

DOE Wizard – Computer Generated Designs

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Summary

The *Computer Generated* designs allow you to create experimental designs which have optimal properties with respect to the estimation of specific statistical models. Given the definition of an experimental region, a model to be estimated, and the number of experimental runs that can be performed, the program searches for a set of runs that maximizes a selected design optimality criteria.

Computer generated designs are included as an option in the Experimental Design Wizard when constructing several types of designs, including screening designs, response surface designs, and mixture experiments. In addition to lower and upper limits for each experimental factor, constraints may be specified based on linear combinations of the factors. The optimality criteria offered include D-optimality, A-optimality, G-optimality, and I-optimality.

The results of previous experimental runs may be included in the design by entering them into the experiment datasheet before requesting that the computer generate new runs. Additional runs will then be added to those already performed to maximize the specified optimality criterion. This allows the procedure to improve a partial design that has already been performed.

Example #1: Optimized Response Surface Experiment

In the book titled Optimal Design of Experiments: A Case Study Approach (2011), Goos and Jones describe an experiment in which the experimenters wished to model the effect of 4 experimental factors on the peel strength of a package. The factors of interest were:

Factor	Type	Low	High	Units
temperature	continuous	193	230	degrees C
pressure	continuous	2.2	3.2	bar
speed	continuous	32	50	cpm
supplier	categorical	1	3	

They wished to estimate a model containing:

1. Main effects of all 4 factors.
2. Two-factor interactions amongst all of the factors.
3. Quadratic effects for the 3 continuous factors.

This document will demonstrate how the DOE Wizard can be used to select a good design for this situation.

Design Creation

To begin the design creation process, start with an empty StatFolio. Select *DOE – Experimental Design Wizard* to load the DOE Wizard’s main window. Then push each button in sequence to create the design.

Step #1 – Define Responses

The first step of the design creation process displays a dialog box used to specify the response variables. For the current example, there is a single response variable:

Design file: <untitled>
 Comment: Computer generated design
 Number of responses: 1 Responses 1-16 Responses 17-32

Response	Name	Units	Analyze	Goal	Target	Impact (1-5)	Sensitivity	Minimum	Maximum
1	peel strength		Mean	Hit target	4.5	3.0	Medium	3.0	6.0
2	Var_2		Mean	Maximize	0.5	3.0	Medium		
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

- **Name:** The name for the variable is *peel strength*.
- **Units:** The units are not relevant in this example.
- **Analyze:** The parameter of interest is the *mean* peel strength.
- **Goal:** The goal of the experiment is to hit a target peel strength close to 4.5.
- **Impact:** This is not relevant since there is only one response.

- **Sensitivity:** The importance of being close to the best desired value has little impact on the optimization result when there is only one response.
- **Minimum and Maximum:** The range of acceptable peel strength was 3.0 to 6.0.

Step #2 – Define Experimental Factors

The second step displays a dialog box on which to specify the factors that will be varied. In the current example, there are 4 controllable process factors:

Design file: peel strength.sgx
 Comment: Computer generated design

Number of controllable process factors: 4 Number of controllable mixture components: 0 Number of noise factors: 0

Factor	Name	Units	Type	Role	Low	High	Levels
A	temperature	degrees C	Continuous	Controllable	193.0	230.0	1,2,3,4
B	pressure	bar	Continuous	Controllable	2.2	3.2	1,2,3,4
C	speed	cpm	Continuous	Controllable	32.0	50.0	1,2,3,4
D	supplier		Categorical	Controllable	-1.0	1.0	1,2,3
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

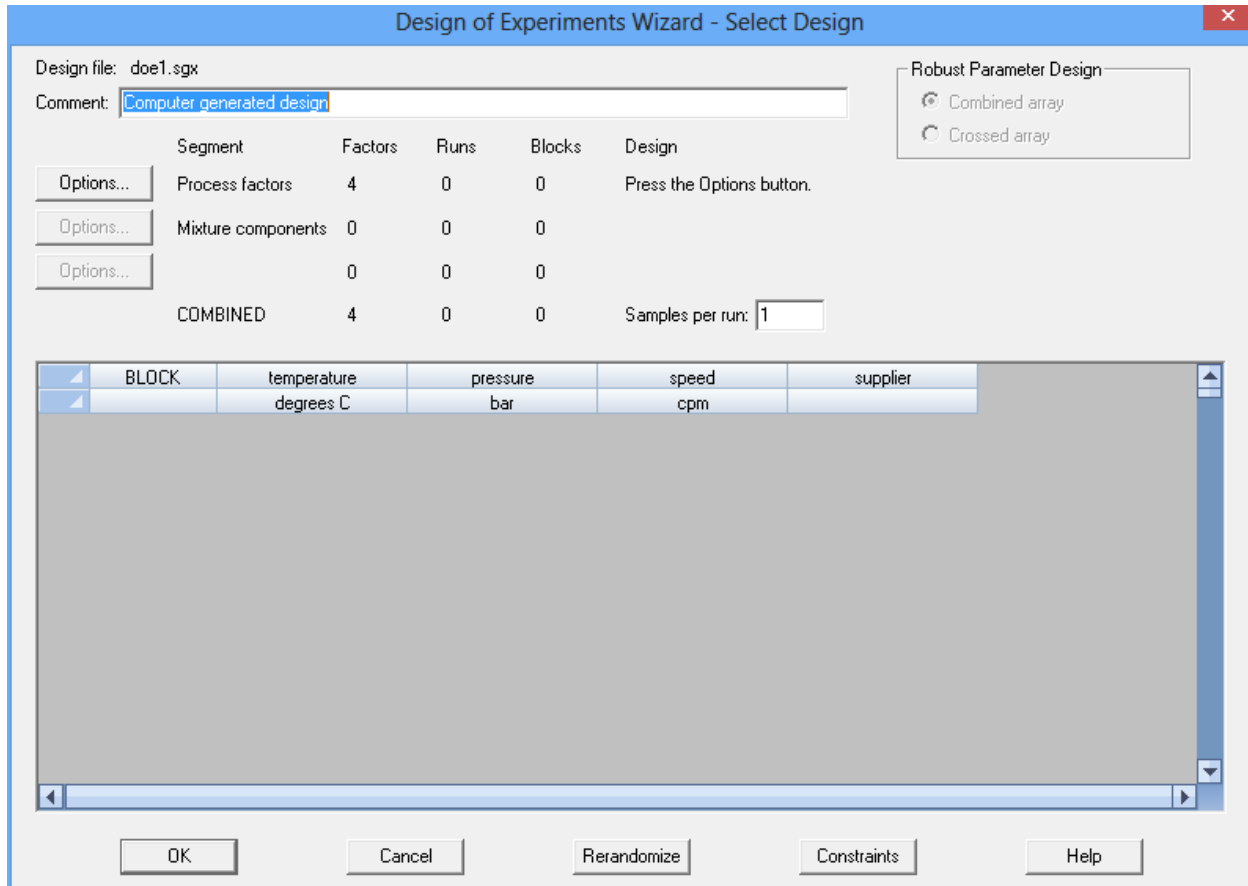
OK Back Cancel Help

- **Name** – Each factor must be assigned a unique name.
- **Units** – Units are optional.
- **Type** – Set the type of the first 3 factors to *Continuous*, since they can be set at any value within a continuous interval. The fourth factor is categorical.
- **Role** - The four factors are all *Controllable*.
- **Low** - the lower level L_j for the continuous factors.
- **High** - the upper level U_j for the continuous factors.

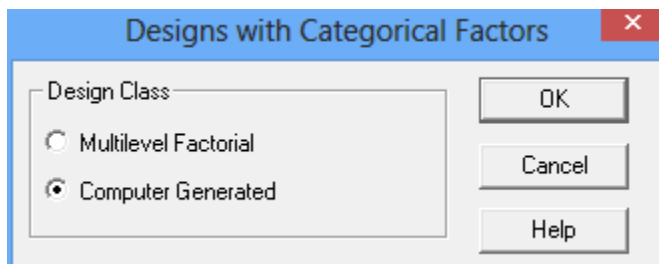
- **Levels** – the allowable levels of the categorical factor *supplier*.

Step #3 - Select Design

The third step begins by displaying the dialog box shown below:



Since all of the factors are controllable process factors, only one *Options* button is enabled. Pressing that button displays a second dialog box:



Since the experiment involves a categorical factor, two types of designs are offered:

1. *Multilevel Factorial* - designs involving all combinations of selected levels of each experimental factor. For example, a 3x3x3x3 factorial design would have 81 runs consisting of all combinations of 3 levels of each factor.

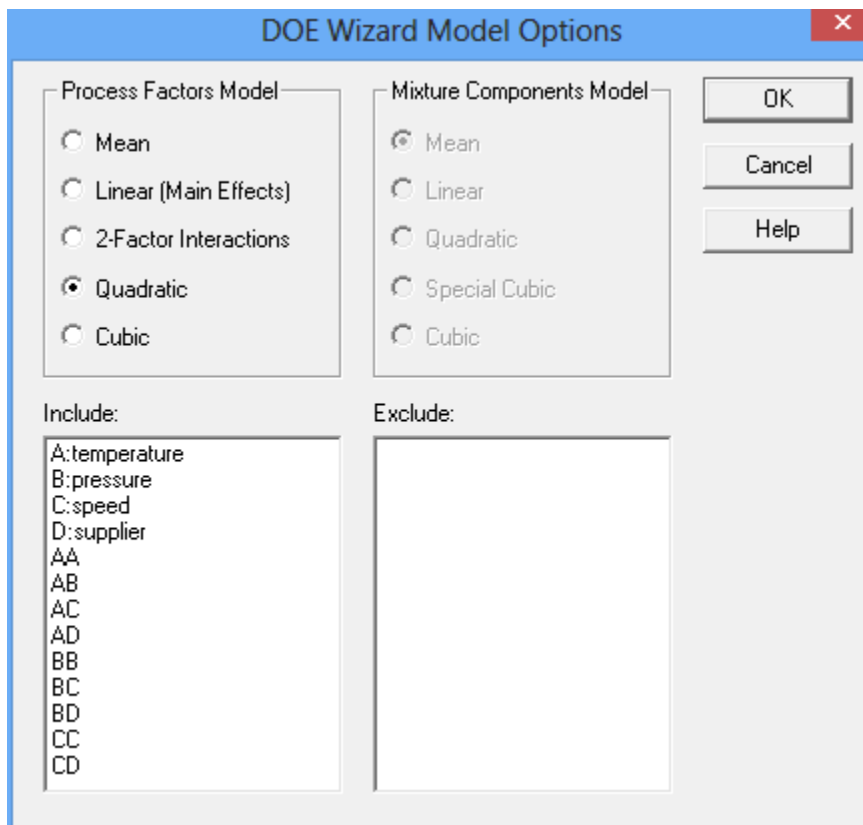
2. *Computer Generated* – If this type of design is selected, the computer will select a set of runs during Step 5 that are optimal for the model to be fit.

Select *Computer Generated* and press *OK*, which will return you to the *Select Design* dialog box:

If satisfied, press *OK* to save the design selection and return to the DOE Wizard's main window, which will now contain a summary of the design:

Step #4: Specify Model

The next step in the design selection process specifies the model that will be fit to the response data. Pressing the fourth button on the DOE Wizard's toolbar displays a dialog box to make that choice:



The *quadratic* model includes main effects for each of the 4 experimental factors, 6 two-factor interactions (shown as two-letter combinations with different factors), and 3 quadratic terms (shown as two-letter combinations with identical factors). Selected terms could be excluded by double-clicking on them with the left mouse button.

Step #5: Select runs

The next step selects the runs to be performed. Press the *Step 5: Select Runs* button on the DOE Wizard toolbar to display the following dialog box:

BLOCK	temperature degrees C	pressure bar	speed cpm	supplier
1				
2				
3				
4				
5				
6				
7				
8				
9				
10				
11				
12				
13				
14				
15				
16				
17				
18				
19				
20				
21				
22				

Optimize:
☒ I-efficiency
☐ D-efficiency
☐ A-efficiency
☐ G-efficiency

Display:
☒ Original units
☐ Coded units

☒ Randomize run order

Number of coefficients: 18
 Number of base runs: 24
 Number of replicates: 0
 Number of centerpoints: 0
☒ Group runs in blocks of size: 1000

Average prediction variance:
 D-efficiency:
 A-efficiency:
 G-efficiency:

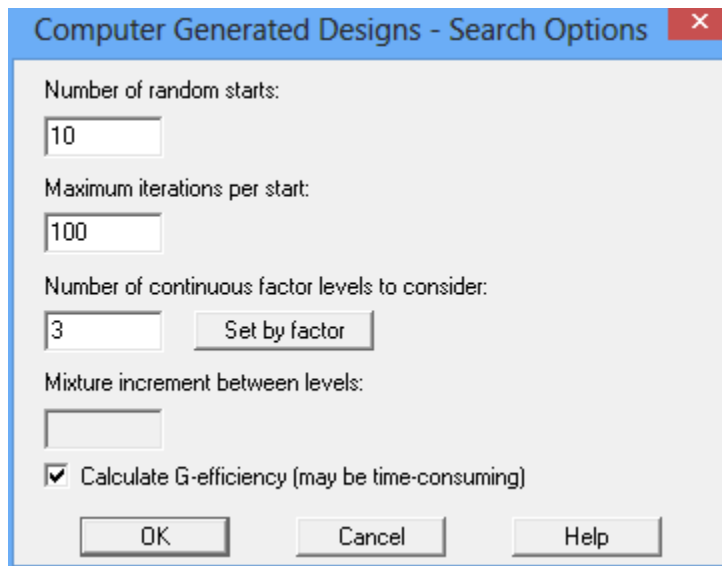
OK
 Cancel
 Help
 Create
 Advanced

The dialog box shows the number of coefficients in the model to be estimated. At least as many runs must be selected as there are coefficients. Typically, at least 3 additional runs will be added to that number in order to estimate the experimental error.

There are several important fields to be completed:

- *Optimize* - the criterion to be used to select the experimental runs. Briefly, D-efficiency measures the information generated by the experiment about the model parameters. A-efficiency measures the average variance of the estimates of the model parameters. G-efficiency measures the maximum variance of the predicted response at the design points. I-efficiency measures the average prediction variance over the design space. It is often recommended that D-efficiency be selected when creating a screening design and I-efficiency selected when creating a response surface design.
- *Display* - whether the runs should be displayed in their original units or coded units.
- *Randomize run order* - whether the order of the runs should be randomized.
- *Number of base runs* - the number of different combinations of the factors that should be generated. This number must be greater than or equal to the number of coefficients in the model that will be fit to the data.

- *Number of replicates* - the number of additional runs to be added that are replicates of one or more of the base runs.
- *Number of centerpoints* - the number of additional runs to be added at the center of the experimental region.
- *Group runs in blocks of size* – If desired, the new runs may be placed in blocks of the specified size. Additional terms will be added to the model to allow for differences between the blocks. Selecting this option also places any experimental runs that have already been performed in a different block than the new runs.
- *Advanced* button – displays a dialog box for changing the search options:



Number of random starts – number of times the algorithm will search for an optimal design from a different random start.

Maximum iterations per start – maximum number of times that the algorithm will try exchanging runs before a solution is accepted.

Number of factor levels to consider - number of levels at which experimental runs may be performed for continuous factors, ranging from the low level of the factor to the high level. Specifying a larger number increases the time required to create the design but may improve the design efficiency. If different numbers of levels are desired for different factors, they may be set by pressing the *Set by factor* button.

Mixture increment between levels – for experiments containing mixture components, the amount by which each component will be changed when attempting to find an optimal set of runs.

Calculate G-efficiency - whether the G-efficiency of the design should be calculated and displayed. This statistic requires calculating the prediction variance at every candidate point considered when constructing the design, which can be very large if there are many factors or factor levels to consider.

In this case, the experimenters decided that they could afford to perform 24 runs, all of which will be allocated to base runs (different combinations of the factors). They also specified that the experiment should include runs at only 3 levels of each continuous factor (the low level, the center level, and the high level).

To generate an I-optimal design, set *Optimize* to *I-efficiency* and press the *Create* button. When the algorithm is complete, the selected experimental runs will be added to the dialog box:

The screenshot shows the 'Computer Generated Designs' dialog box. It contains a table with 24 rows of experimental runs. The columns are BLOCK, temperature (degrees C), pressure (bar), speed (cpm), and supplier. Below the table, there are settings for optimization (I-efficiency selected), display (Original units selected), and various efficiency metrics (D-efficiency: 42.73%, A-efficiency: 30.37%, G-efficiency: 76.23%). The 'Number of base runs' is set to 24, and 'Group runs in blocks of size' is set to 1000. The 'Create' button is highlighted.

	BLOCK	temperature degrees C	pressure bar	speed cpm	supplier
1	1	193.0	2.7	32.0	3
2	1	230.0	3.2	50.0	1
3	1	230.0	3.2	50.0	2
4	1	211.5	2.7	41.0	2
5	1	230.0	2.7	50.0	3
6	1	193.0	3.2	50.0	3
7	1	211.5	2.7	41.0	2
8	1	230.0	2.2	41.0	1
9	1	193.0	3.2	32.0	2
10	1	193.0	2.2	32.0	2
11	1	230.0	2.7	32.0	2
12	1	211.5	2.7	41.0	1
13	1	211.5	3.2	32.0	3
14	1	193.0	2.2	50.0	1
15	1	230.0	3.2	32.0	1
16	1	193.0	2.2	32.0	1
17	1	230.0	2.2	50.0	2
18	1	193.0	2.7	50.0	2
19	1	193.0	2.2	41.0	3
20	1	193.0	3.2	41.0	1
21	1	211.5	2.7	41.0	1
22	1	230.0	2.2	32.0	3

Optimize:
☒ I-efficiency
☐ D-efficiency
☐ A-efficiency
☐ G-efficiency

Display:
☒ Original units
☐ Coded units
☒ Randomize run order

Number of coefficients: 18
 Number of base runs: 24
 Number of replicates: 0
 Number of centerpoints: 0
☒ Group runs in blocks of size: 1000

Average prediction variance: 0.483778
 D-efficiency: 42.73%
 A-efficiency: 30.37%
 G-efficiency: 76.23%

OK
 Cancel
 Help
 Create
 Advanced

The efficiencies of the selected design and the average prediction variance are also displayed.

Note: The efficiency values should only be used to compare alternative experiments containing the same number of runs. Their absolute magnitude is usually not important.

If you uncheck the button labeled *Randomize run order*, the runs will be displayed in standard order:

Computer Generated Designs

	BLOCK	temperature degrees C	pressure bar	speed cpm	supplier
1	1	193.0	2.2	32.0	1
2	1	230.0	3.2	32.0	1
3	1	230.0	2.2	41.0	1
4	1	211.5	2.7	41.0	1
5	1	211.5	2.7	41.0	1
6	1	193.0	3.2	41.0	1
7	1	193.0	2.2	50.0	1
8	1	230.0	3.2	50.0	1
9	1	193.0	2.2	32.0	2
10	1	230.0	2.7	32.0	2
11	1	193.0	3.2	32.0	2
12	1	211.5	2.7	41.0	2
13	1	211.5	2.7	41.0	2
14	1	230.0	2.2	50.0	2
15	1	193.0	2.7	50.0	2
16	1	230.0	3.2	50.0	2
17	1	230.0	2.2	32.0	3
18	1	193.0	2.7	32.0	3
19	1	211.5	3.2	32.0	3
20	1	193.0	2.2	41.0	3
21	1	230.0	3.2	41.0	3
22	1	211.5	2.2	50.0	3

Optimize

☒ I-efficiency

☐ D-efficiency

☐ A-efficiency

☐ G-efficiency

Display

☒ Original units

☐ Coded units

☐ Randomize run order

Number of coefficients: 18

Number of base runs:

Number of replicates:

Number of centerpoints:

☒ Group runs in blocks of size:

Average prediction variance: 0.483778

D-efficiency: 42.73%

A-efficiency: 30.37%

G-efficiency: 76.23%

OK

Cancel

Help

Create

Advanced

Note that 8 runs are performed for each supplier.

You can change some settings and try again or press *OK* to accept the selection, at which point the selected runs will be placed in datasheet A:

C:\Data\Version17 Tests\doewiz compgen rsm.sgx						
	BLOCK	temperature degrees C	pressure bar	speed cpm	supplier	peel strength
1	1	193.0	2.7	32.0	3	
2	1	230.0	3.2	50.0	1	
3	1	230.0	3.2	50.0	2	
4	1	211.5	2.7	41.0	2	
5	1	230.0	2.7	50.0	3	
6	1	193.0	3.2	50.0	3	
7	1	211.5	2.7	41.0	2	
8	1	230.0	2.2	41.0	1	
9	1	193.0	3.2	32.0	2	
10	1	193.0	2.2	32.0	2	
11	1	230.0	2.7	32.0	2	
12	1	211.5	2.7	41.0	1	
13	1	211.5	3.2	32.0	3	
14	1	193.0	2.2	50.0	1	
15	1	230.0	3.2	32.0	1	
16	1	193.0	2.2	32.0	1	
17	1	230.0	2.2	50.0	2	
18	1	193.0	2.7	50.0	2	
19	1	193.0	2.2	41.0	3	
20	1	193.0	3.2	41.0	1	
21	1	211.5	2.7	41.0	1	
22	1	230.0	2.2	32.0	3	
23	1	230.0	3.2	41.0	3	
24	1	211.5	2.2	50.0	3	

The main DOE Wizard window will reflect the design:

Experimental Design Wizard									
Step 1: Define responses		Step 3: Specify model		Step 5: Select runs		Step 7: Save experiment		Step 9: Optimize responses	
Step 2: Define exp. factors		Step 4: Select design		Step 6: Evaluate design		Step 8: Analyze data		Step 10: Save results	
Step 11: Augment design		Step 12: Extrapolate							
Experimental Design Wizard									
Step 1: Define the response variables to be measured									
Name	Units	Analyze	Goal	Target	Impact	Sensitivity	Low	High	
peel strength		Mean	Hit target	4.5	3.0	Medium	3.0	6.0	
Step 2: Define the experimental factors to be varied									
Name	Units	Type	Role	Low	High	Levels			
A:temperature	degrees C	Continuous	Controllable	193.0	230.0				
B:pressure	bar	Continuous	Controllable	2.2	3.2				
C:speed	cpm	Continuous	Controllable	32.0	50.0				
D:supplier		Categorical	Controllable			1,2,3			
Step 3: Specify the initial model to be fit to the experimental results									
Factors	Model	Coefficients	Excluded effects						
Process	quadratic	18							
Step 4: Select the experimental design									
Type of	Design	Centerpoints	Centerpoint	Design is	Number of	Total	Total	Error	
Factors	Type	Per Block	Placement	Randomized	Replicates	Runs	Blocks	D.F.	
Process	Computer generated design								
Number of samples per run: 1									
Step 5: Select an optimal subset of the runs (optional)									
24 runs selected									

If the selection is acceptable, press *Step 7: Save experiment* to save the design.

Evaluate Design

After the design has been created, press the button labeled *Step 6: Evaluate Design* on the DOE Wizard toolbar to display various design diagnostics:

Tables and Graphs	
TABLES	GRAPHS
<input checked="" type="checkbox"/> Analysis Summary	<input type="checkbox"/> Design Points
<input type="checkbox"/> Design Worksheet	<input type="checkbox"/> Prediction Variance Plot
<input type="checkbox"/> ANOVA Table	<input type="checkbox"/> Prediction Profile
<input checked="" type="checkbox"/> Model Coefficients	<input type="checkbox"/> Variance Dispersion Graph
<input type="checkbox"/> Alias Matrix	<input checked="" type="checkbox"/> Fraction of Design Space Plot
<input type="checkbox"/> Correlation Matrix	<input type="checkbox"/> Power Curve
<input type="checkbox"/> Leverage	<input type="checkbox"/> Desirability Plot
<input type="checkbox"/> Desirability	<input type="checkbox"/> Overlaid Contour Plots
<input type="button" value="OK"/> <input type="button" value="Cancel"/> <input type="button" value="All"/> <input type="button" value="Store"/> <input type="button" value="Help"/>	

The *Model Coefficients* table shows the relative standard error of each coefficient in the model to be estimated:

Model Coefficients						
				Power at	Power at	Power at
Coefficient	Standard Error	VIF	Ri-Squared	SN = 0.5	SN = 1.0	SN = 2.0
constant	0.466817			7.41%	14.85%	43.68%
A	0.245327	1.08333	0.0769231	13.90%	40.32%	92.11%
B	0.259094	1.07407	0.0689655	12.96%	36.90%	89.23%
C	0.259094	1.07407	0.0689655	12.96%	36.90%	89.23%
D	0.311438	1.5519	0.355627	10.47%	27.32%	76.28%
D	0.296604	1.40759	0.289564	11.04%	29.58%	80.10%
AA	0.584816	1.53904	0.350246	6.53%	11.22%	30.27%
AB	0.280009	1.0846	0.0780028	11.79%	32.50%	84.30%
AC	0.280009	1.0846	0.0780028	11.79%	32.50%	84.30%
AD	0.350264	1.47222	0.320755	9.31%	22.65%	66.48%
AD	0.340207	1.38889	0.28	9.57%	23.71%	68.95%
BB	0.505853	1.36473	0.267254	7.05%	13.36%	38.37%
BC	0.312182	1.16949	0.144928	10.44%	27.21%	76.08%
BD	0.387896	1.50463	0.335385	8.50%	19.36%	57.89%
BD	0.350264	1.47222	0.320755	9.31%	22.65%	66.48%
CC	0.505853	1.36473	0.267254	7.05%	13.36%	38.37%
CD	0.360041	1.2963	0.228571	9.07%	21.69%	64.14%
CD	0.350264	1.22685	0.184906	9.31%	22.65%	66.48%

alpha = 5.0%, sigma estimated from total error with 6 d.f.

The standard error is relative in the sense that it is the multiple of the residual standard error, which is not known until the experiment has been performed. Of particular interest are the VIFs (Variance Inflation Factors), which show how much the variance of each coefficient has been

increased relative to a perfectly orthogonal design. Since the largest VIF is less than 1.4, there has been relatively little variance inflation.

Example #2: Adding Runs to an Existing Experiment

After running a set of experimental runs, it is not uncommon to desire that additional runs be added to the original design. This may happen because of various reasons:

1. The initial design might have been constructed poorly. It is not uncommon to find experimenters who begin with a haphazard approach to factor level selection and only realize later that the interpretation of their results would be much easier with a designed experiment.
2. In other cases, unexpected effects may be observed in the first design and additional runs may be desired to follow up on the initial discoveries.
3. In the case of screening designs involving many factors, there may be considerable confounding amongst the effects in the initial design. Breaking apart specific confounding patterns then requires additional runs.
4. Conversion of a screening design to a response design may require additional runs to add higher-order terms to the statistical model.

Goos and Jones (2011) describe a situation where a 12-run experiment was performed involving 6 factors, each at 2 levels. The design was constructed to estimate a model involving all 6 main effects and 1 specific 2-factor interaction. After analyzing the results of the first experiment, they wished to augment the design so that it could estimate 5 additional interactions.

To reconstruct their experiment, start with a StatFolio and select *DOE – Experimental Design Wizard* from the main menu. In Step 1, enter the following information about the response variable:

Design of Experiments Wizard - Define Responses

Design file: <untitled>

Comment: computer augmented design

Number of responses: 1 Responses 1-16 Responses 17-32

Response	Name	Units	Analyze	Goal	Target	Impact (1-5)	Sensitivity	Minimum	Maximum
1	yield	mg	Mean	Maximize	0.5	3.0	Medium		
2	Var_2		Mean	Maximize	0.5	3.0	Medium		
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

In step 2, enter the following information about the experimental factors:

Design of Experiments Wizard - Define Factors

Design file: chapter3.sgx

Comment: computer augmented design

Number of controllable process factors: 6 Number of controllable mixture components: 0 Number of noise factors: 0

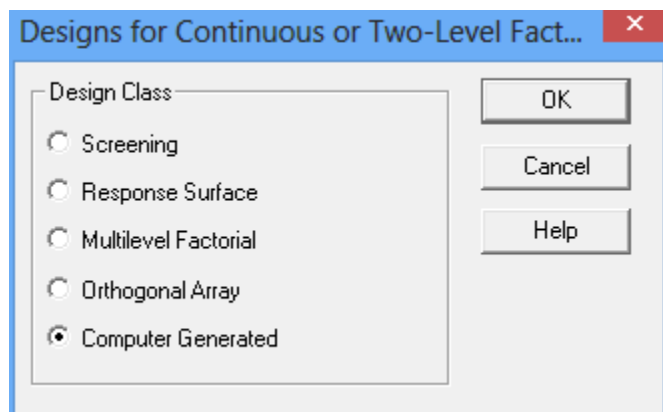
Factor	Name	Units	Type	Role	Low	High	Levels
A	methanol		Continuous	Controllable	0.0	10.0	1,2,3,4
B	ethanol		Continuous	Controllable	0.0	10.0	1,2,3,4
C	propanol		Continuous	Controllable	0.0	10.0	1,2,3,4
D	butanol		Continuous	Controllable	0.0	10.0	1,2,3,4
E	pH		Continuous	Controllable	6.0	9.0	1,2,3,4
F	time		Continuous	Controllable	1.0	2.0	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

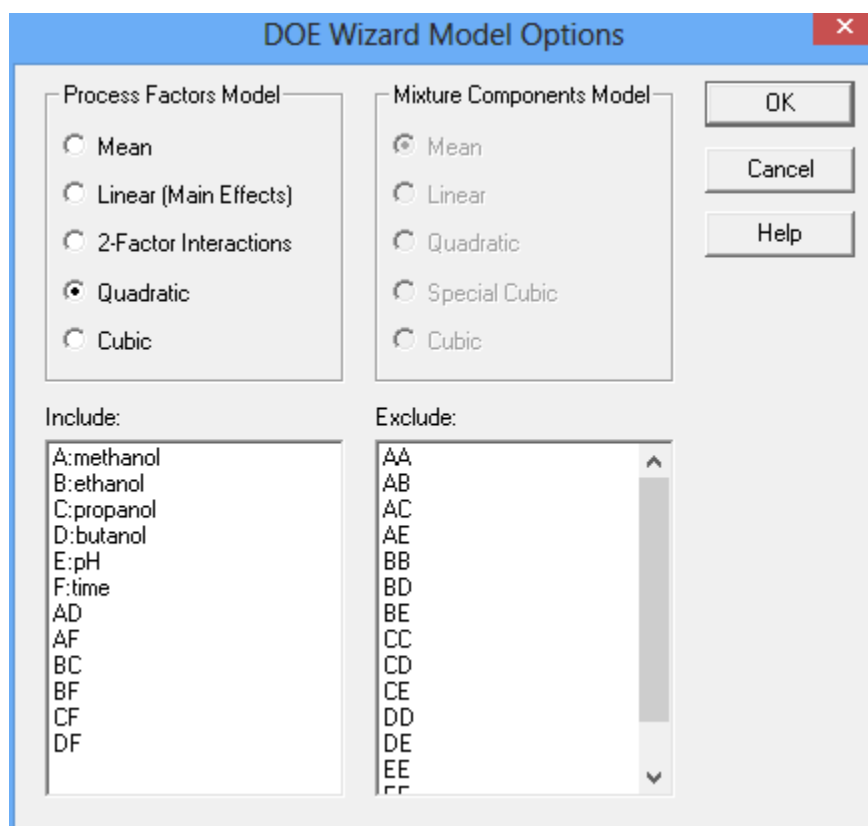
Factors A-M Factors N-Z

OK Back Cancel Help

In Step 3, select a *Computer Generated* design:



In Step 4, select a model involving all 6 main effects and 6 two-factor interactions:



Before selecting the experimental runs, go to the DataBook and put in information about the 12 runs that have already been performed:

	BLOCK	methanol	ethanol	propanol	butanol	pH	time	yield mg
1	1	0	0	0	10	6	1	10.94
2	1	0	10	0	0	9	1	15.79
3	1	0	10	0	10	9	2	25.96
4	1	10	10	10	0	6	1	35.92
5	1	0	0	10	0	6	2	22.92
6	1	0	10	10	10	6	1	23.54
7	1	10	10	0	0	6	2	47.44
8	1	10	0	0	0	9	1	19.80
9	1	10	0	10	10	9	1	29.48
10	1	0	0	10	0	9	2	17.13
11	1	10	10	10	10	9	2	43.75
12	1	10	0	0	10	6	2	40.86
13								
14								
15								

Be sure to include the values for *Yield*, so that the algorithm will know that those runs have already been performed.

Now return to the DOE Wizard and press the button labeled *Step 5: Select runs*. The dialog box will show the 12 runs that have already been performed:

	BLOCK	methanol	ethanol	propanol	butanol	pH	time
1	1	0.0	0.0	0.0	10.0	6.0	1.0
2	1	0.0	10.0	0.0	0.0	9.0	1.0
3	1	0.0	10.0	0.0	10.0	9.0	2.0
4	1	10.0	10.0	10.0	0.0	6.0	1.0
5	1	0.0	0.0	10.0	0.0	6.0	2.0
6	1	0.0	10.0	10.0	10.0	6.0	1.0
7	1	10.0	10.0	0.0	0.0	6.0	2.0
8	1	10.0	0.0	0.0	0.0	9.0	1.0
9	1	10.0	0.0	10.0	10.0	9.0	1.0
10	1	0.0	0.0	10.0	0.0	9.0	2.0
11	1	10.0	10.0	10.0	10.0	9.0	2.0
12	1	10.0	0.0	0.0	10.0	6.0	2.0
13							
14							
15							
16							
17							
18							
19							
20							
21							
22							

Optimize:
☒ D-efficiency
☐ G-efficiency
☐ A-efficiency
☐ I-efficiency

Display:
☒ Original units
☐ Coded units
☒ Randomize run order

Number of coefficients: 14
 Number of base runs: 20
 Number of replicates: 0
 Number of centerpoints: 0
☒ Group runs in blocks of size: 1000

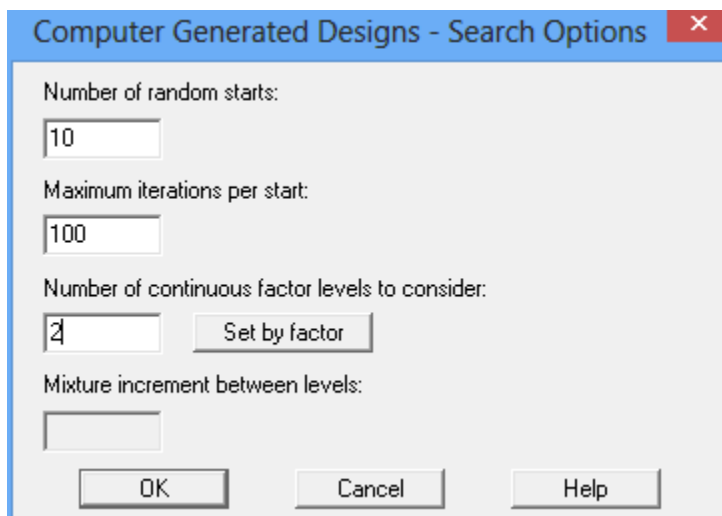
D-efficiency:
 G-efficiency:
 A-efficiency:
 Average prediction variance:

Create Advanced

OK Cancel Help

Now:

1. Set *Optimize* to *D-efficiency* to create a D-optimal design.
2. Set *Number of base runs* to 20 to add 8 additional runs to the original 12 runs.
3. Push the *Advanced* button and set *Number of factor levels to consider* to 2 to consider only runs involving the low and high levels of each factor:



Computer Generated Designs - Search Options

Number of random starts:
10

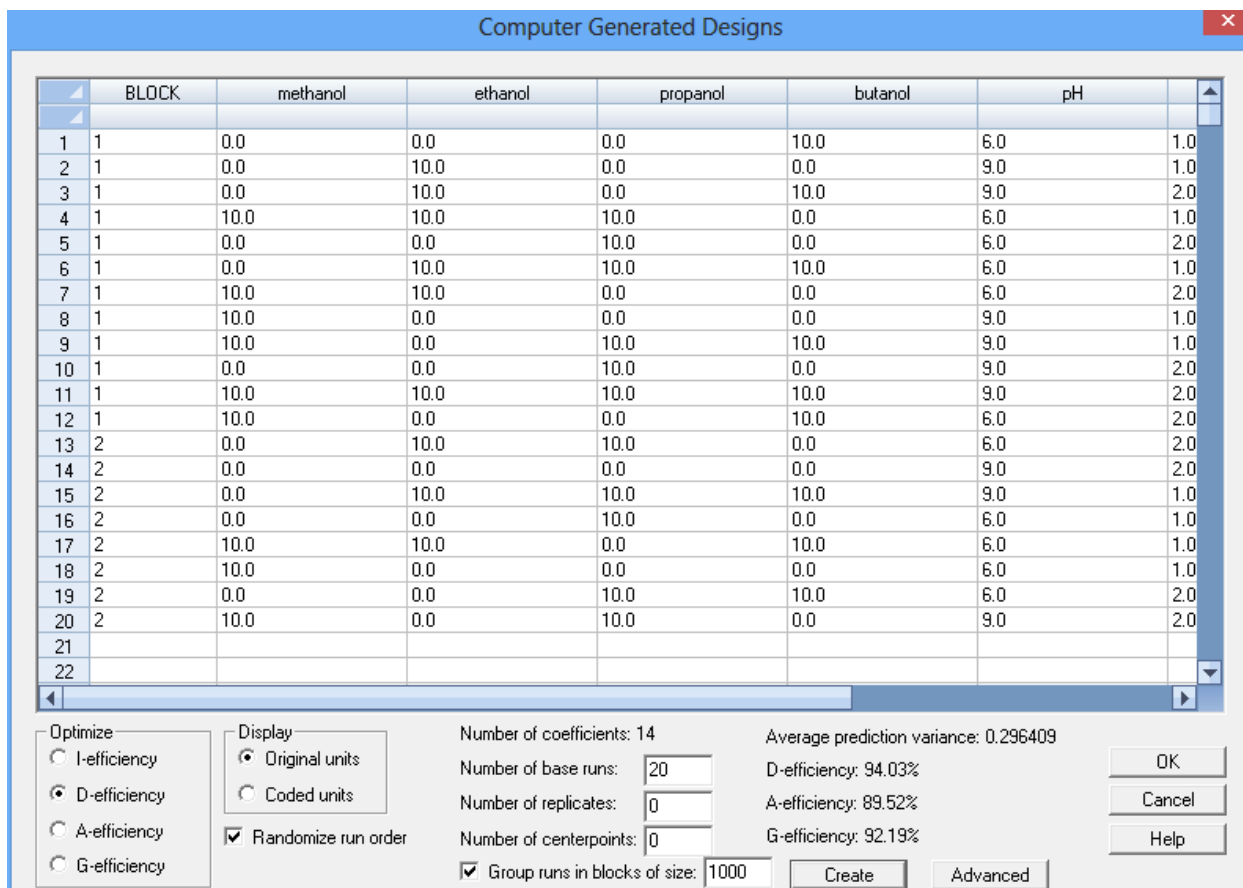
Maximum iterations per start:
100

Number of continuous factor levels to consider:
2 Set by factor

Mixture increment between levels:
[empty box]

OK Cancel Help

4. Push the *Create* button to initiate the design creation process. When the algorithm is complete, 8 additional runs will be added to the dialog box:



Computer Generated Designs

	BLOCK	methanol	ethanol	propanol	butanol	pH	
1	1	0.0	0.0	0.0	10.0	6.0	1.0
2	1	0.0	10.0	0.0	0.0	9.0	1.0
3	1	0.0	10.0	0.0	10.0	9.0	2.0
4	1	10.0	10.0	10.0	0.0	6.0	1.0
5	1	0.0	0.0	10.0	0.0	6.0	2.0
6	1	0.0	10.0	10.0	10.0	6.0	1.0
7	1	10.0	10.0	0.0	0.0	6.0	2.0
8	1	10.0	0.0	0.0	0.0	9.0	1.0
9	1	10.0	0.0	10.0	10.0	9.0	1.0
10	1	0.0	0.0	10.0	0.0	9.0	2.0
11	1	10.0	10.0	10.0	10.0	9.0	2.0
12	1	10.0	0.0	0.0	10.0	6.0	2.0
13	2	0.0	10.0	10.0	0.0	6.0	2.0
14	2	0.0	0.0	0.0	0.0	9.0	2.0
15	2	0.0	10.0	10.0	10.0	9.0	1.0
16	2	0.0	0.0	10.0	0.0	6.0	1.0
17	2	10.0	10.0	0.0	10.0	6.0	1.0
18	2	10.0	0.0	0.0	0.0	6.0	1.0
19	2	0.0	0.0	10.0	10.0	6.0	2.0
20	2	10.0	0.0	10.0	0.0	9.0	2.0
21							
22							

Optimize:
☐ I-efficiency
☒ D-efficiency
☐ A-efficiency
☐ G-efficiency

Display:
☒ Original units
☐ Coded units

☒ Randomize run order

Number of coefficients: 14
 Number of base runs: 20
 Number of replicates: 0
 Number of centerpoints: 0
☒ Group runs in blocks of size: 1000

Average prediction variance: 0.296409
 D-efficiency: 94.03%
 A-efficiency: 89.52%
 G-efficiency: 92.19%

Create Advanced

OK Cancel Help

5. Push *OK* to save the design.

The new runs have now been added to the DataBook:

C:\Data\Version17 Tests\doewiz compgen augment.sgx								
	BLOCK	methanol	ethanol	propanol	butanol	pH	time	yield
								mg
1	1	0.0	0.0	0.0	10.0	6.0	1.0	10.94
2	1	0.0	10.0	0.0	0.0	9.0	1.0	15.79
3	1	0.0	10.0	0.0	10.0	9.0	2.0	25.96
4	1	10.0	10.0	10.0	0.0	6.0	1.0	35.92
5	1	0.0	0.0	10.0	0.0	6.0	2.0	22.92
6	1	0.0	10.0	10.0	10.0	6.0	1.0	23.54
7	1	10.0	10.0	0.0	0.0	6.0	2.0	47.44
8	1	10.0	0.0	0.0	0.0	9.0	1.0	19.80
9	1	10.0	0.0	10.0	10.0	9.0	1.0	29.48
10	1	0.0	0.0	10.0	0.0	9.0	2.0	17.13
11	1	10.0	10.0	10.0	10.0	9.0	2.0	43.75
12	1	10.0	0.0	0.0	10.0	6.0	2.0	40.86
13	2	0.0	10.0	10.0	0.0	6.0	2.0	
14	2	0.0	0.0	0.0	0.0	9.0	2.0	
15	2	0.0	10.0	10.0	10.0	9.0	1.0	
16	2	0.0	0.0	10.0	0.0	6.0	1.0	
17	2	10.0	10.0	0.0	10.0	6.0	1.0	
18	2	10.0	0.0	0.0	0.0	6.0	1.0	
19	2	0.0	0.0	10.0	10.0	6.0	2.0	
20	2	10.0	0.0	10.0	0.0	9.0	2.0	

Example #3: Incorporating Design Region Constraints

It is not infrequent to find when designing an experiment that the feasible region in which design points may be placed is not cuboidal. In other words, having set low and high ranges for each of the factors, certain combinations of factor levels falling between the lows and the highs may not correspond to acceptable locations at which to perform an experiment. Statgraphics allows you to specify constraints on linear combinations of the factors that limit the locations at which experiments may be run.

Goos and Jones (2011) describe an experiment intended to maximize the yield of a chemical process. The first factor (Time) was allowed to vary between 430 and 640 seconds. The second factor (Temperature) was allowed to vary between 500 and 550 degrees Kelvin. However, experiments could only be run in regions where two additional constraints were satisfied:

$$0.3 \text{ Time} + \text{Temperature} \geq 539.8$$

$$0.09 \text{ Time} + \text{Temperature} \leq 587.8$$

Outside that constrained region, it was thought that the process would behave much differently than within the region, so that any experimental points outside the region could potentially distort the estimated statistical model.

To reconstruct their experiment, start with an StatFolio and select *DOE – Experimental Design Wizard* from the main menu. In Step 1, enter the following information about the response variable:

Design of Experiments Wizard - Define Responses

Design file: <untitled>

Comment: rsm with constraints

Number of responses: 1

Response	Name	Units	Analyze	Goal	Target	Impact (1-5)	Sensitivity	Minimum	Maximum
1	yield	%	Mean	Maximize	0.5	3.0	Medium		
2	Var_2		Mean	Maximize	0.5	3.0	Medium		
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

In step 2, enter the following information about the experimental factors:

Design of Experiments Wizard - Define Factors

Design file: <untitled>
 Comment: rsm with constraints

Number of controllable process factors: 2 Number of controllable mixture components: 0 Number of noise factors: 0

Factor	Name	Units	Type	Role	Low	High	Levels
A	time	seconds	Continuous	Controllable	430	650	1,2,3,4
B	temperature	degrees K	Continuous	Controllable	500	550	1,2,3,4
C	Factor_C		Continuous		-1.0	1.0	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

In Step 3, select a *Computer Generated* design on the first dialog box:

Designs for Continuous or Two-Level Fact...

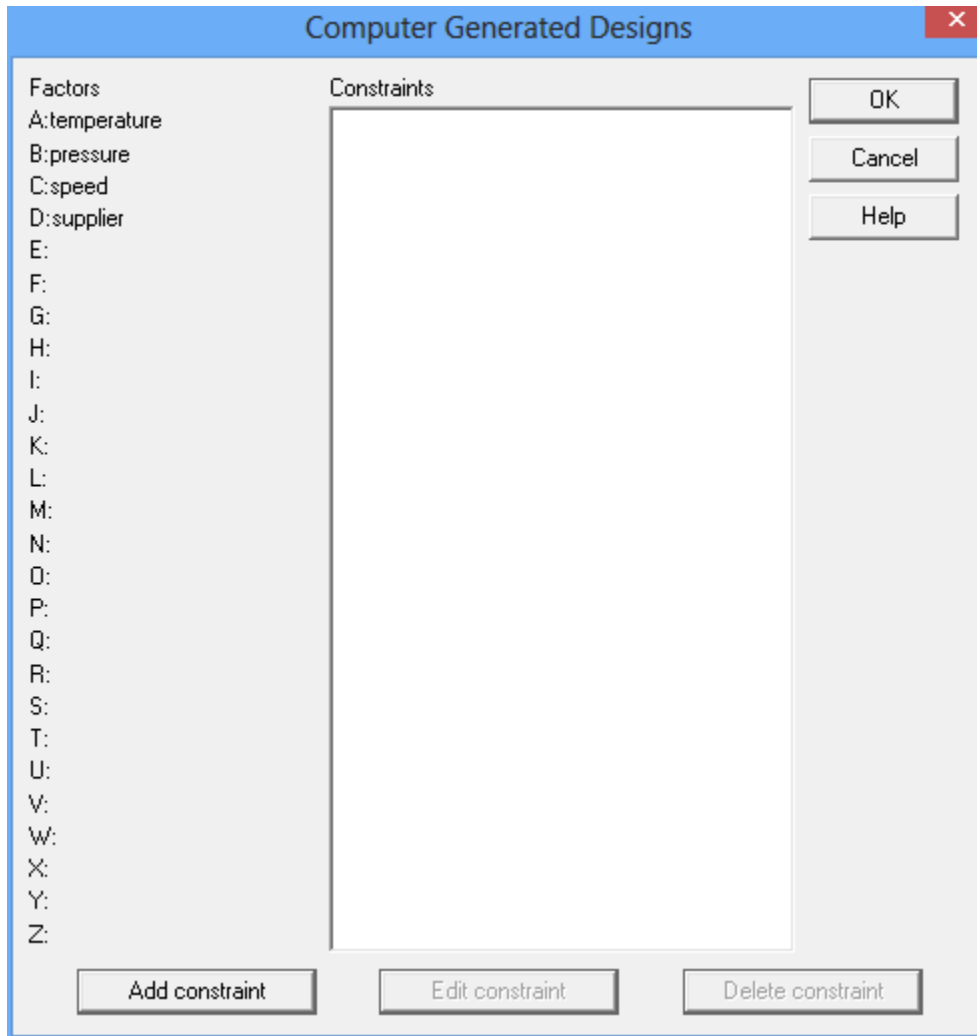
Design Class

- ☐ Screening
- ☐ Response Surface
- ☐ Multilevel Factorial
- ☐ Orthogonal Array
- ☒ Computer Generated

OK Cancel Help

Press *OK* to return to the *Select Design* dialog box.

After *Computer Generated* is selected, the *Constraints* button at the bottom of the *Select Design* dialog box will be enabled. Pressing that button displays a dialog box in which up to 20 constraints involving the experimental factors may be entered:



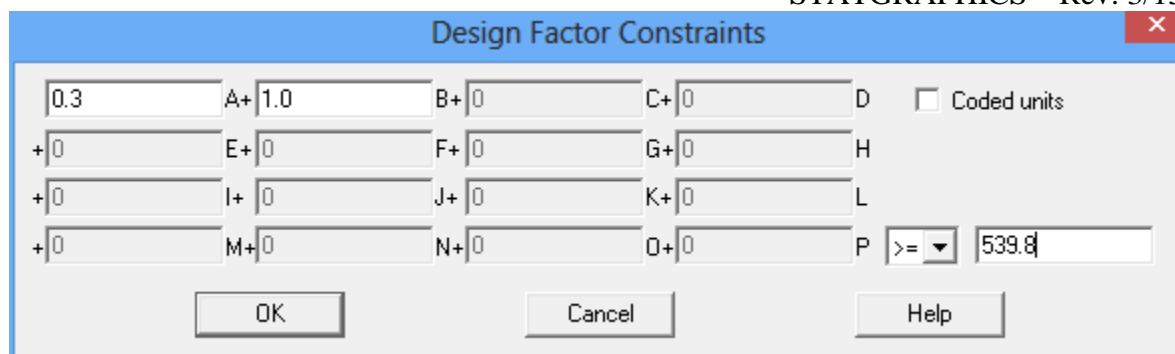
You may enter constraints of the form

$$C_1X_1 + C_2X_2 + C_3X_3 \leq d$$

or

$$C_1X_1 + C_2X_2 + C_3X_3 \geq d$$

by pressing the *Add constraint* button and entering the values of C_1 , C_2 and C_3 . For the current example, the first constraint should be added by entering the following:



Design Factor Constraints

0.3 A+ 1.0 B+ 0 C+ 0 D ☐ Coded units

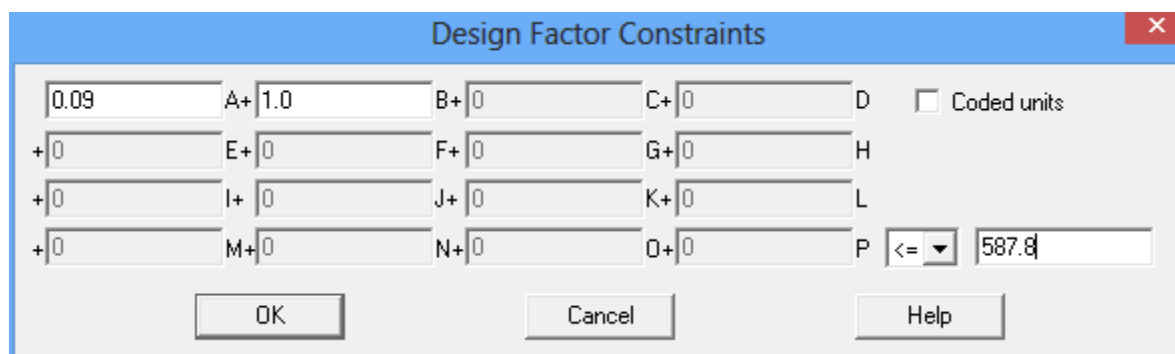
+ 0 E+ 0 F+ 0 G+ 0 H

+ 0 I+ 0 J+ 0 K+ 0 L

+ 0 M+ 0 N+ 0 O+ 0 P \geq 539.8

OK Cancel Help

Press *OK* and then *Add constraint* again to add the second constraint:



Design Factor Constraints

0.09 A+ 1.0 B+ 0 C+ 0 D ☐ Coded units

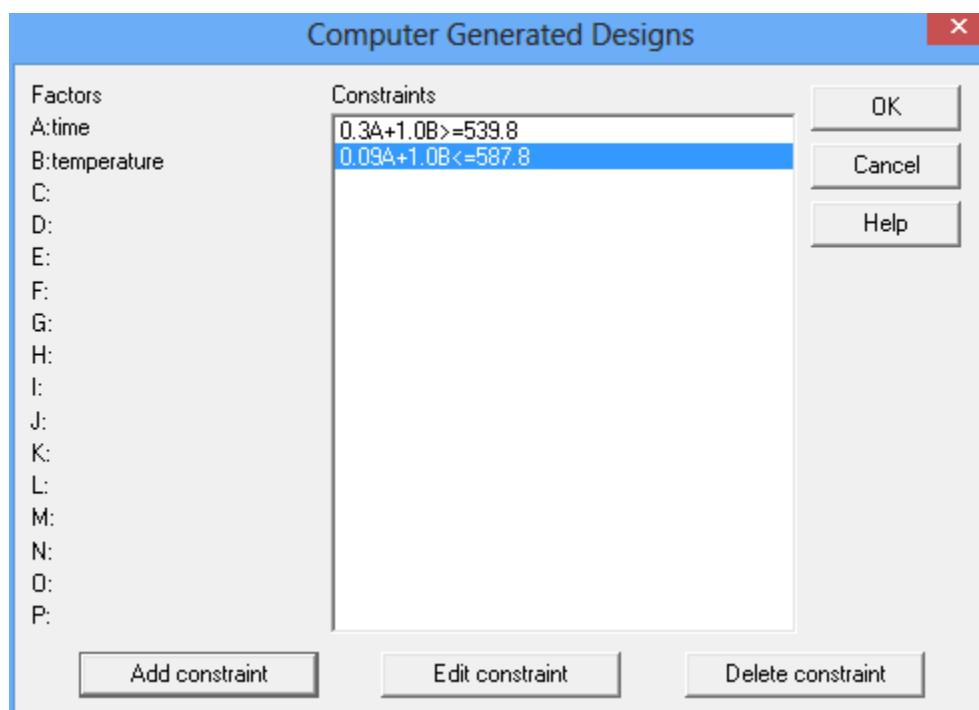
+ 0 E+ 0 F+ 0 G+ 0 H

+ 0 I+ 0 J+ 0 K+ 0 L

+ 0 M+ 0 N+ 0 O+ 0 P \leq 587.8

OK Cancel Help

Press *OK* again and review the entered constraints:



Computer Generated Designs

Factors

A: time

B: temperature

C:

D:

E:

F:

G:

H:

I:

J:

K:

L:

M:

N:

O:

P:

Constraints

0.3A+1.0B \geq 539.8

0.09A+1.0B \leq 587.8

OK

Cancel

Help

Add constraint Edit constraint Delete constraint

Note: if your design contains both process factors and mixture components, each constraint may involve only one type of factor.

Press *OK* twice to return to the main DOE Wizard window, which will display the entered constraints:

Experimental Design Wizard

Step 1: Define responses Step 3: Select design Step 5: Select runs Step 7: Save experiment Step 9: Optimize responses Step 11: Augment design
 Step 2: Define exp. factors Step 4: Specify model Step 6: Evaluate design Step 8: Analyze data Step 10: Save results Step 12: Extrapolate

Experimental Design Wizard

Step 1: Define the response variables to be measured

Name	Units	Analyze	Goal	Target	Impact	Sensitivity	Low	High
yield	%	Mean	Maximize		3.0	Medium		

Step 2: Define the experimental factors to be varied

Name	Units	Type	Role	Low	High	Levels
A:time	seconds	Continuous	Controllable	430.0	650.0	
B:temperature	degrees K	Continuous	Controllable	500.0	550.0	

Step 3: Select the experimental design

Type of	Design	Centerpoints	Centerpoint	Design is	Number of	Total	Total	Error
Factors	Type	Per Block	Placement	Randomized	Replicates	Runs	Blocks	D.F.
Process	Computer generated design							

Number of samples per run: 1

Constraints

0.3A+1.0B>=539.8
0.09A+1.0B<=587.8

In Step 4, select a cubic model:

DOE Wizard Model Options

Process Factors Model

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

Mixture Components Model

☒ Mean
☐ Linear
☐ Quadratic
☐ Special Cubic
☐ Cubic

Include:

A:time
 B:temperature
 AA
 AB
 BB
 AAA
 AAB
 ABB
 BBB

Exclude:

OK
 Cancel
 Help

This model involves 2 main effects, 1 two-factor interaction, 2 quadratic effects, 2 cubic terms of the form x_j^3 , and 2 mixed cubic terms of the form $x_i x_j^2$.

Now press the button labeled *Step 5: Select runs*. Complete the dialog box as shown below:

BLOCK	time seconds	temperature degrees K
1		
2		
3		
4		
5		
6		
7		
8		
9		
10		
11		
12		
13		
14		
15		
16		
17		
18		
19		
20		
21		
22		

Optimize
☒ D-efficiency
☐ G-efficiency
☐ A-efficiency
☐ I-efficiency

Display
☒ Original units
☐ Coded units
☒ Randomize run order

Number of coefficients: 10
 Number of base runs: 13
 Number of replicates: 2
 Number of centerpoints: 0
☒ Block old runs versus new

D-efficiency:
 G-efficiency:
 A-efficiency:
 Average prediction variance:

Create Advanced OK Cancel Help

The settings request a D-optimal design with a total of 15 runs, 2 of which are to be replicates of 2 of the 13 base runs. Press the *Create* button to generate the design:

Computer Generated Designs

	BLOCK	time seconds	temperature degrees K
1	1	720.0	523.0
2	1	605.0	527.5
3	1	360.0	529.0
4	1	475.838	525.525
5	1	499.363	542.857
6	1	360.0	535.0
7	1	360.0	529.0
8	1	590.544	534.651
9	1	360.0	544.75
10	1	643.83	520.485
11	1	457.222	537.9
12	1	720.0	520.0
13	1	360.0	550.0
14	1	475.838	525.525
15	1	420.0	550.0
16			
17			
18			
19			
20			
21			
22			

Optimize

☐ I-efficiency

☒ D-efficiency

☐ A-efficiency

☐ G-efficiency

Display

☒ Original units

☐ Coded units

☒ Randomize run order

Number of coefficients: 10

Number of base runs:

Number of replicates:

Number of centerpoints:

☒ Group runs in blocks of size:

Average prediction variance: 0.618091

D-efficiency: 5.46%

A-efficiency: 0.27%

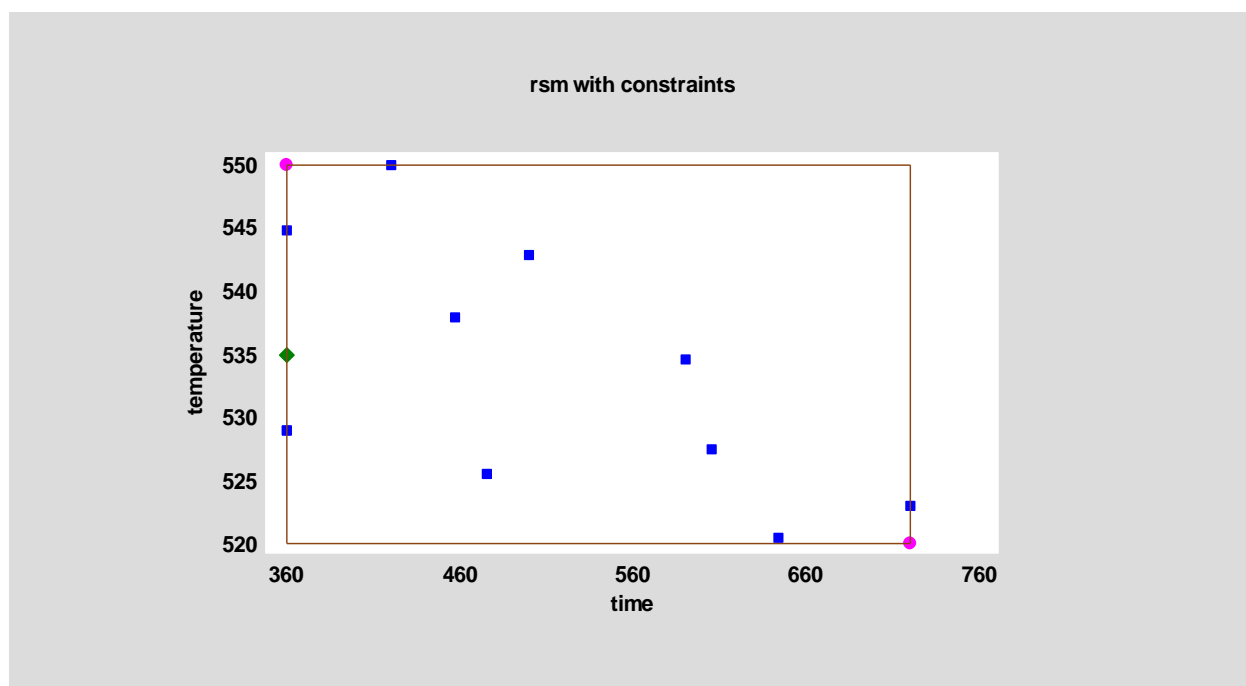
OK
Cancel
Help
Create
Advanced

Push *OK* to save the design.

Once the design has been saved to the datasheet, you may round off the levels if desired:

C:\Data\Version17 Tests\doewiz compgen constraints.sgx				
	BLOCK	time	temperature	yield
		seconds	degrees K	%
1	1	720.0	523.0	
2	1	605.0	527.5	
3	1	360.0	529.0	
4	1	476	526	
5	1	499	543	
6	1	360.0	535.0	
7	1	360.0	529.0	
8	1	591	535	
9	1	360.0	545	
10	1	644	520	
11	1	457	538	
12	1	720.0	520.0	
13	1	360.0	550.0	
14	1	476	526	
15	1	420.0	550.0	
16				

To display the design points, select *Step 6: Evaluate design* from the DOE Wizard toolbar. The *Design Points* graph displays the data as shown below:



Original vertices are shown as round point symbols.

Example #4: Designs with Mixture Variables

Many experiments involve determining tradeoffs between components which must sum to a fixed value. A typical example is a formulation which consists of 3 components. While the experimenter may be able to tradeoff one component for another, the sum of the percentages of each component must equal 100%. Such “mixture” experiments may or may not include additional process factors.

A typical example of a mixture problem, discussed by Myers and Montgomery (2002), involves the formulation of a rocket propellant. The propellant is a mixture of three components: a fuel, an oxidizer, and a binder. The researcher wished to find a combination of these three components which achieved a satisfactory burn rate. Since an inert component made up 10% of the propellant, the factors were constrained by:

$$fuel + oxidizer + binder = 90\%.$$

In addition, there were lower bounds for each of the three components:

$$\begin{aligned} 30\% &\leq fuel \\ 20\% &\leq oxidizer \\ 20\% &\leq binder \end{aligned}$$

Given the constraints, there is a remaining 20% of the mixture that can be any combination of *fuel*, *oxidizer*, and/or *binder*.

To reconstruct their experiment, start with an StatFolio and select *DOE – Experimental Design Wizard* from the main menu. In Step 1, enter the following information about the response variable:

Design of Experiments Wizard - Define Responses

Design file: propellant.sgx

Comment: Rocket propellant example

Number of responses: 1 Responses 1-16 Responses 17-32

Response	Name	Units	Analyze	Goal	Target	Impact (1-5)	Sensitivity	Minimum	Maximum
1	burn rate	cm per second	Mean	Hit target	85.0	3.0	Medium		
2	Var_2		Mean	Maximize	0.5	3.0	Medium		
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

The goal of the experiment was to achieve a burn rate close to 85 cm per second.

In step 2, enter the following information about the experimental factors:

Design of Experiments Wizard - Define Factors

Design file: propellant.sgx
 Comment: Rocket propellant example

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

Factor	Name	Units	Type	Role	Low	High	Levels
A	fuel	percent	Mixture	Controllable	30.0	50.0	30.0,50.0
B	oxidizer	percent	Mixture	Controllable	20.0	40.0	20.0,40.0
C	binder	percent	Mixture	Controllable	20.0	40.0	20.0,40.0
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: 90.0

Factors A-M Factors N-Z

There are 3 mixture components which may sum to 90%.

Pushing the button labeled *Step 3: Select design* displays the dialog box shown below:

Design of Experiments Wizard - Select Design

Design file: propellant.sgx
 Comment: Rocket propellant example

Robust Parameter Design
☒ Combined array
☐ Crossed array

Segment	Factors	Runs	Blocks	Design
Options...	Process factors	0	0	0
Options...	Mixture components	3	0	0
Options...		0	0	0
COMBINED	3	0	0	Samples per run: 1

Press the Options button.

BLOCK	fuel	oxidizer	binder
	percent	percent	percent

OK Cancel Rerandomize Constraints Help

Press the *Options* button for the mixture components to display a list of designs appropriate for 3 mixture components:

Mixture Design Selection

Name	Linear	Quadratic	Special Cubic	Cubic
Simplex-Lattice	3	6	10	10
Simplex-Lattice	3	6	10	10
Simplex-Centroid	7	7	7	
Extreme vertices	3			
Computer generated design				
User-specified design				

☒ Display Blocked Designs

OK Cancel Back Help

Select *Computer generated design* and press *OK* to return to the previous dialog box:

Design of Experiments Wizard - Select Design

Design file: propellant.sgx
 Comment: Rocket propellant example

Robust Parameter Design
☒ Combined array
☐ Crossed array

Options...	Segment	Factors	Runs	Blocks	Design
Options...	Process factors	0	0	0	
Options...	Mixture components	3	0	0	Computer generated design
Options...		0	0	0	
	COMBINED	3	0	0	Samples per run: 1

BLOCK	fuel	oxidizer	binder
	percent	percent	percent

OK Cancel Rerandomize Constraints Help

Press *OK* again to return to the main DOE Wizard window:

Experimental Design Wizard

Step 1: Define responses Step 3: Select design Step 5: Select runs Step 7: Save experiment Step 9: Optimize responses Step 11: Augment design
 Step 2: Define exp. factors Step 4: Specify model Step 6: Evaluate design Step 8: Analyze data Step 10: Save results Step 12: Extrapolate

Experimental Design Wizard

Step 1: Define the response variables to be measured

Name	Units	Analyze	Goal	Target	Impact	Sensitivity	Low	High
burn rate	cm per second	Mean	Hit target	85.0	3.0	Medium		

Step 2: Define the experimental factors to be varied

Name	Units	Type	Role	Low	High	Levels
A: fuel	percent	Mixture	Controllable	30.0	50.0	
B: oxidizer	percent	Mixture	Controllable	20.0	40.0	
C: binder	percent	Mixture	Controllable	20.0	40.0	

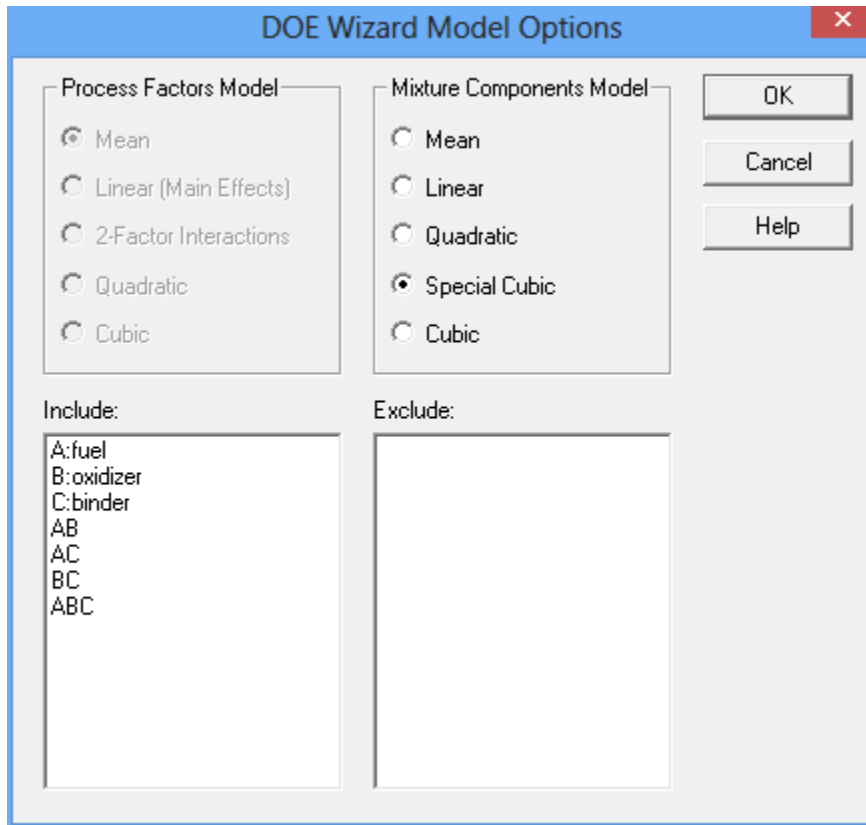
Mixture total = 0.0

Step 3: Select the experimental design

Type of	Design	Centerpoints	Centerpoint	Design is	Number of	Total	Total	Error
Factors	Type	Per Block	Placement	Randomized	Replicates	Runs	Blocks	D.F.
Mixture	Computer generated design							

Number of samples per run: 1

Press the *Step 4* button to select the desired model:



In the example, the researchers choose the popular *Special Cubic* model which has 7 coefficients that must be estimated.

Now press the button labeled *Step 5: Select runs*. Complete the dialog box as shown below:

Computer Generated Designs

BLOCK	fuel percent	oxidizer percent	binder percent
1			
2			
3			
4			
5			
6			
7			
8			
9			
10			
11			
12			
13			
14			
15			
16			
17			
18			
19			
20			
21			
22			

Optimize:
☐ I-efficiency
☒ D-efficiency
☐ A-efficiency
☐ G-efficiency

Display:
☒ Original units
☐ Coded units
☒ Randomize run order

Number of coefficients: 7
 Number of base runs: 10
 Number of replicates: 0
 Number of centerpoints: 0
☒ Group runs in blocks of size: 1000

Average prediction variance:
 D-efficiency:
 A-efficiency:
 G-efficiency:

Create Advanced

OK Cancel Help

The settings request a D-optimal design with a total of 10 runs.

Before creating the design, press the *Advanced* button and set the *Mixture increment* field to 6.6667:

Computer Generated Designs - Search Options

Number of random starts:
 10

Maximum iterations per start:
 100

Number of continuous factor levels to consider:
 5 Set by factor

Mixture increment between levels:
 6.6667

☒ Calculate G-efficiency (may be time-consuming)

OK Cancel Help

This tells the program to consider experimental runs spaced at increments of $6\frac{2}{3}\%$ between the low and high levels of each component.

Press the *Create* button to generate the design:

	BLOCK	fuel percent	oxidizer percent	binder percent
1	1	36.6667	33.3333	20.0
2	1	30.0	40.0	20.0
3	1	50.0	20.0	20.0
4	1	30.0	20.0	40.0
5	1	43.3333	26.6667	20.0
6	1	36.6667	20.0	33.3333
7	1	30.0	33.3333	26.6667
8	1	30.0	26.6667	33.3333
9	1	43.3333	20.0	26.6667
10	1	36.6667	26.6667	26.6667
11				
12				
13				
14				
15				
16				
17				
18				
19				
20				
21				
22				

Optimize:
☐ I-efficiency
☒ D-efficiency
☐ A-efficiency
☐ G-efficiency

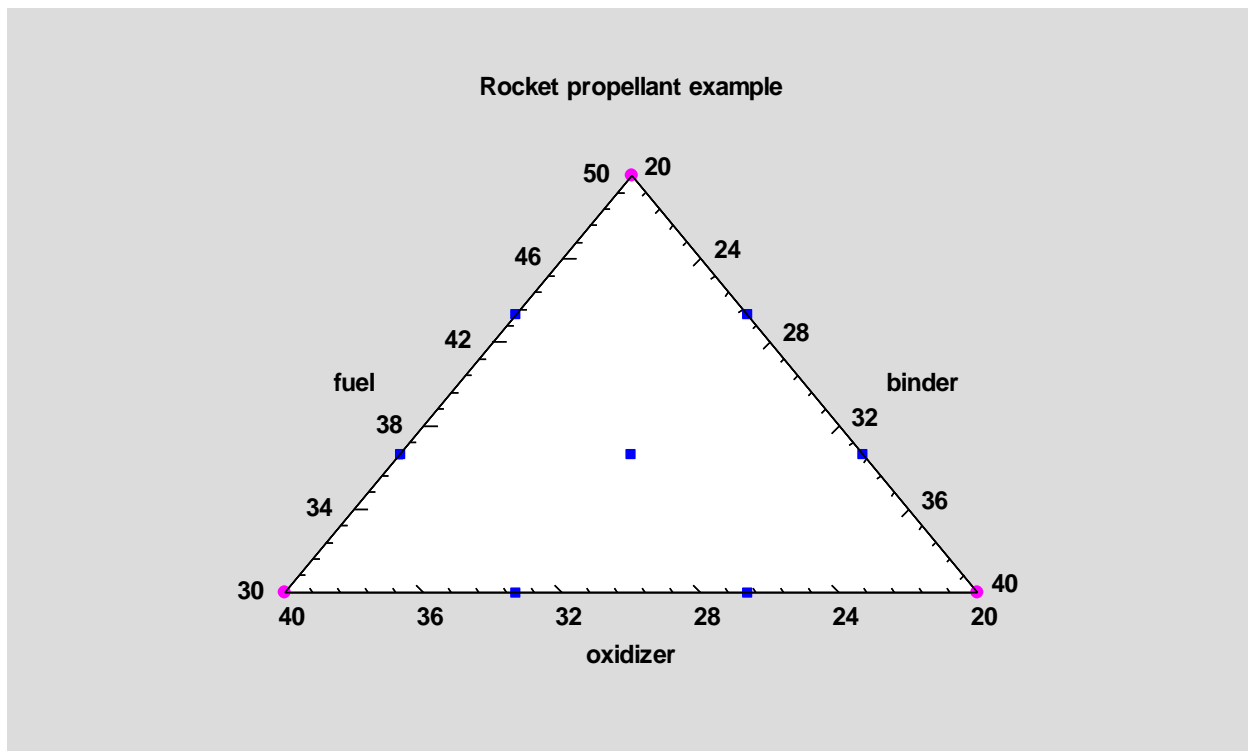
Display:
☒ Original units
☐ Coded units
☒ Randomize run order

Number of coefficients: 7
 Number of base runs: 10
 Number of replicates: 0
 Number of centerpoints: 0
☒ Group runs in blocks of size: 1000

Average prediction variance: 0.522307
 D-efficiency: 13.35%
 A-efficiency: 1.12%

OK Cancel Help Create Advanced

To display the design points, select *Step 6: Evaluate design* from the DOE Wizard toolbar. The *Design Points* graph displays the data as shown below:



The selected runs include the 3 vertices, 2 points on each face, and the centerpoint.

Example #5: Designs with Both Process and Mixture Variables

Many experiments involve determining tradeoffs between components which must sum to a fixed value. A typical example is a formulation which consists of 3 components. While the experimenter may be able to tradeoff one component for another, the sum of the percentages of each component must equal 100%. Such “mixture” experiments may or may not include additional process factors.

Goos and Jones (2011) describe an experiment intended to study the effects on *reflectivity* in a rolling mill producing sheet aluminum. The experiment involved two process factors (*spray volume* and *oil-water ratio*) and three mixture components (percentage of thickness reduction assigned to each of 3 *rollers*).

To reconstruct their experiment, start with a StatFolio and select *DOE – Experimental Design Wizard* from the main menu. In Step 1, enter the following information about the response variable:

Design of Experiments Wizard - Define Responses

Design file: <untitled>

Comment: milling experiment

Number of responses: 1

Responses 1-16 Responses 17-32

Response	Name	Units	Analyze	Goal	Target	Impact (1-5)	Sensitivity	Minimum	Maximum
1	reflectivity		Mean	Maximize	0.5	3.0	Medium		
2	Var_2		Mean	Maximize	0.5	3.0	Medium		
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

In step 2, enter the following information about the experimental factors:

Design of Experiments Wizard - Define Factors

Design file: <untitled>

Comment: milling experiment

Number of controllable process factors: 2 Number of controllable mixture components: 3 Number of noise factors: 0

Factor	Name	Units	Type	Role	Low	High	Levels
A	spray volume		Categorical	Controllable	-1.0	1.0	low,high
B	oil-water		Categorical	Controllable	-1.0	1.0	low,high
C	roller 1	reduction	Mixture	Controllable	0.1	0.8	1,2,3,4
D	roller 2	reduction	Mixture	Controllable	0.1	0.8	1,2,3,4
E	roller 3	reduction	Mixture	Controllable	0.1	0.8	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

The two process variables are treated as categorical factors with 2 levels each. The 3 mixture components, which represent the proportion of thickness reduction performed by each roller, are each constrained to range between 0.1 and 0.8, summing to 1.

Pushing the button labeled *Step 3: Select design* displays the dialog box shown below:

Design of Experiments Wizard - Select Design

Design file: C:\Data\Version17 Tests\chapter6.sgx

Comment: milling experiment

Robust Parameter Design

☒ Combined array

☐ Crossed array

	Segment	Factors	Runs	Blocks	Design
Options...	Process factors	2	0	0	Press the Options button.
Options...	Mixture components	3	0	0	Press the Options button.
Options...		0	0	0	
	COMBINED	5	0	0	Samples per run: <input type="text" value="1"/>

BLOCK	spray volume	oil-water	roller 1 reduction	roller 2 reduction	roller 3 reduction

OK Cancel Rerandomize Constraints Help

Press the *Options* button for the process factors to display the following choices:

Designs for Continuous or Two-Level Fact...

Design Class

☐ Screening

☐ Response Surface

☐ Multilevel Factorial

☐ Orthogonal Array

☒ Computer Generated

OK Cancel Help

Select *Computer Generated* and press *OK* to return to the *Select Design* dialog box:

Design of Experiments Wizard - Select Design

Design file: C:\Data\Version17 Tests\chapter6.sgx

Comment: milling experiment

Robust Parameter Design

☒ Combined array

☐ Crossed array

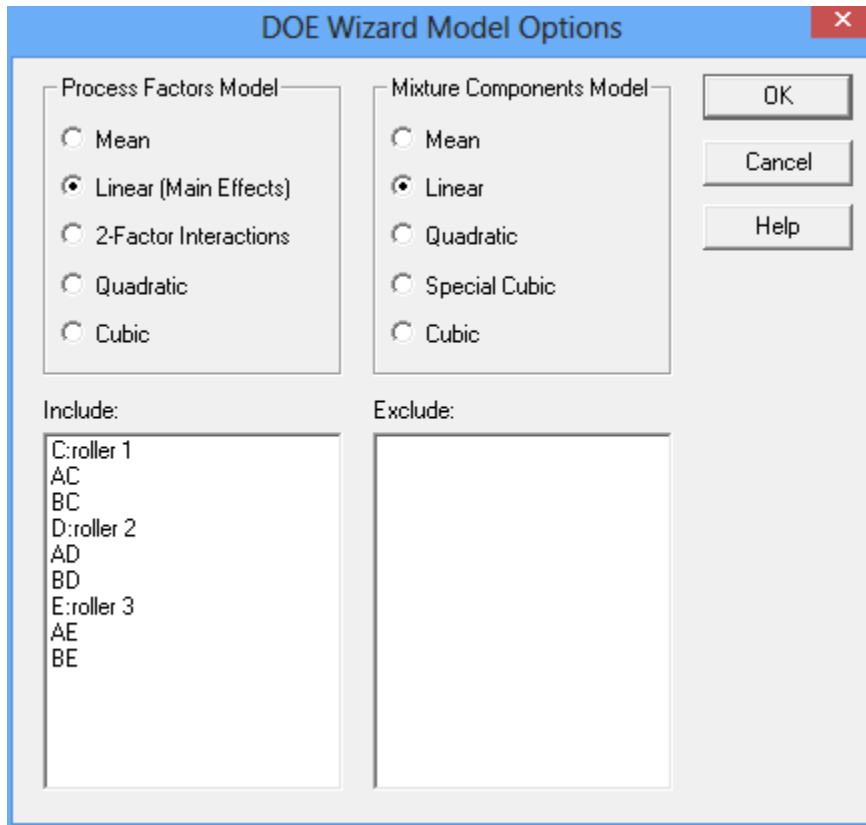
	Segment	Factors	Runs	Blocks	Design
Options...	Process factors	2	0	0	Computer generated design
Options...	Mixture components	3	0	0	Computer generated design
Options...		0	0	0	
	COMBINED	5	0	0	Samples per run: 1

BLOCK	spray volume	oil-water	roller 1 reduction	roller 2 reduction	roller 3 reduction

OK Cancel Rerandomize Constraints Help

Notice that the *Design* for the mixture components has also been set to *Computer Generated Design*, since a single design will be generated for all 5 factors.

Next, push the button labeled *Step 4: Specify model* to display the dialog box shown below:



Selecting a linear model for both the process factors and the mixture components results in a model containing 9 coefficients that must be estimated.

After saving the choice of models, press the button labeled Step 5: Select runs to display the design creation dialog box:

Computer Generated Designs

	BLOCK	spray volume	oil-water	roller 1 reduction	roller 2 reduction	roller 3 reduction
1						
2						
3						
4						
5						
6						
7						
8						
9						
10						
11						
12						
13						
14						
15						
16						
17						
18						
19						
20						
21						
22						

Optimize:
☐ I-efficiency
☒ D-efficiency
☐ A-efficiency
☐ G-efficiency

Display:
☒ Original units
☐ Coded units
☒ Randomize run order

Number of coefficients: 9
 Number of base runs: 12
 Number of replicates: 0
 Number of centerpoints: 0
☒ Group runs in blocks of size: 1000

Average prediction variance:
 D-efficiency:
 A-efficiency:
 G-efficiency:

OK
 Cancel
 Help
 Create
 Advanced

Be sure that “D-efficiency” is checked and that the requested number of base runs is 12.

Press the Advanced button and set the *Mixture increment* field to 0.1:

Computer Generated Designs - Search Options

Number of random starts:
 10

Maximum iterations per start:
 100

Number of continuous factor levels to consider:
 5 Set by factor

Mixture increment between levels:
 0.1

☒ Calculate G-efficiency (may be time-consuming)

OK Cancel Help

Press *OK* and then *Create* to create the design as shown below:

Computer Generated Designs

BLOCK		spray volume	oil-water	roller 1 reduction	roller 2 reduction	roller 3 reduction
1	1	low	high	0.1	0.1	0.8
2	1	high	high	0.1	0.8	0.1
3	1	low	low	0.8	0.1	0.1
4	1	high	low	0.1	0.8	0.1
5	1	low	low	0.1	0.8	0.1
6	1	high	low	0.8	0.1	0.1
7	1	low	high	0.8	0.1	0.1
8	1	high	high	0.1	0.1	0.8
9	1	low	low	0.1	0.1	0.8
10	1	high	high	0.8	0.1	0.1
11	1	high	low	0.1	0.1	0.8
12	1	low	high	0.1	0.8	0.1
13						
14						
15						
16						
17						
18						
19						
20						
21						
22						

Optimize

☐ I-efficiency

☒ D-efficiency

☐ A-efficiency

☐ G-efficiency

Display

☒ Original units

☐ Coded units

☒ Randomize run order

Number of coefficients: 9

Number of base runs:

Number of replicates:

Number of centerpoints:

☒ Group runs in blocks of size:

Average prediction variance: 0.373462

D-efficiency: 83.99%

A-efficiency: 66.67%

G-efficiency: 100.00%

OK

Cancel

Help

Create

Advanced

To display the design points, select *Step 6: Evaluate design* from the DOE Wizard toolbar. The *Design Points* graph displays the experimental points as shown below

