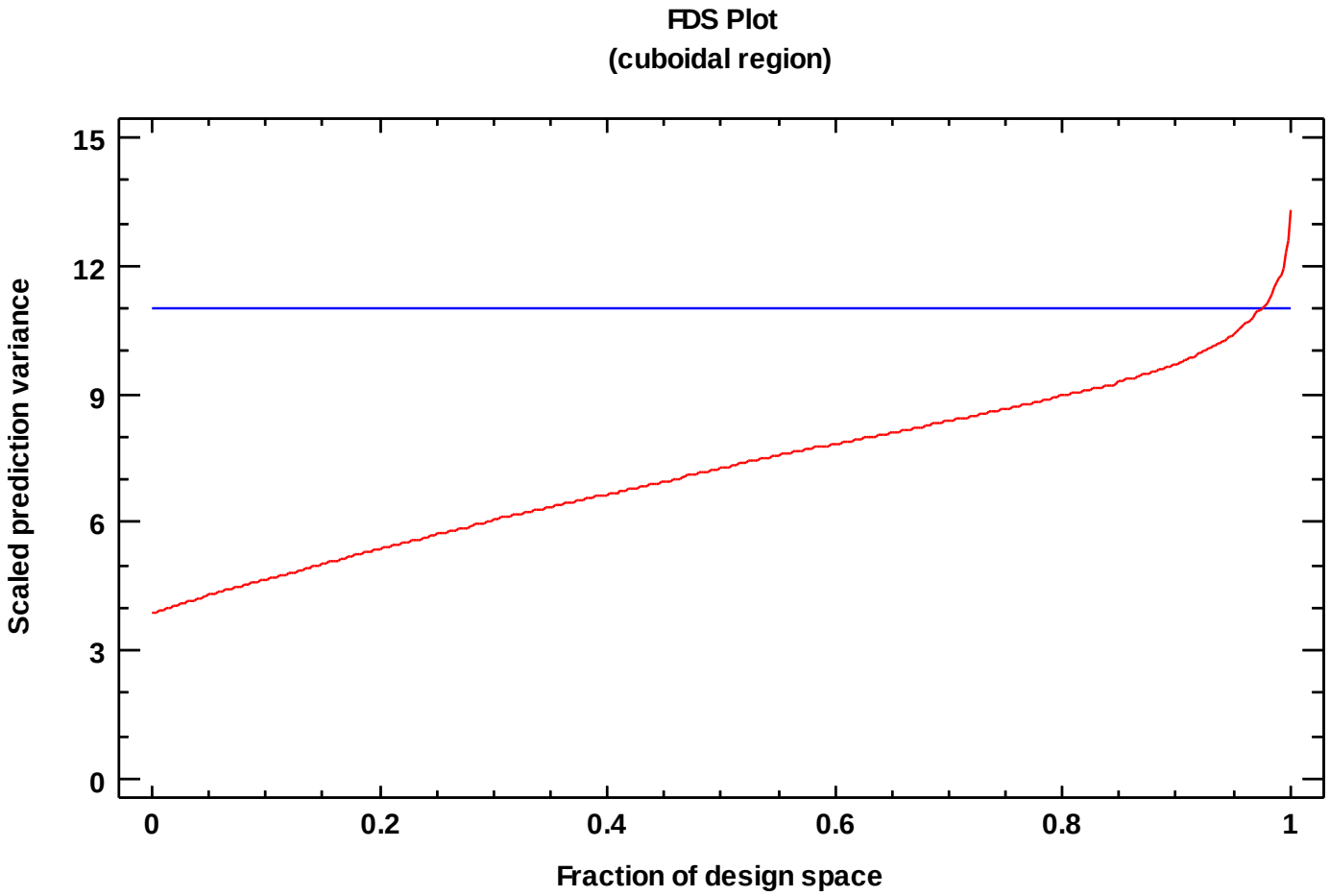
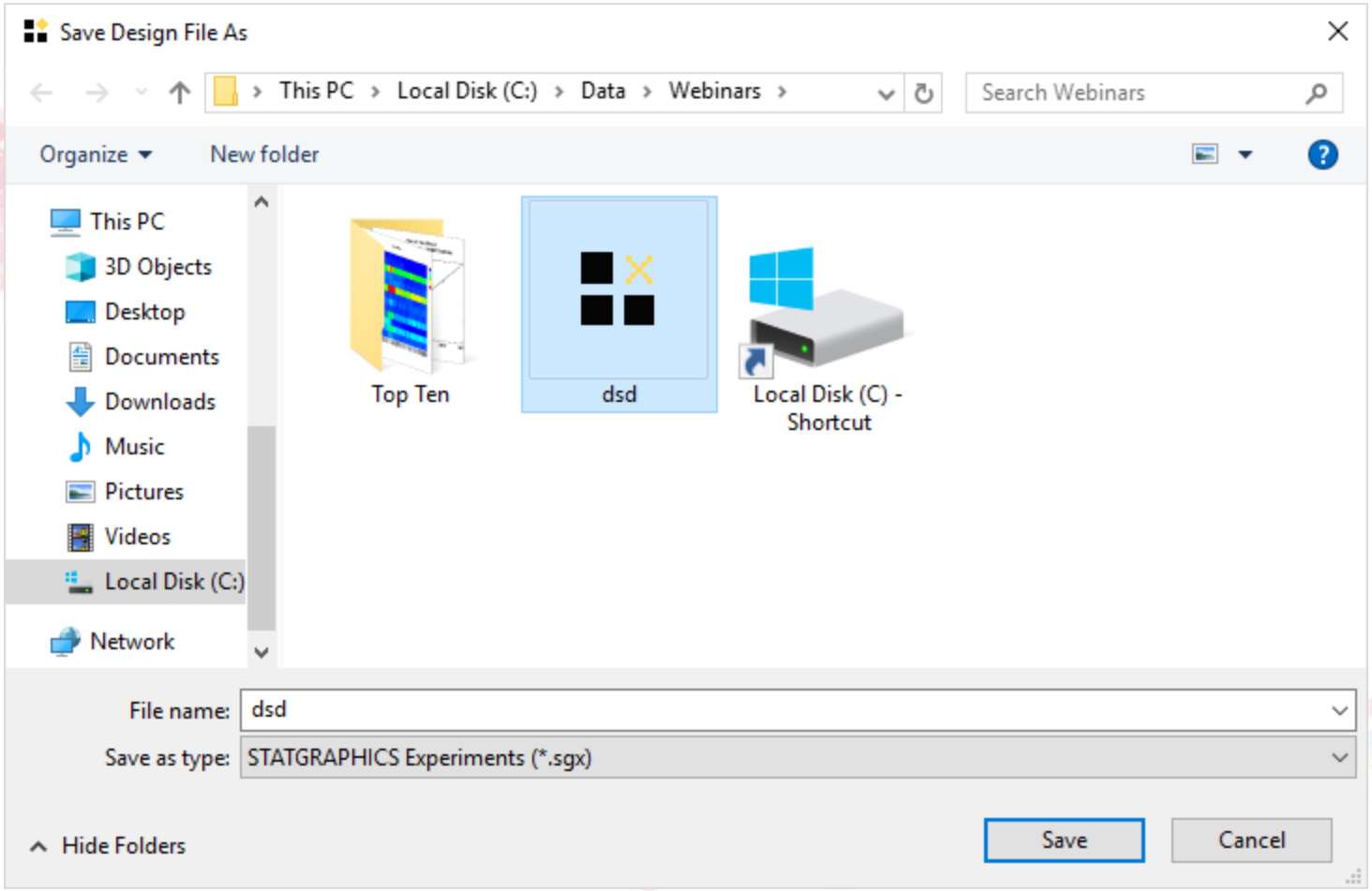
Step 6: Evaluate Design (cont.)



Step 7: Save Experiment



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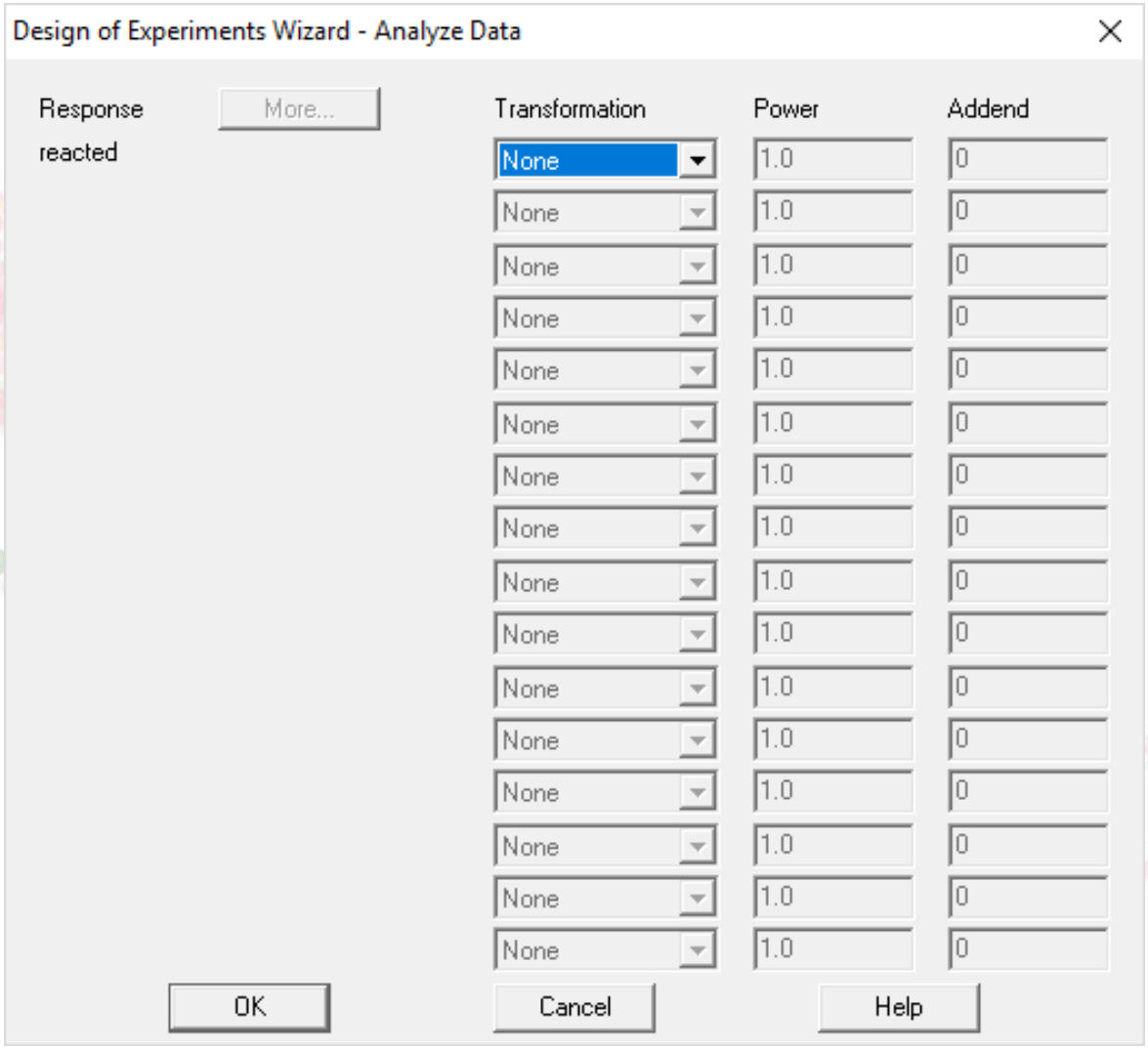
Step 8: Analyze Experiment



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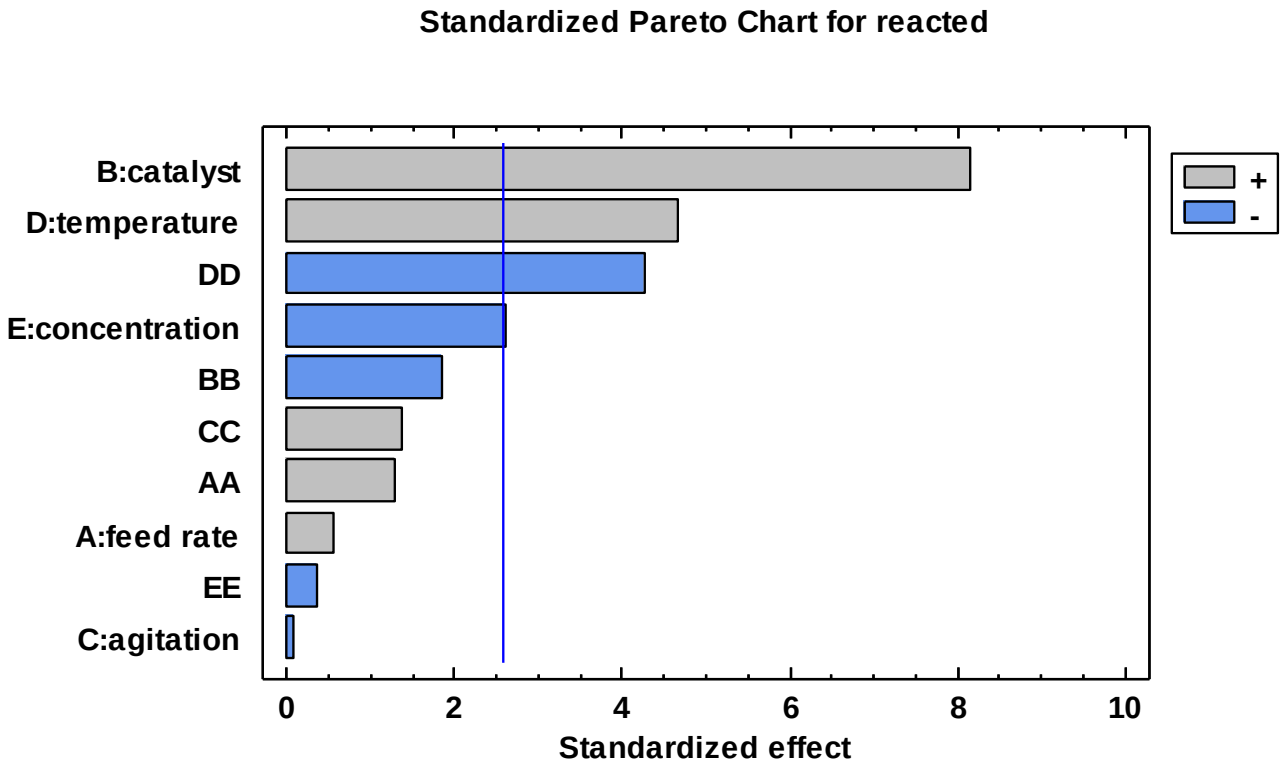
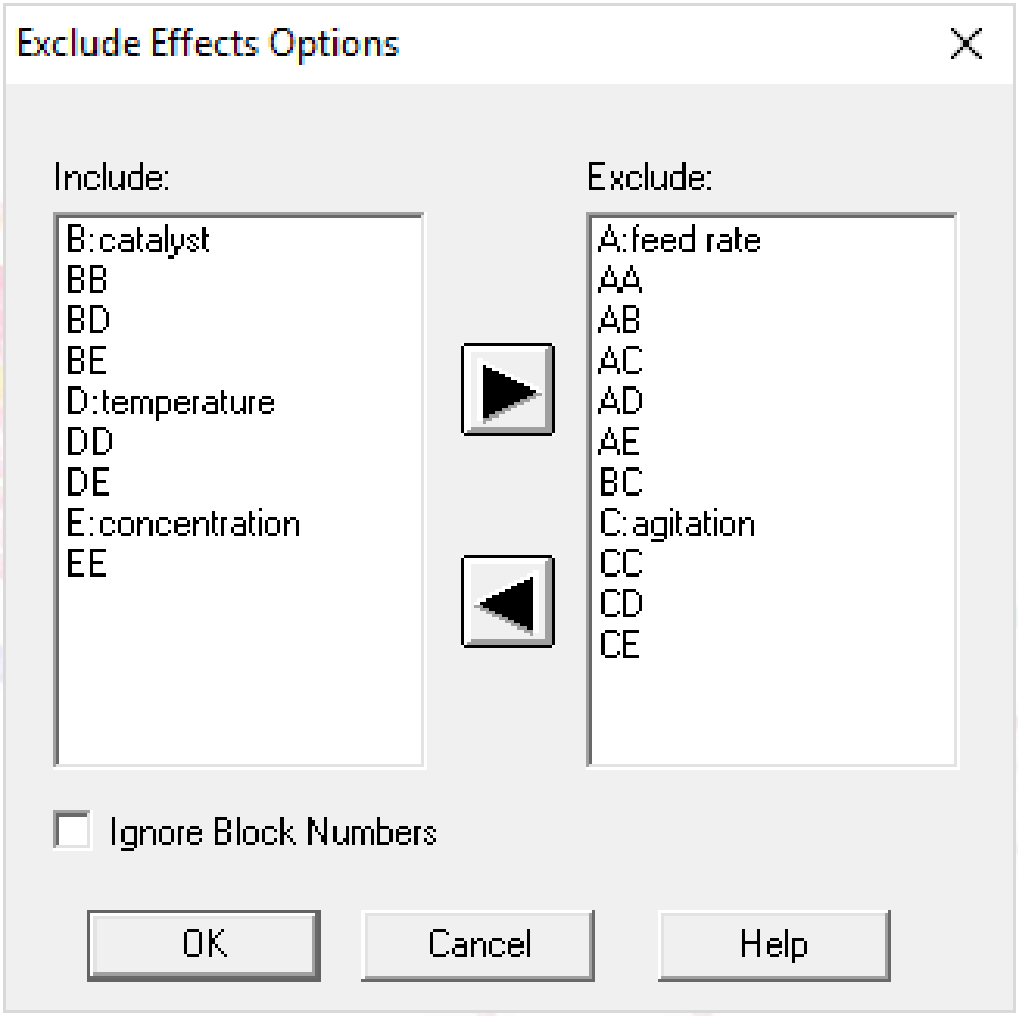
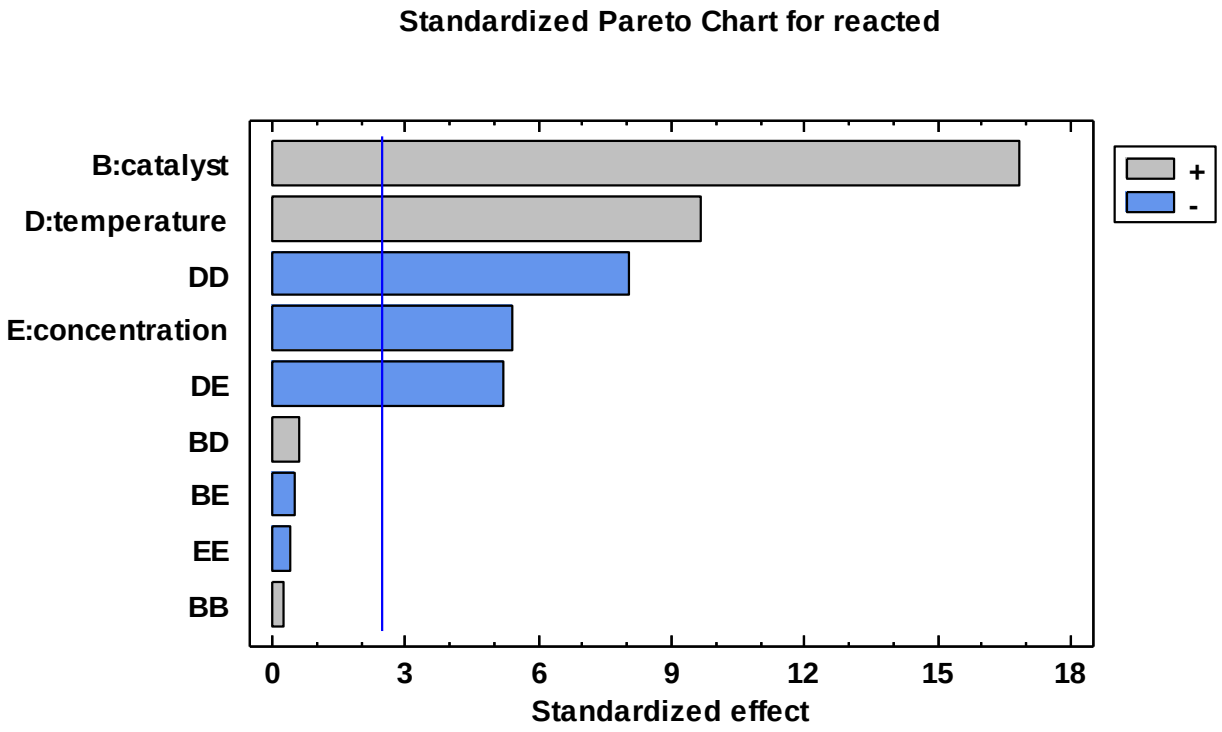
Pareto Chart of Effects



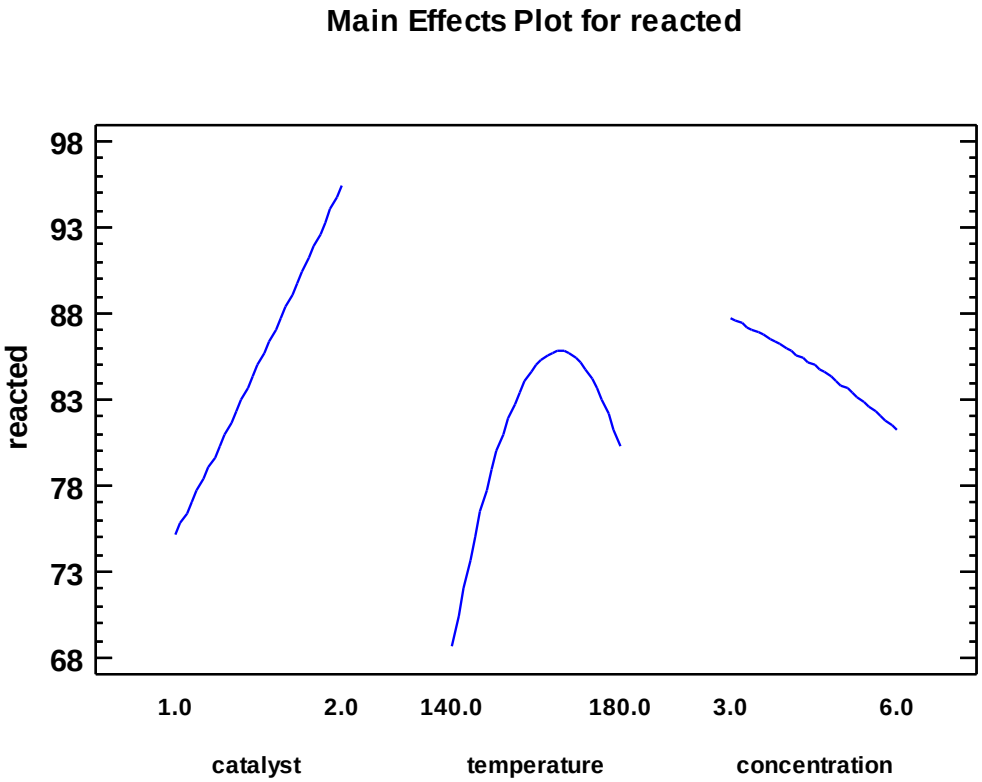
Collapse Design



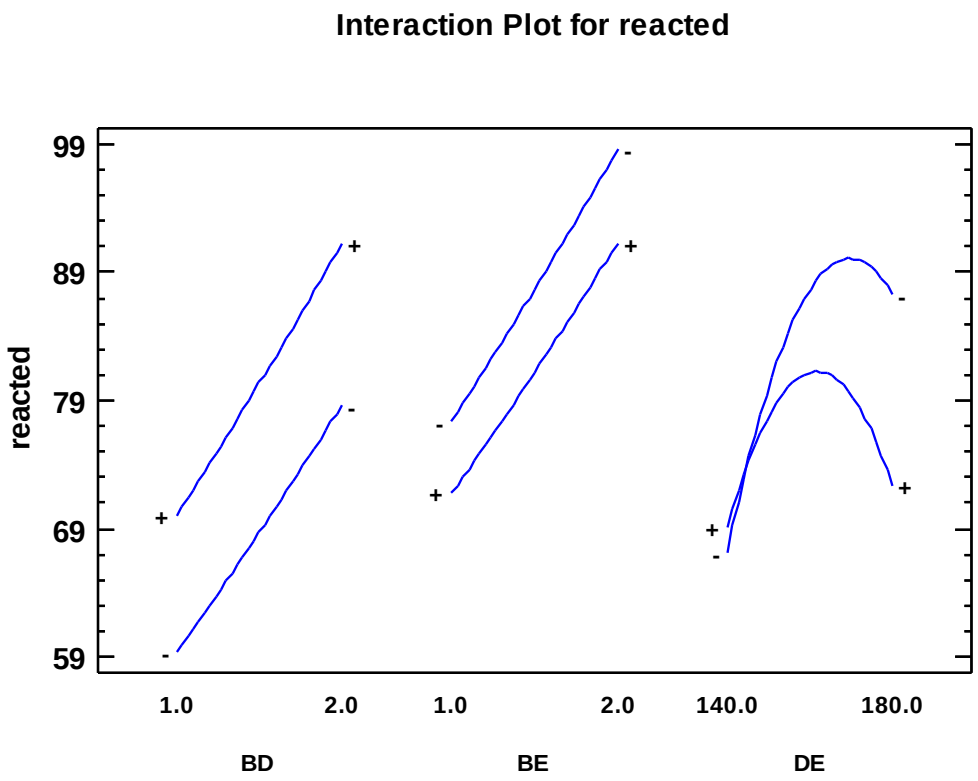
Pareto Chart for Collapsed Design



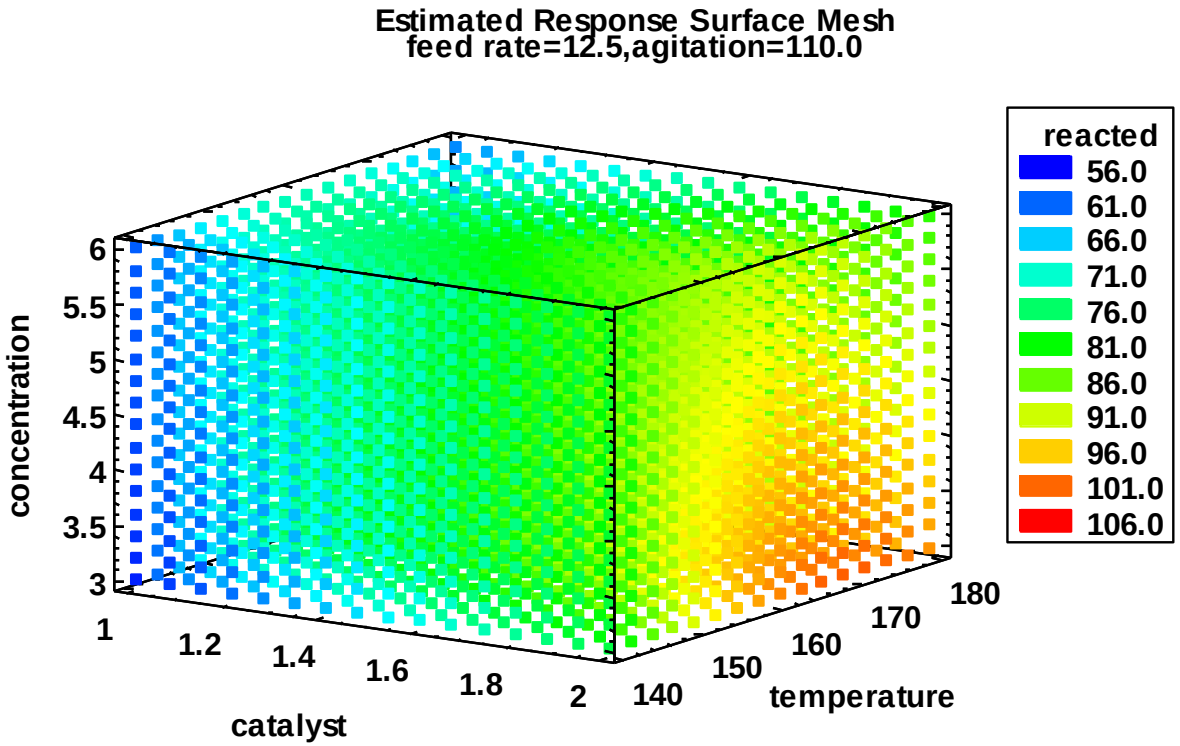
Main Effects Plot



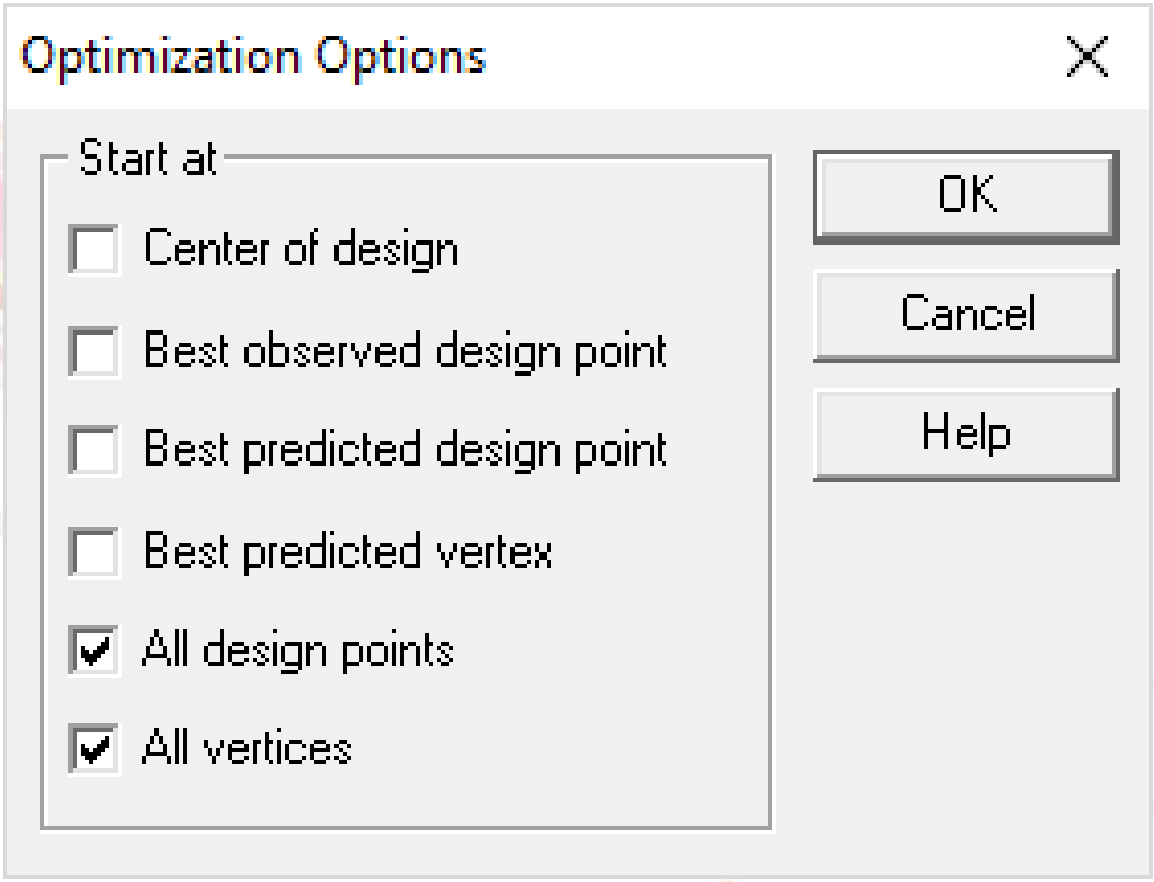
Interactions Plot



Mesh Plot



Step 9: Optimize Responses



Step 9: Optimize Responses (cont.)

Step 9: Optimize the responses

Response Values at Optimum

Response	*Optimized*	*Prediction*	*Lower 95.0% Limit*	*Upper 95.0% Limit*	*Desirability*
reacted	yes	100.484	96.4202	104.548	1.0

Factor Settings at Optimum

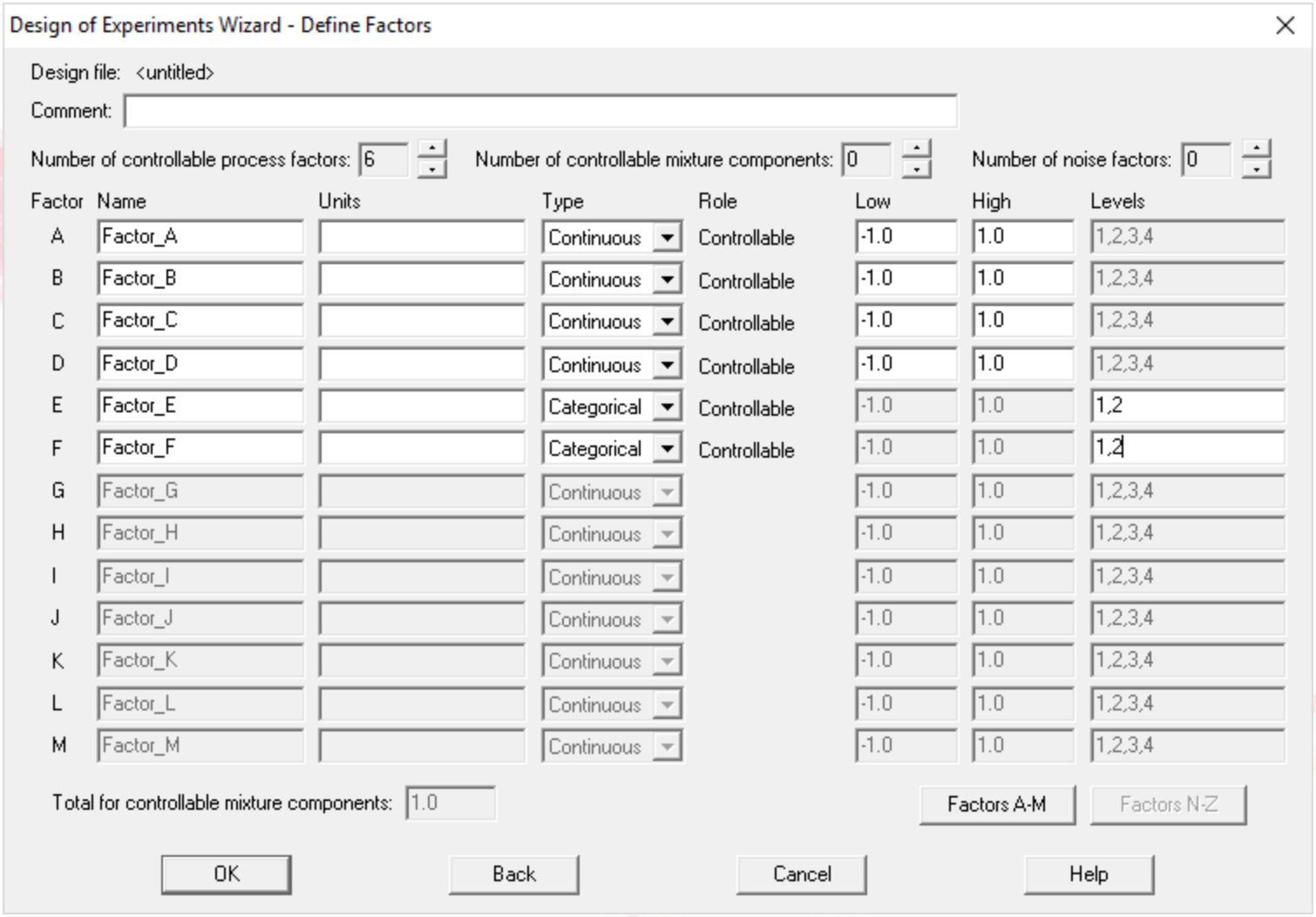
Factor	*Setting*
feed rate	11.1915
catalyst	1.99574
agitation	110.873
temperature	174.566
concentration	3.01764

Designs with Categorical Factors

- DSDs may also contain 2-level categorical factors.

- The next example shows a design with 4 continuous factors and 2 categorical factors.

Example #2



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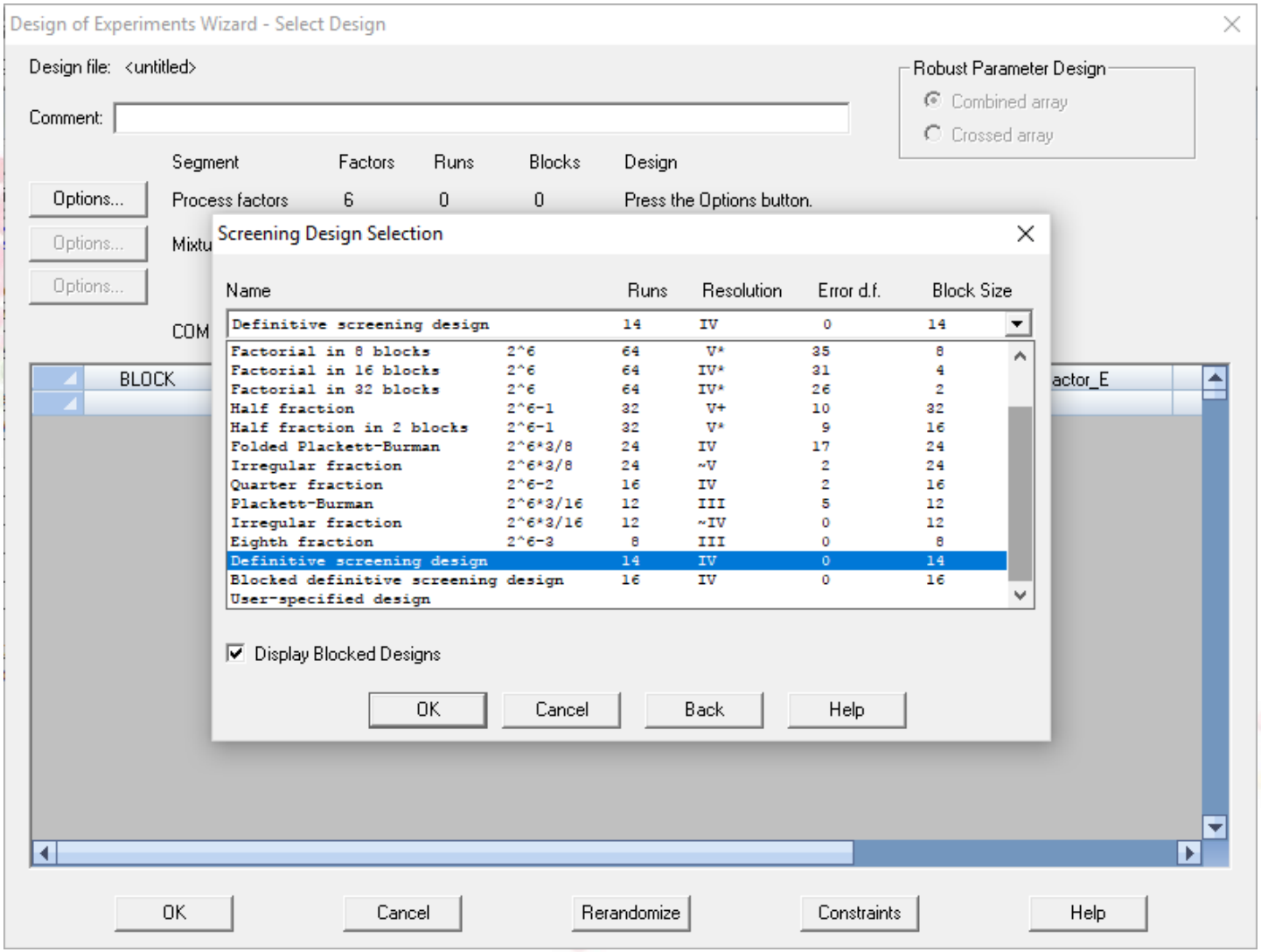
Example #2 (cont.)



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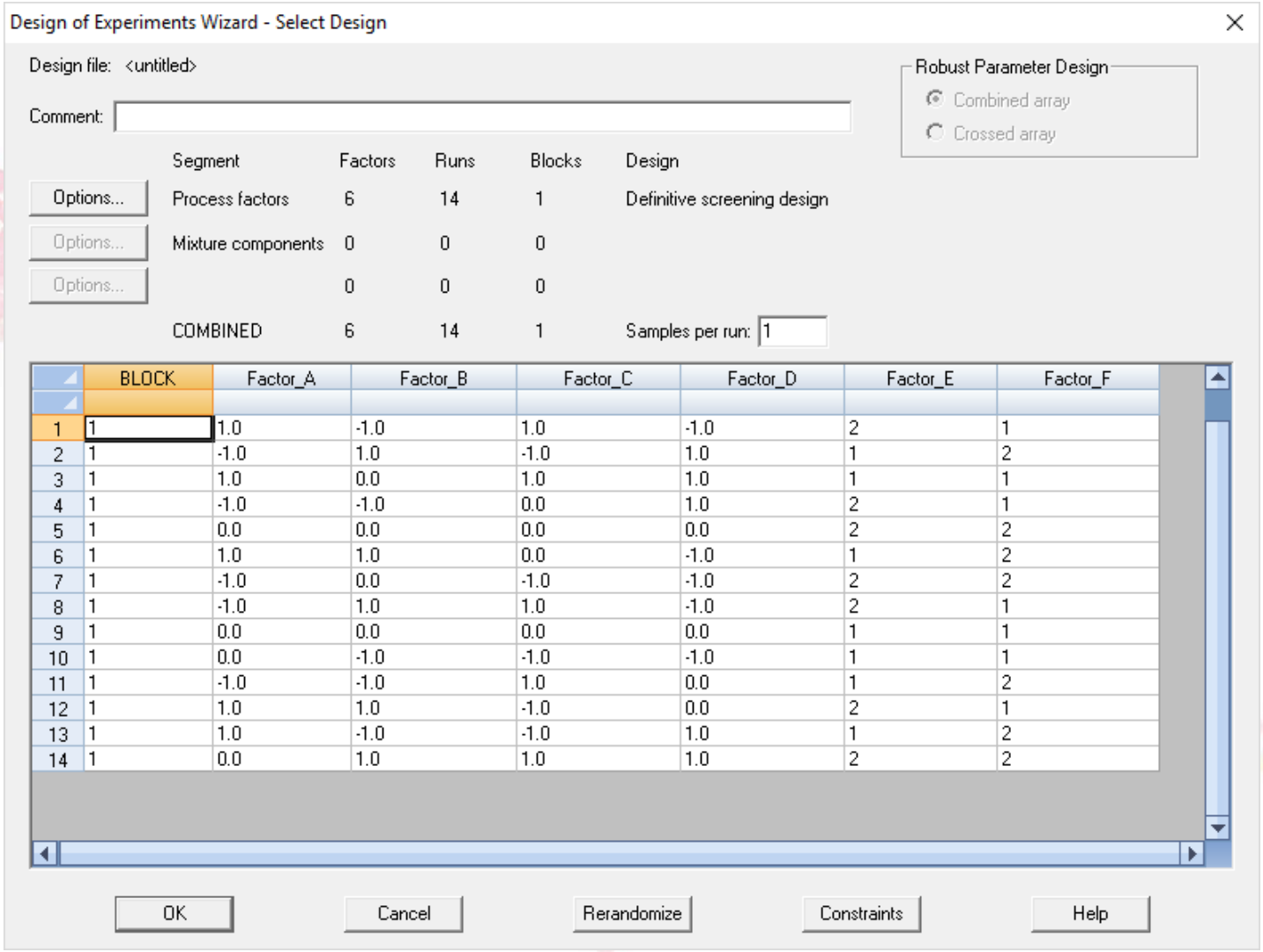
Example #2 (cont.)

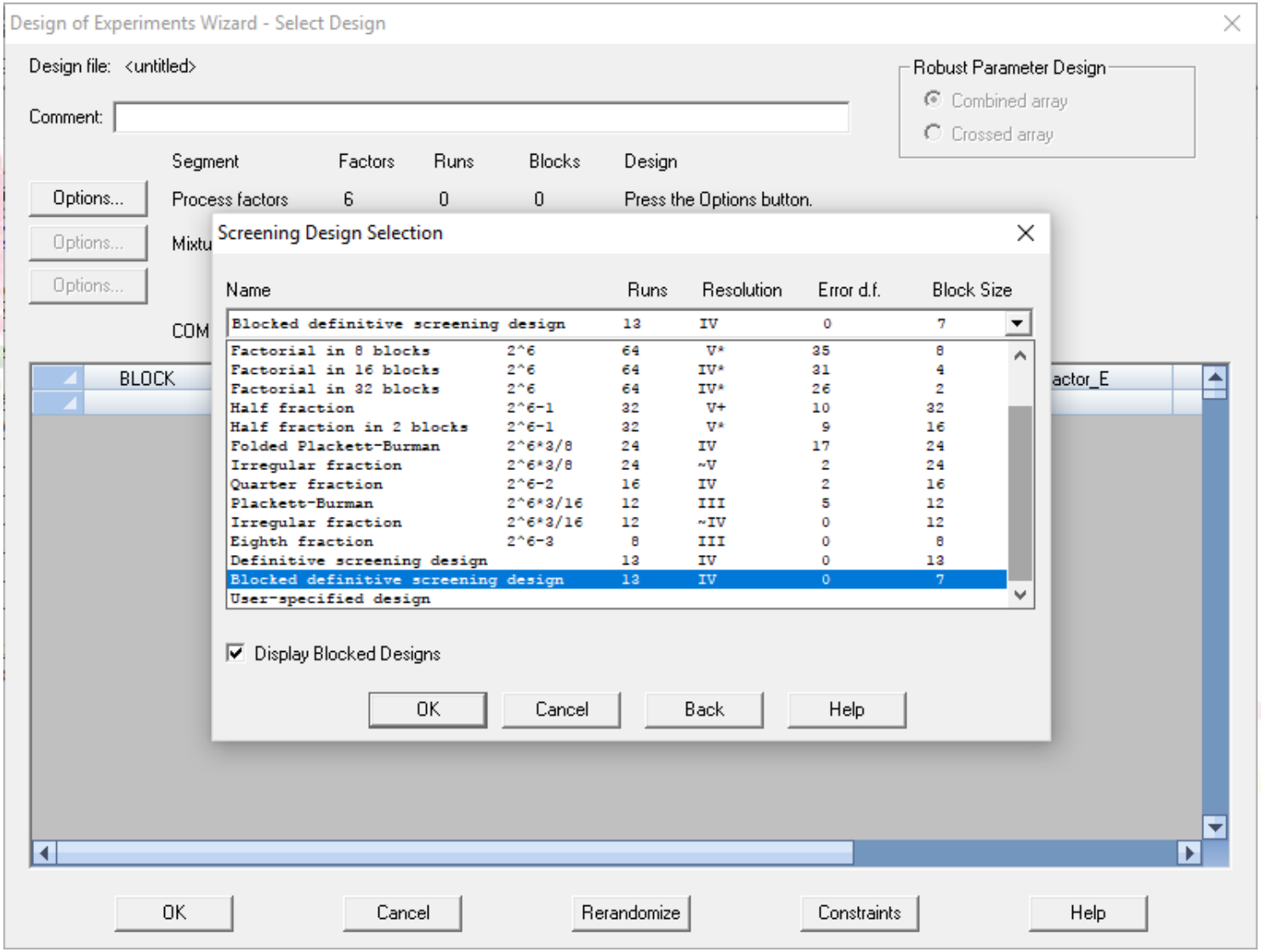


	BLOCK	Factor_A	Factor_B	Factor_C	Factor_D	Factor_E	Factor_F
1	1	1.0	-1.0	1.0	-1.0	2	1
2	1	-1.0	1.0	-1.0	1.0	1	2
3	1	1.0	0.0	1.0	1.0	1	1
4	1	-1.0	-1.0	0.0	1.0	2	1
5	1	0.0	0.0	0.0	0.0	2	2
6	1	1.0	1.0	0.0	-1.0	1	2
7	1	-1.0	0.0	-1.0	-1.0	2	2
8	1	-1.0	1.0	1.0	-1.0	2	1
9	1	0.0	0.0	0.0	0.0	1	1
10	1	0.0	-1.0	-1.0	-1.0	1	1
11	1	-1.0	-1.0	1.0	0.0	1	2
12	1	1.0	1.0	-1.0	0.0	2	1
13	1	1.0	-1.0	-1.0	1.0	1	2
14	1	0.0	1.0	1.0	1.0	2	2

Designs with Blocking

- DSDs may be run in more than one block.
- The next example shows a design with 6 continuous factors divided into 2 blocks.

Example #3



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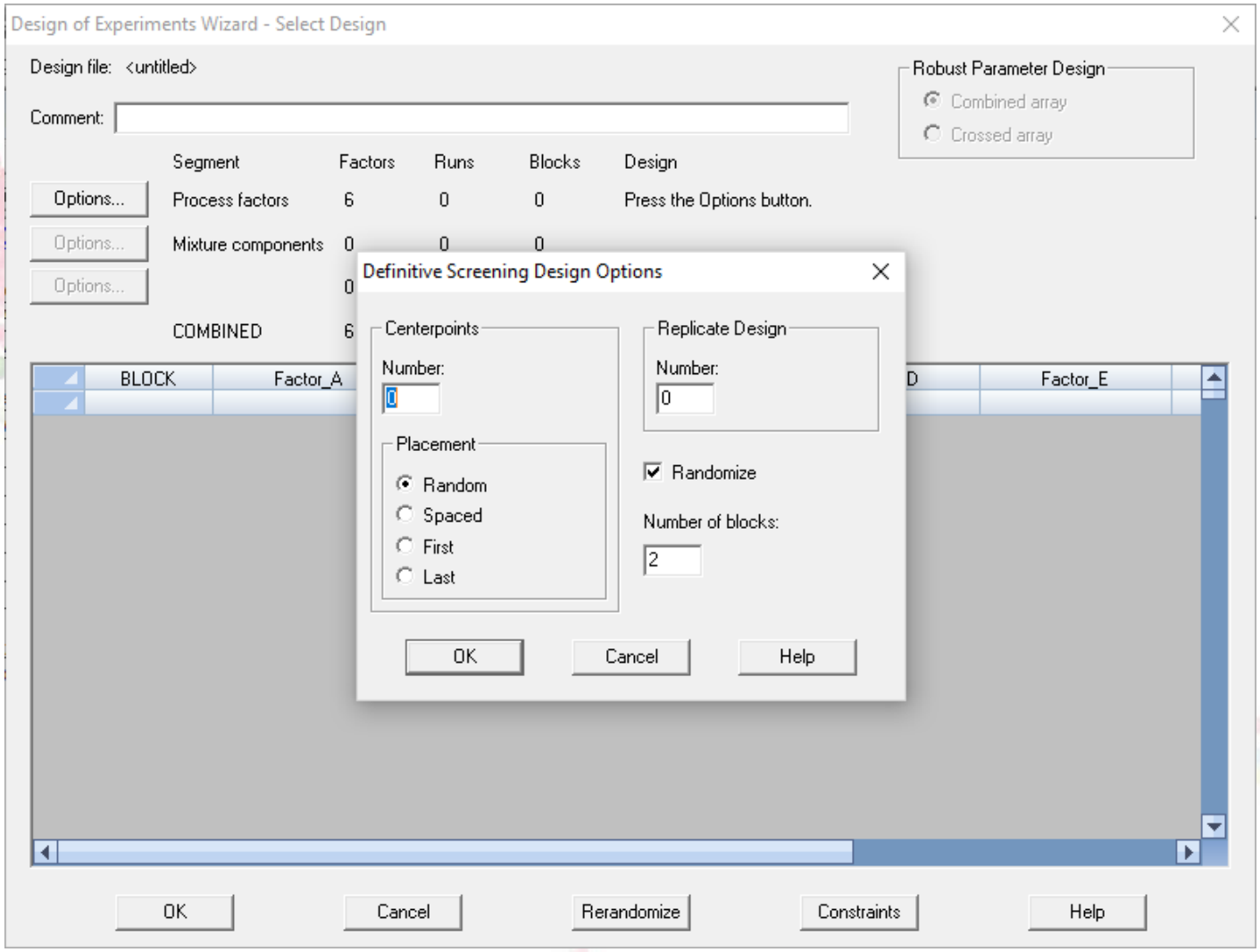
Example #3 (cont.)



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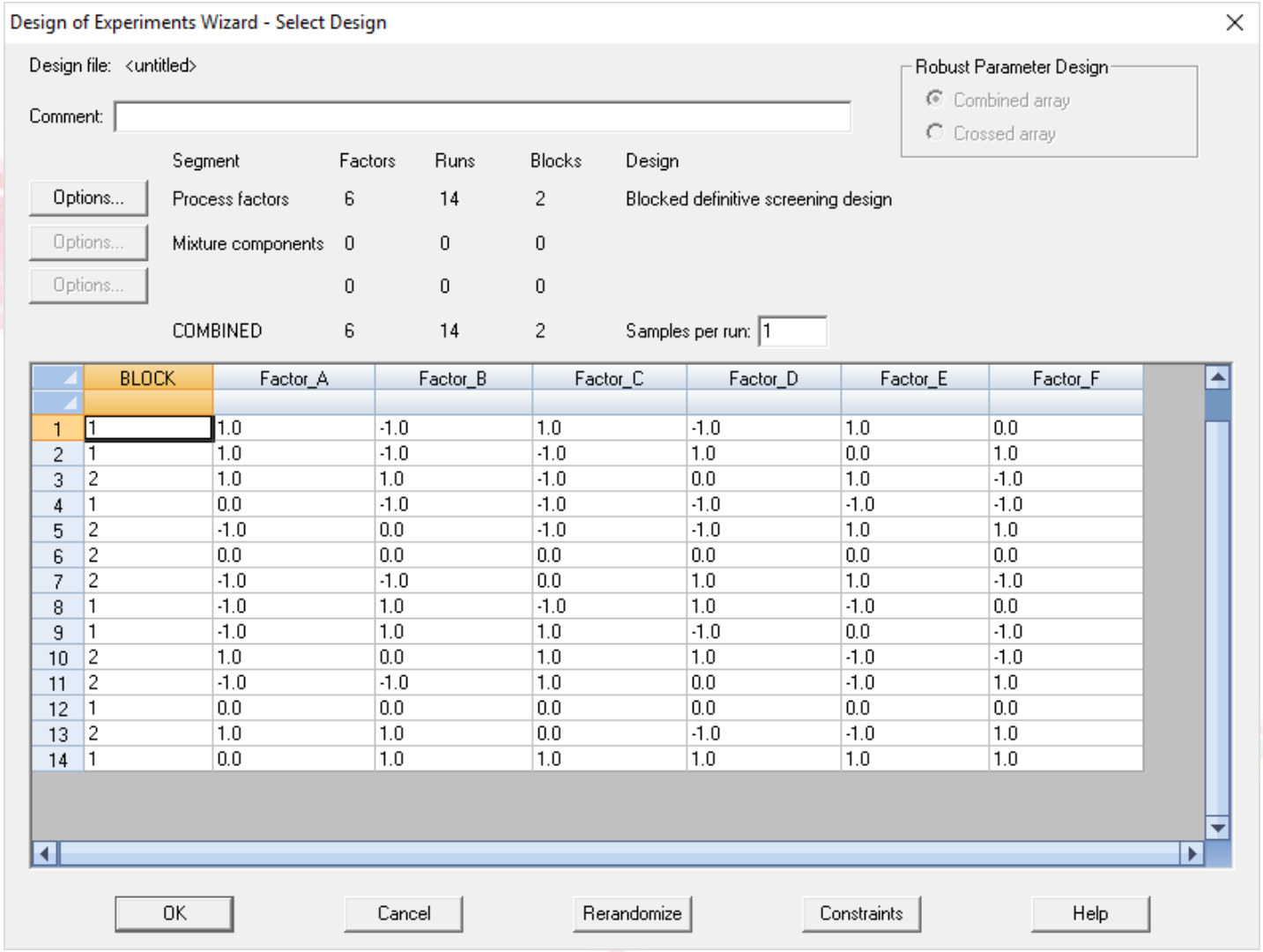
Example #3 (cont.)



	BLOCK	Factor_A	Factor_B	Factor_C	Factor_D	Factor_E	Factor_F
1	1	1.0	-1.0	1.0	-1.0	1.0	0.0
2	1	1.0	-1.0	-1.0	1.0	0.0	1.0
3	2	1.0	1.0	-1.0	0.0	1.0	-1.0
4	1	0.0	-1.0	-1.0	-1.0	-1.0	-1.0
5	2	-1.0	0.0	-1.0	-1.0	1.0	1.0
6	2	0.0	0.0	0.0	0.0	0.0	0.0
7	2	-1.0	-1.0	0.0	1.0	1.0	-1.0
8	1	-1.0	1.0	-1.0	1.0	-1.0	0.0
9	1	-1.0	1.0	1.0	-1.0	0.0	-1.0
10	2	1.0	0.0	1.0	1.0	-1.0	-1.0
11	2	-1.0	-1.0	1.0	0.0	-1.0	1.0
12	1	0.0	0.0	0.0	0.0	0.0	0.0
13	2	1.0	1.0	0.0	-1.0	-1.0	1.0
14	1	0.0	1.0	1.0	1.0	1.0	1.0

References

StatFolios and data files are at: *www.statgraphics.com/webinars*

Articles:

Box, G. E. P., Hunter, W. G. and Hunter, J. S. (2005). Statistics for Experimenters: An Introduction to Design, Data Analysis, and Model Building, 2nd edition. New York: John Wiley and Sons.

Jones, B. and Nachtsheim, C.J. (2011) "A Class of Three-Level Designs for Definitive Screening in the Presence of Second-Order Effects", Journal of Quality Technology 43(1), pp. 1-15.

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