

DOE Wizard – Response Surface Designs

Summary

Once the important factors affecting a process have been identified, additional experiments usually need to be performed to locate the optimal settings of those factors. Since “optimal” often implies a minimum or maximum, optimization designs involve at least three levels of each factor so that curvature may be estimated. In STATGRAPHICS, several popular types of designs for response optimization have been grouped together under *Response Surface Designs*. These include:

1. central composite designs
2. three-level factorial designs
3. Box-Behnken designs
4. Draper-Lin designs

This document concentrates on the creation of response surface designs. Since the analysis of the data once collected parallels that of screening designs, refer to the *DOE – Screening Design* documentation for a detailed discussion of the output generated from the analysis process.

Example

Myers and Montgomery (1995) describe a typical example of an experiment performed to optimize the strength of breadwrapper stock. The design involves the following experimental factors and the range of values over which they were to be varied.

Factor	Low	High	Units
sealing temperature	225	285	°F
cooling bar temperature	46	64	°F
polyethylene	0.5	1.7	%

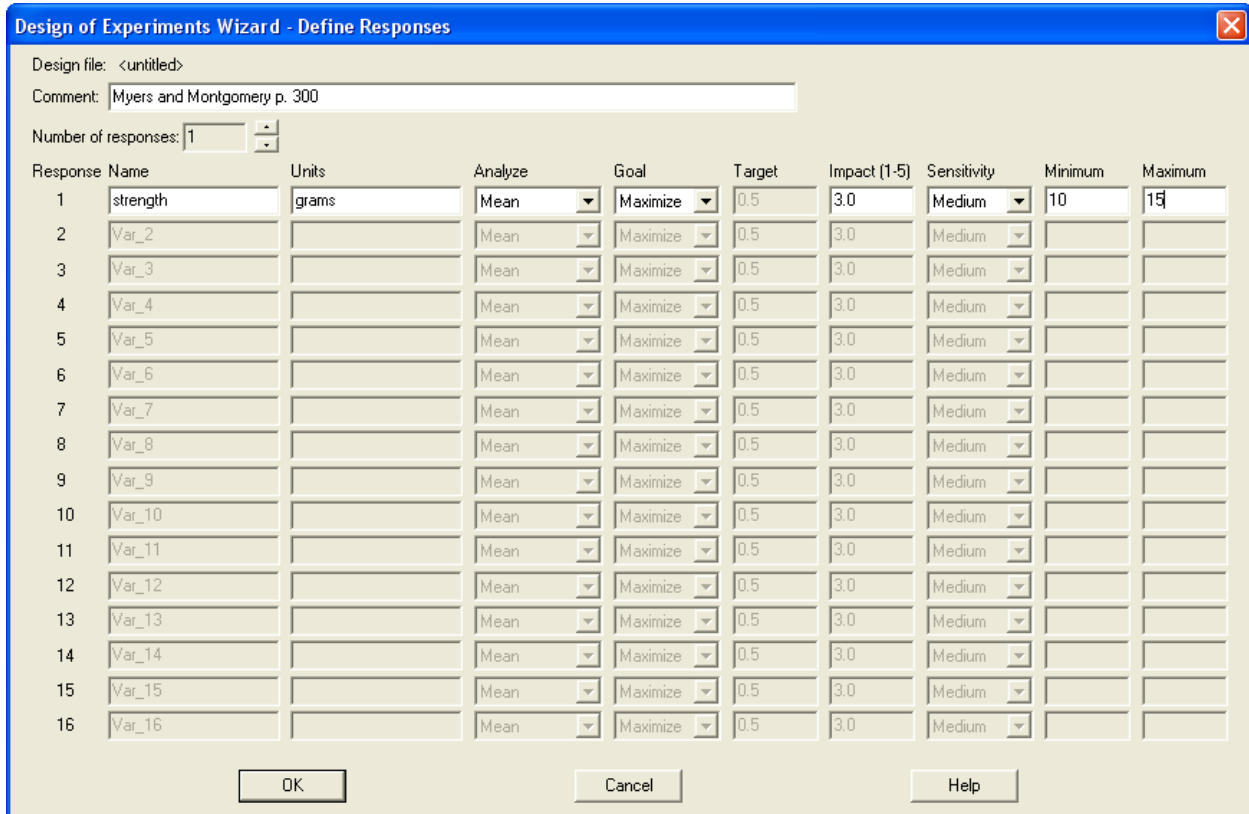
Sample StatFolio: doewiz rsm.sgp

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:

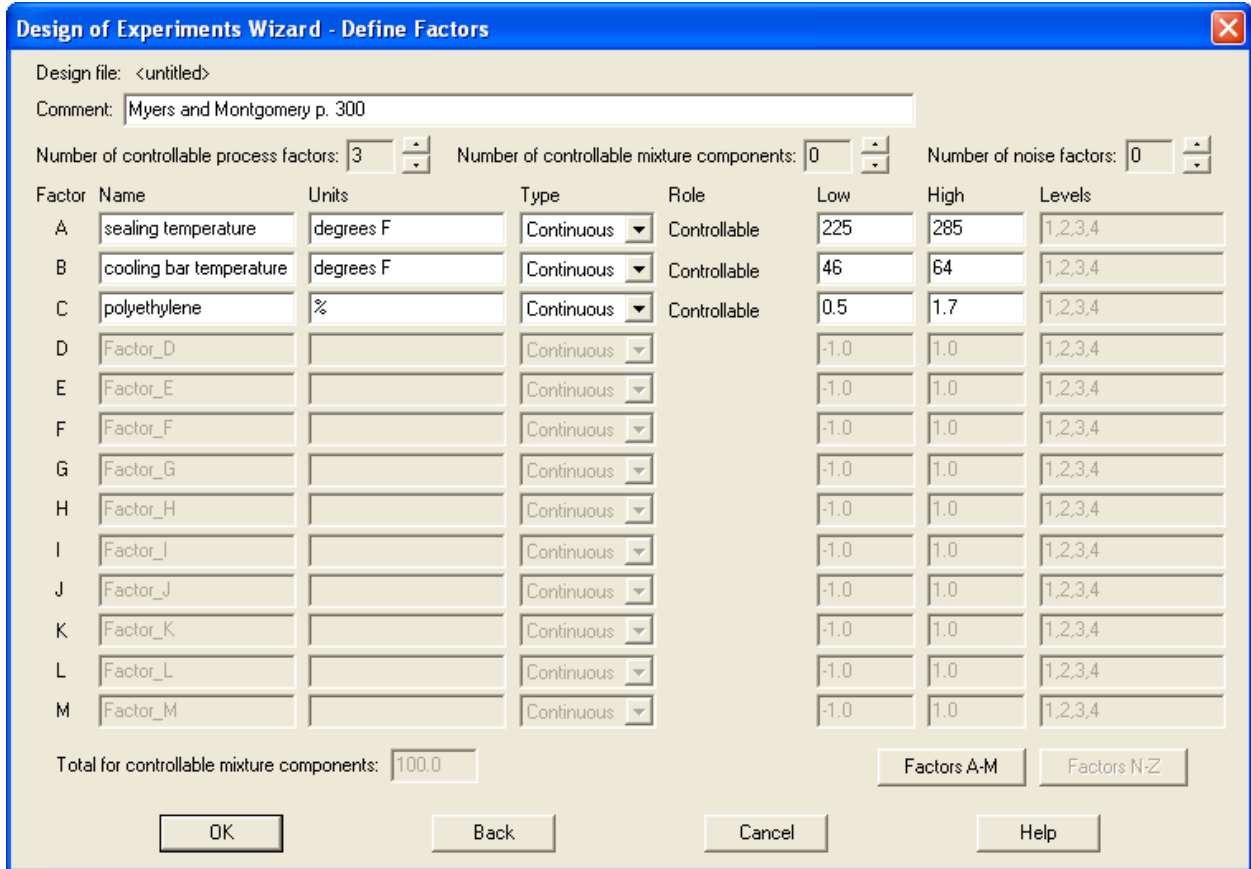


- **Name:** The name for the variable is *strength*.
- **Units:** Strength is measured in grams.
- **Analyze:** The parameter of interest is the *mean* strength.
- **Goal:** The goal of the experiment is to maximize the strength.
- **Impact:** The relative importance of each response (not relevant if only one response).
- **Sensitivity:** The importance of being close to the best desired value (in this case, the *Maximum*). Setting *Sensitivity* to *Medium* implies that the desirability attributed to the response rises linearly between the *Minimum* and *Maximum* values indicated.

- **Minimum and Maximum:** The range of acceptable values for strength is 10 or above, with 15 or above being most desirable.

Step #2 – Define Experimental Factors

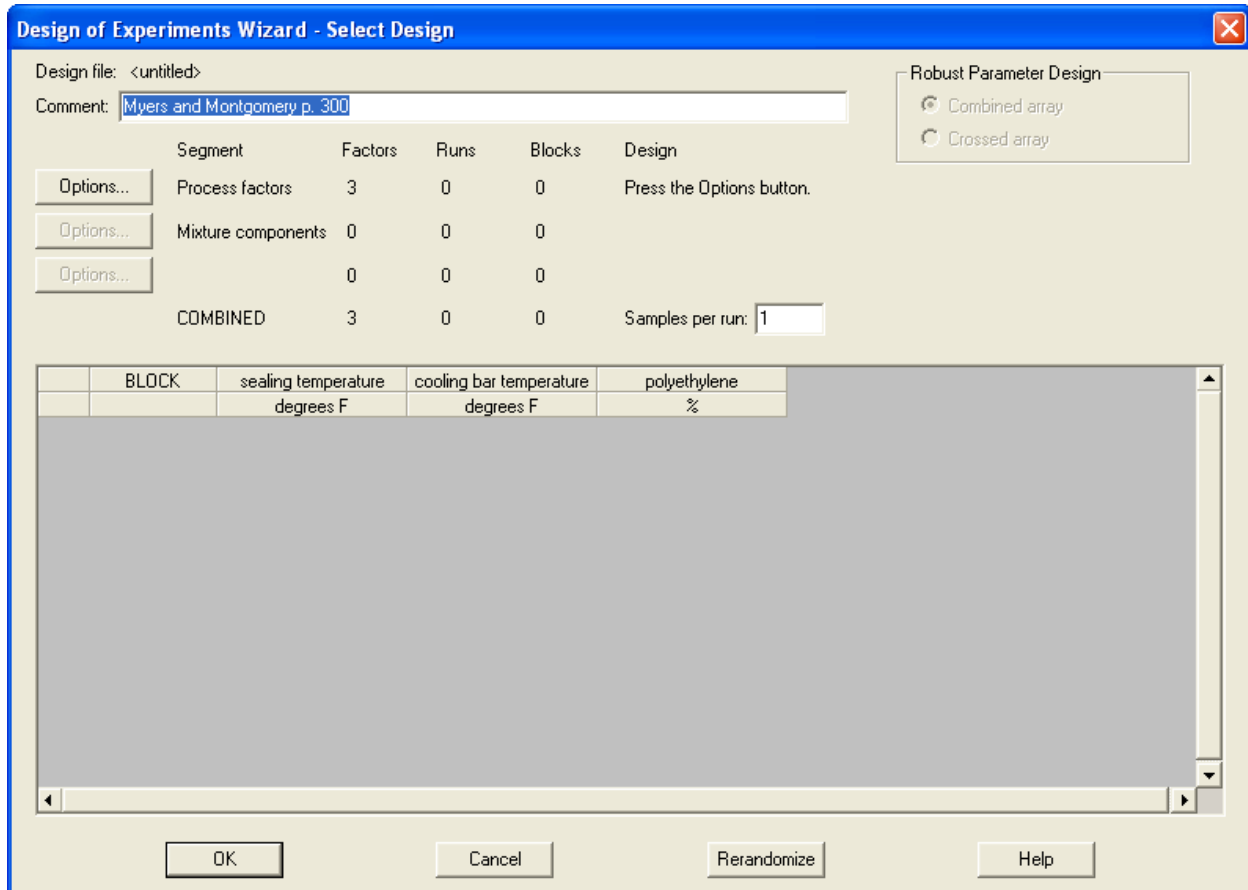
The second step displays a dialog box on which to specify the factors that will be varied. In the chemical reaction example, there are 3 factors:



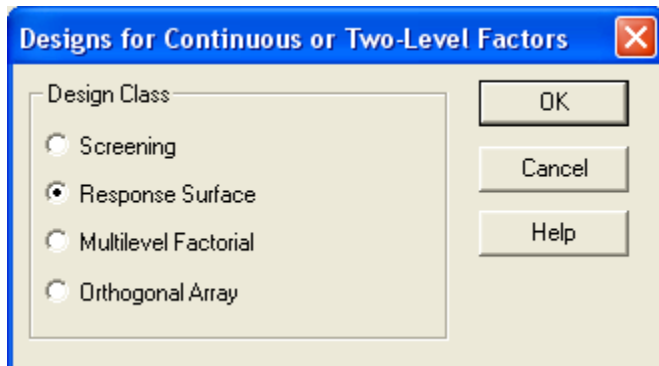
- **Name** – Each factor must be assigned a unique name.
- **Units** – Units are optional.
- **Type** – Set the type of each component to *Continuous*, since they can be set at any value within a continuous interval.
- **Role** – Set the role of each component to *Controllable*.
- **Low** - the lower level L_j for the factor.
- **High** - the upper level U_j for the factor.

Step #3 – Select Design

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



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

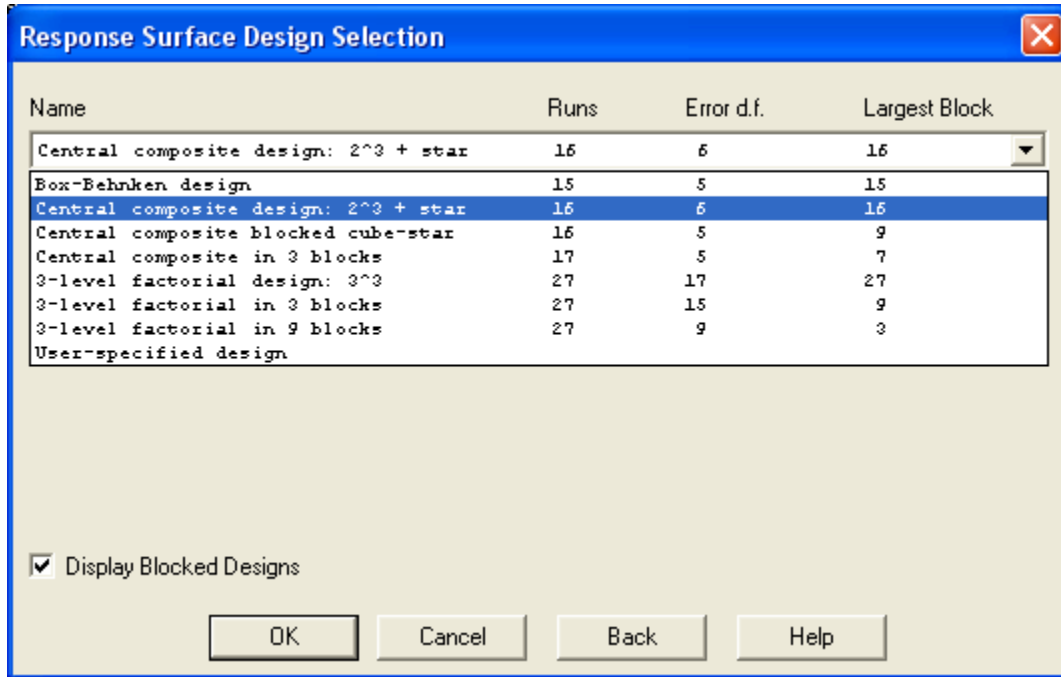


Four general classes of designs are offered:

1. *Screening* - designs intended to select the most important factors affecting a response. Most of the designs involve only 2 levels of each factor. The factors may be quantitative or categorical.
2. *Response Surface* - designs intended to select the optimal settings of a set of experimental factors. The designs involve at least 3 levels of the experimental factors, which must be quantitative.

3. *Multilevel Factorial* - designs involving different numbers of levels for each experimental factor. The factors must be quantitative.
4. *Orthogonal Array* – a general class of designs developed by Genichi Taguchi. The factors may be quantitative or categorical.

If *Response Surface Designs* is selected, a third dialog box will be displayed listing all of the response surface designs available for 3 experimental factors:

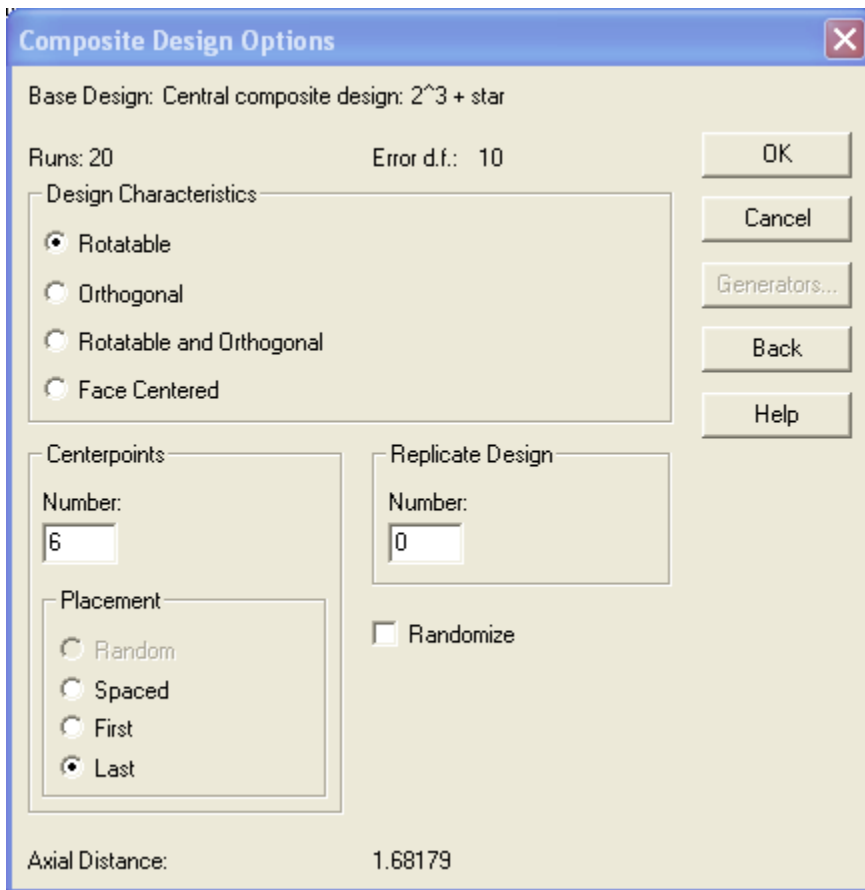


- **Name** - the design name, including an abbreviation such as 3³ if relevant. For response surface designs, the following types may appear in the list, depending upon the number of experimental factors:
 1. *Central composite designs* – designs consisting of a central two-level factorial or resolution V fractional factorial design, plus additional star points used to model curvature with respect to each factor.
 2. *Three level factorial designs* – designs consisting of all combinations of 3 levels of each experimental factor.
 3. *Box-Behnken designs* – 3-level designs including a subset of the runs in the full three level factorial.
 4. *Draper-Lin designs* – small central composite designs in which the central portion of the design is less than resolution V.
- **Runs** - the number of runs in the base design, before adding any additional replicates or centerpoints.

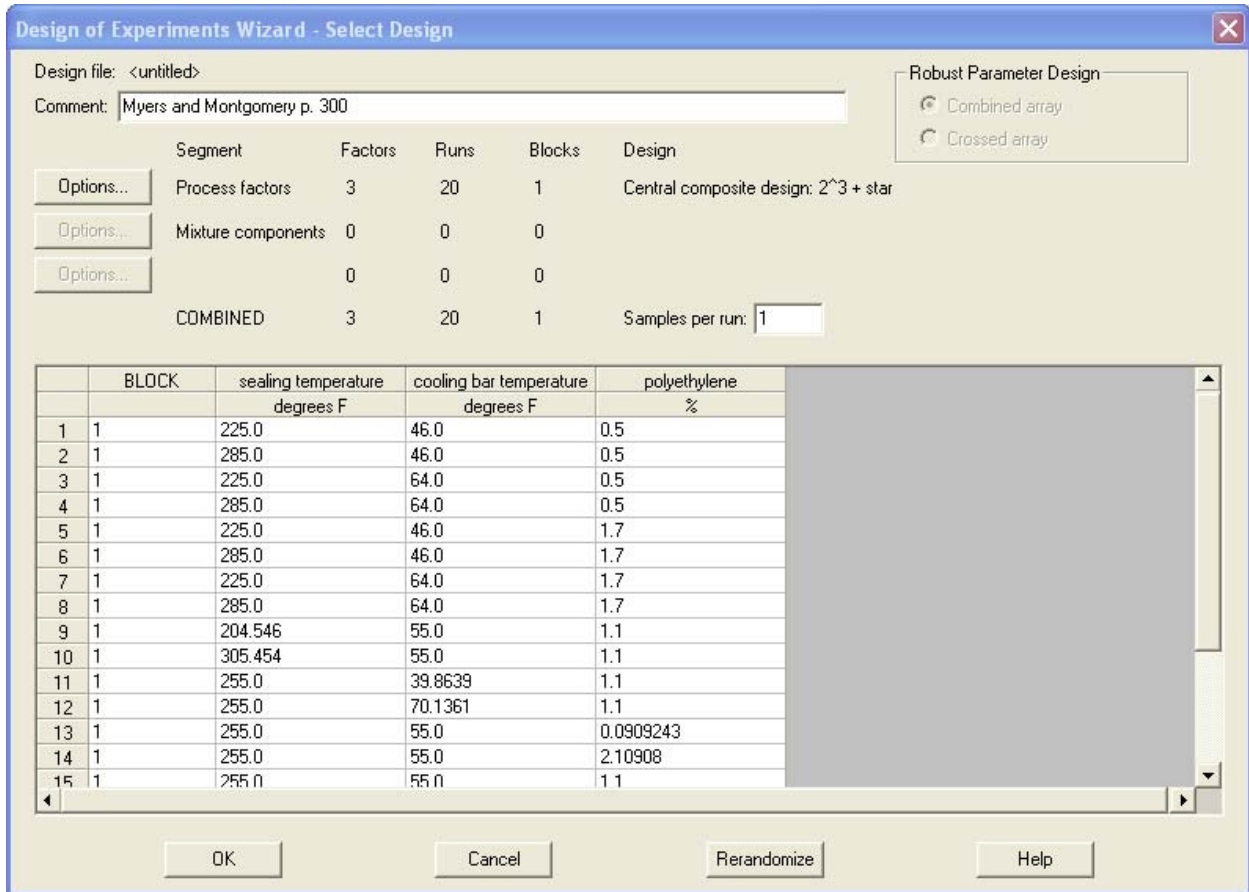
- **Error d.f.** - the number of degrees of freedom from which the experimental error may be estimated remaining after estimating all main effects, second-order interactions, and quadratic effects (if relevant). This is prior to any replication or addition of centerpoints. In general, at least 3 d.f. must be available if the statistical tests to be performed during the analysis are to have reasonable statistical power.
- **Block Size** - for a design that is run in more than 1 block, the number of runs in the largest block.
- **Display Blocked Designs** - check to include designs with more than one block.

For the Myers and Montgomery example, a central composite design with 20 runs was selected.

The final dialog box depends upon the type of design selected. It will be discussed separately for each type in the sections below. For the current example, set the options as:



After completing the final dialog box, the tentatively selected design is displayed in the *Select Design* dialog box:



If the design is acceptable, press OK to save it to the STATGRAPHICS DataBook and return to the DOE Wizard’s main window, which should now contain a summary of the design:

Central Composite Designs

A popular type of optimization experiment begins with a standard two-level factorial design and adds two additional runs for each factor. The additional runs, called *star points*, are located a small distance below the low level of a factor and that same distance above the high level, thus allowing for the estimation of curvature with respect to that factor. While each factor is being varied, the other factors are held at their central values.

For example, consider the 2^3 factorial design shown below:

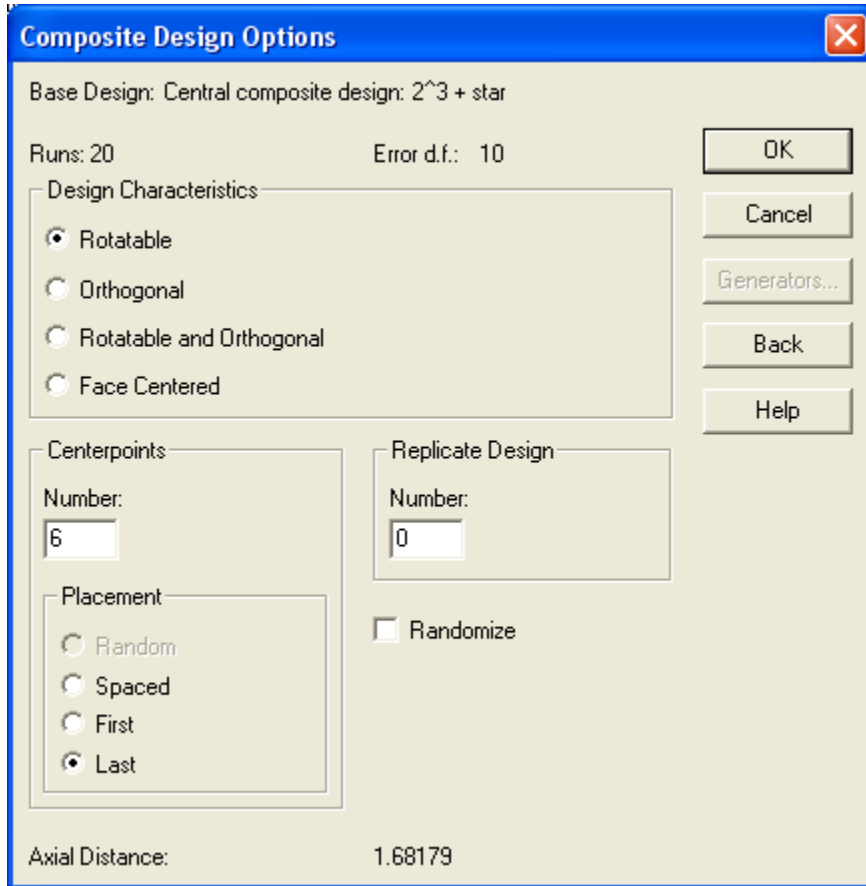
Run	X_1	X_2	X_3
1	-1.0	-1.0	-1.0
2	1.0	-1.0	-1.0
3	-1.0	1.0	-1.0
4	1.0	1.0	-1.0
5	-1.0	-1.0	1.0
6	1.0	-1.0	1.0
7	-1.0	1.0	1.0
8	1.0	1.0	1.0

The design is expressed in standard units where -1 represents the low level of the factor and +1 represents the high level. The additional star points are located at:

Run	X_1	X_2	X_3
9	$-\alpha$	0	0
10	α	0	0
11	0	$-\alpha$	0
12	0	α	0
13	0	0	$-\alpha$
14	0	0	α

where α , the *axial distance*, is ≥ 1 . By setting α equal to specific values, desirable properties can be achieved. At least one centerpoint must also be added to the design.

When constructing a central composite design, the final dialog box has the following form:



- **Design Characteristics:** specifies the properties of the design from the following choices:

1. **Rotatable** - places the star points at a distance that makes the variance of the predicted response the same at all points which are the same distance from the center of the design (in standard units). This is intuitively reasonable, since the experimenter typically does not know beforehand in which direction the optimum point is likely to be located. Rotatability is achieved by setting the axial distance at

$$\alpha = \sqrt[4]{F} \tag{1}$$

where F is the number of runs in the factorial portion of the design (not counting any centerpoints). Any number of centerpoints may be added (3-5 centerpoints are usually desirable), which may be placed in a separate block if desired. For a 2³ factorial, the star points are placed at $\alpha = 1.68179$.

2. **Orthogonal** - places the star points at an axial distance that insures that all second order terms are orthogonal to one another. The proper axial distance depends on the number of centerpoints n_c added to the design:

$$\alpha = \sqrt[4]{\left(\sqrt{2k + n_c + F} - \sqrt{F}\right)^2 F / 4} \tag{2}$$

For a 2³ factorial with 2 centerpoints in the axial block, the star points are placed at $\alpha = 1.28719$.

3. **Rotatable and Orthogonal** - achieves both properties by proper selection of the number of centerpoints. This is done by setting the axial distance equal to that required to achieve rotatability, and then selecting a value for n_c which makes the axial distance for orthogonality the same as for rotatability. For a 2^3 factorial, the star points are placed at $\alpha = 1.68179$ and 9 centerpoints are added to the design.
 4. **Face Centered** - places the star points at the low and high levels of the factorial design, i.e., sets $\alpha = 1.0$. Although less desirable from a statistical perspective, such a design may be easier to run since it involves only low, medium, and high levels of each factor. For such designs, 1-2 centerpoints are usually sufficient.
- **Centerpoints (number)** - the number of centerpoints to be added to the base design, which are additional experimental runs located at a point midway between the low and high level of all the factors. Each additional centerpoint adds one degree of freedom from which to estimate experimental error.
 - **Centerpoints (placement)** - positioning of the centerpoints with respect to the runs in the base design. They may be *randomly* scattered throughout the other experimental runs, *spaced* evenly throughout the other runs, or placed at the *beginning* or *end* of the experiment. The first two options are usually preferable.
 - **Replicate design** - if a number other than 0 is entered, the entire design will be repeated the indicated number of times.
 - **Randomize** - check this box to randomly order the runs in the experiment. Randomization is generally a good idea, since it can reduce the effect of lurking variables such as trends over time. However, when replicating the examples in this documentation, **do not** randomize the designs.

For the example, a rotatable central composite design with 6 centerpoints will be selected. This yields a total of 20 runs, as displayed in the worksheet below:

Worksheet for breadwrapper.sfx - Myers and Montgomery p. 300				
run	sealing temperature (degrees F)	cooling bar temperature (degrees F)	polyethylene (%)	strength (grams per square inch)
1	225.0	46.0	0.5	
2	285.0	46.0	0.5	
3	225.0	64.0	0.5	
4	285.0	64.0	0.5	
5	225.0	46.0	1.7	
6	285.0	46.0	1.7	
7	225.0	64.0	1.7	
8	285.0	64.0	1.7	
9	204.546	55.0	1.1	
10	305.454	55.0	1.1	
11	255.0	39.8639	1.1	
12	255.0	70.1361	1.1	
13	255.0	55.0	0.0909243	
14	255.0	55.0	2.10908	
15	255.0	55.0	1.1	
16	255.0	55.0	1.1	
17	255.0	55.0	1.1	
18	255.0	55.0	1.1	
19	255.0	55.0	1.1	
20	255.0	55.0	1.1	

The design consists of:

- Runs 1-8: a 2^3 factorial.
- Runs 9-14: the star points.
- Runs 15-20: the replicated centerpoints.

When STATGRAPHICS sets up the design, the levels of the star points are placed at the exact distance to achieve rotatability. These levels may be rounded by hand to more reasonable values by changing them in the datasheet.

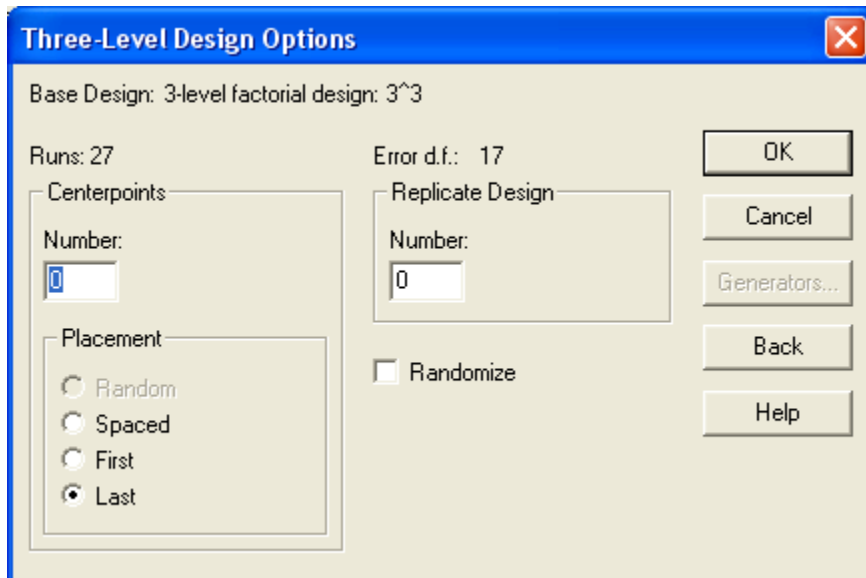
Three-Level Factorial Designs

The central composite designs involve five levels of each experimental factor. Simpler designs can be achieved by using only three levels of each factor, a low level (-), a central level (0), and a high level (+). The three level factorial designs generate runs at each combination of those three levels. With 3 experimental factors, there would be 27 runs, as displayed in the worksheet below:

Run	X ₁	X ₂	X ₃
1	-1	-1	-1
2	0	-1	-1
3	1	-1	-1
4	-1	0	-1
5	0	0	-1
6	1	0	-1
7	-1	1	-1
8	0	1	-1
9	1	1	-1
10	-1	-1	0
11	0	-1	0
12	1	-1	0
13	-1	0	0
14	0	0	0
15	1	0	0
16	-1	1	0
17	0	1	0
18	1	1	0
19	-1	-1	1
20	0	-1	1
21	1	-1	1
22	-1	0	1
23	0	0	1
24	1	0	1
25	-1	1	1
26	0	1	1
27	1	1	1

STATGRAPHICS includes 3-level factorial designs for 2, 3, and 4 factors. In every case, however, the central composite designs are equal or smaller in size than the three-level factorials. By using face-centered star points, the central composite design can also be constrained to the same 3 low, medium, and high levels. Unless the number of runs is not a concern, the 3-level factorial design is usually not the best choice.

If a three-level factorial design is selected, the final dialog box takes the following form:



- **Centerpoints (number)** - the number of centerpoints to be added to the base design, which are additional experimental runs located at a point midway between the low and high level of all the factors. Each additional centerpoint adds one degree of freedom from which to estimate experimental error.
- **Centerpoints (placement)** - positioning of the centerpoints with respect to the runs in the base design. They may be *randomly* scattered throughout the other experimental runs, *spaced* evenly throughout the other runs, or placed at the *beginning* or *end* of the experiment. The first two options are usually preferable.
- **Replicate design** - if a number other than 0 is entered, the entire design will be repeated the indicated number of times.
- **Randomize** - check this box to randomly order the runs in the experiment. Randomization is generally a good idea, since it can reduce the effect of lurking variables such as trends over time. However, when replicating the examples in this documentation, **do not** randomize the designs.

Box-Behnken Designs

A type of design which *does* present a reasonable alternative to the central composites was developed by Box and Behnken for situations when the experimenter wishes to run only three levels of the factors and yet desires a design that is close to rotatable. While the central composite design with face-centered centerpoints also has 3 levels, it places most of the design points at the corners of the experimental region. If that region defines the feasible conditions for the process, the face-centered central composite is a natural choice. However, if one is starting at a particular combination of factors and is simply searching for better conditions, a more spherical arrangement of design points will be more efficient.

The Box-Behnken designs consist of sets of runs in which each pair of factors is varied between their low and high levels, while the other experimental factors are held at the medium level. For example, a 3-factor Box-Behnken design (with centerpoints omitted) is shown below:

Run	X ₁	X ₂	X ₃
1	-1	-1	0
2	1	-1	0
3	-1	1	0
4	1	1	0
5	-1	0	-1
6	1	0	-1
7	-1	0	1
8	1	0	1
9	0	-1	-1
10	0	1	-1
11	0	-1	1
12	0	1	1

Each set of 4 consecutive runs is a 2-level experimental design involving a selected pair of factors. In addition, 3-5 centerpoints at (0,0,0) should be added to the design. The design is comparable in size to a central composite and considerably smaller than a 3-level factorial. For a Box-Behnken design, the final dialog box is the same as for the three-level factorial design.

Draper-Lin Designs

When the cost of experimentation is high, the experimenter may wish to keep the number of runs as small as possible. The Draper-Lin designs in the STATGRAPHICS design catalog are small composite designs that consist of a fractional factorial or Plackett-Burman design of less than resolution V, with added star points. For example, a Draper-Lin design for 4 factors is shown below (omitting centerpoints):

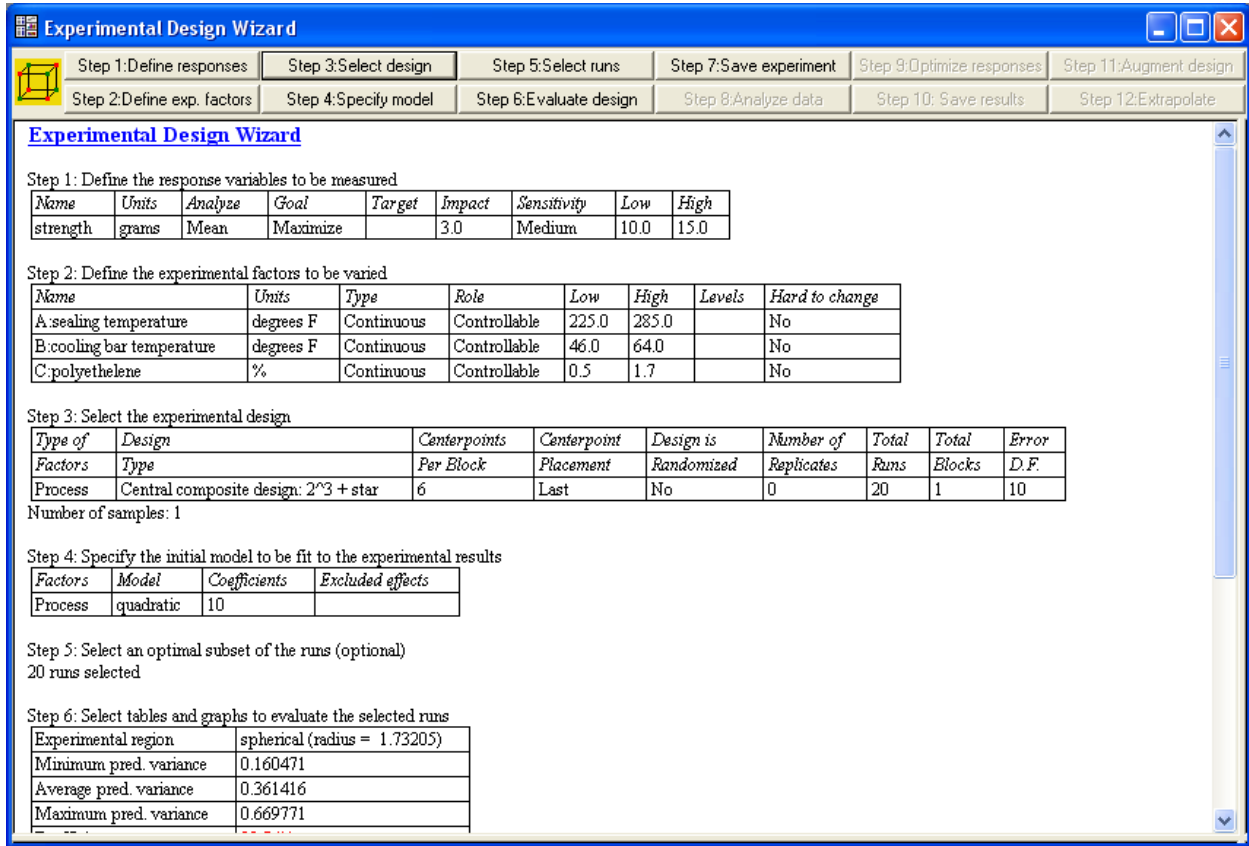
Run	X ₁	X ₂	X ₃	X ₄
1	1	1	1	-1
2	1	1	-1	-1
3	1	-1	1	1
4	-1	1	-1	1
5	1	-1	-1	1
6	-1	-1	1	-1
7	-1	1	1	1
8	-1	-1	-1	-1
9	- α	0	0	0
10	α	0	0	0
11	0	- α	0	0
12	0	α	0	0
13	0	0	- α	0
14	0	0	α	0
15	0	0	0	- α
16	0	0	0	α

The first 8 runs comprise a half-fraction of a 2⁴ factorial, which is resolution IV. The second set of 8 runs are the star points, where α is the axial distance as defined for central composite designs. Several centerpoints would also be added. The resulting design is capable of estimating the full second-order model, although some correlation will exist among the estimated model coefficients. For cases in which the cost of each run is very large, however, the saving of 8 runs over the full central composite design can be significant.

For a Draper-Lin design, the final dialog box is the same as for the central composite design.

Selecting an Initial Model

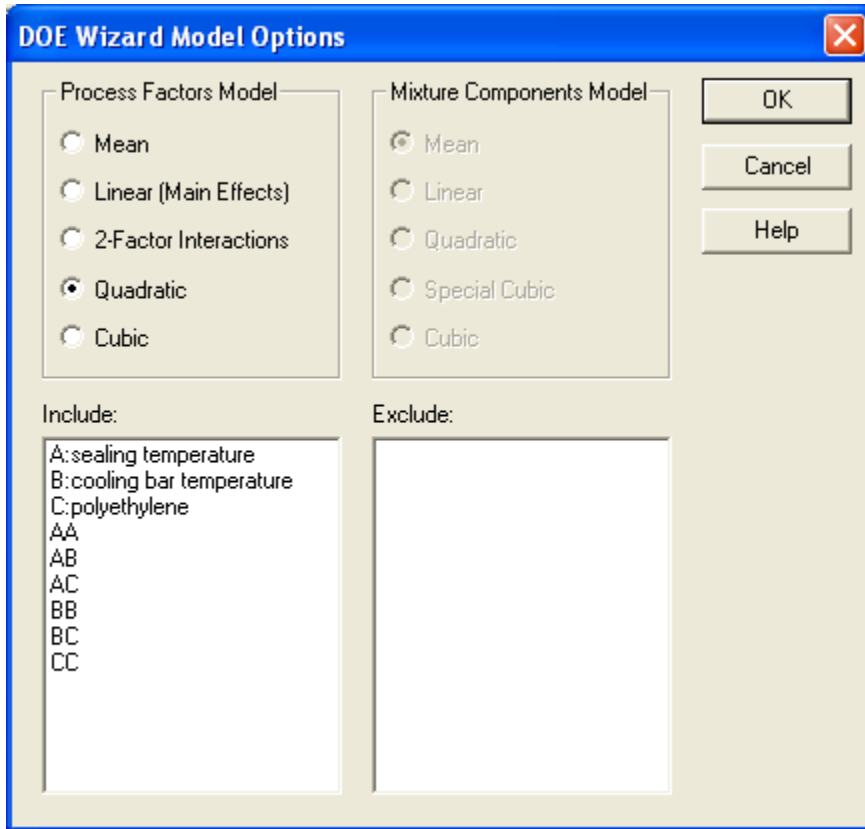
Once the design is selected, a summary will be added to the main DOE Wizard window:



Step #4: Specify Model

Before evaluating the properties of the design, a tentative model must be specified. Pressing the fourth button on the DOE Wizard’s toolbar displays a dialog box to make that choice:

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The statistical model upon which the analysis of response surface designs is based expresses the response variable Y as a linear function of the experimental factors, interactions between the factors, quadratic terms, and an error term. Select from the following models:

1. Mean model – contains only a constant term plus error:

$$Y = \beta_0 + \varepsilon \tag{3}$$

2. *Linear model* – contains terms representing main effects:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \varepsilon \tag{4}$$

3. *Two factor interaction model* – contains terms representing main effects and second-order interactions:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \beta_{12} X_1 X_2 + \beta_{13} X_1 X_3 + \beta_{23} X_2 X_3 + \varepsilon \tag{5}$$

4. *Quadratic model* – contains terms representing main effects, second-order interactions, and quadratic effects.

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \beta_{12} X_1 X_2 + \beta_{13} X_1 X_3 + \beta_{23} X_2 X_3 + \beta_{11} X_1^2 + \beta_{22} X_2^2 + \beta_{33} X_3^2 + \varepsilon \tag{6}$$

The experimental error ε is assumed to be randomly drawn from a normal distribution with a mean of 0 and a standard deviation equal to σ .

The only difference in the analysis between response surface designs and screening designs is the inclusion of the quadratic effects. These appear on the Pareto chart and other output as effects labeled AA, BB, and CC:

The default model is the quadratic model. This allows for estimating curved surfaces such as hills, valleys, ridges, saddle points, and the like. Selected terms could be excluded by double-clicking on them with the left mouse button.

Step #5: Select Runs

Since we intend to run all of the runs in the base design, this step can be omitted.

Design Properties

Step #6: Evaluate Design

Several of the selections presented when pressing button #6 are helpful in evaluating the selected design:

Design Worksheet

The design worksheet shows the 20 runs that have been created, in the order they are to be run:

Worksheet for <untitled> - Myers and Montgomery p. 300				
<i>run</i>	<i>sealing temperature</i>	<i>cooling bar temperature</i>	<i>polyethelene</i>	<i>strength</i>
	<i>degrees F</i>	<i>degrees F</i>	<i>%</i>	<i>grams</i>
1	225.0	46.0	0.5	
2	285.0	46.0	0.5	
3	225.0	64.0	0.5	
4	285.0	64.0	0.5	
5	225.0	46.0	1.7	
6	285.0	46.0	1.7	
7	225.0	64.0	1.7	
8	285.0	64.0	1.7	
9	204.546	55.0	1.1	
10	305.454	55.0	1.1	
11	255.0	39.8639	1.1	
12	255.0	70.1361	1.1	
13	255.0	55.0	0.0909243	
14	255.0	55.0	2.10908	
15	255.0	55.0	1.1	
16	255.0	55.0	1.1	
17	255.0	55.0	1.1	
18	255.0	55.0	1.1	
19	255.0	55.0	1.1	
20	255.0	55.0	1.1	

ANOVA Table

The ANOVA table shows the breakdown of the degrees of freedom in the design:

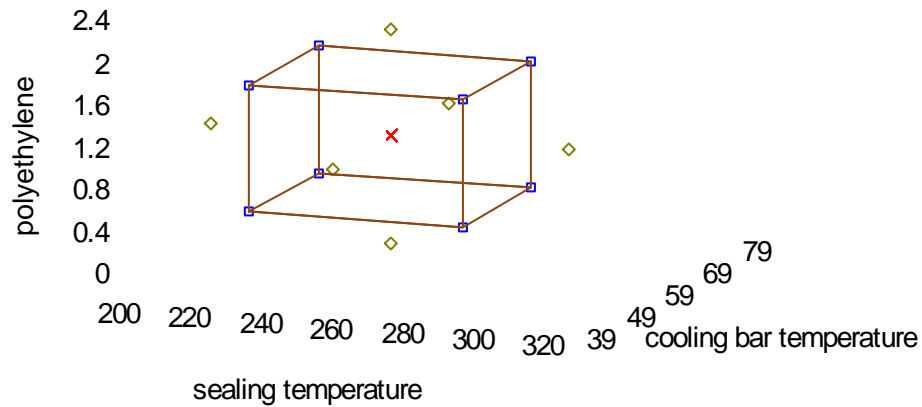
ANOVA Table	
Source	D.F.
Model	9
Total Error	10
Lack-of-fit	5
Pure error	5
Total (corr.)	19

10 of the 20 total degrees of freedom are used to estimate the model coefficients. 5 degrees of freedom are available from replicates to estimate pure error. 5 degrees of freedom are available to test the adequacy of the quadratic model (“lack-of-fit”).

Design Points

This graph displays the runs in the selected design:

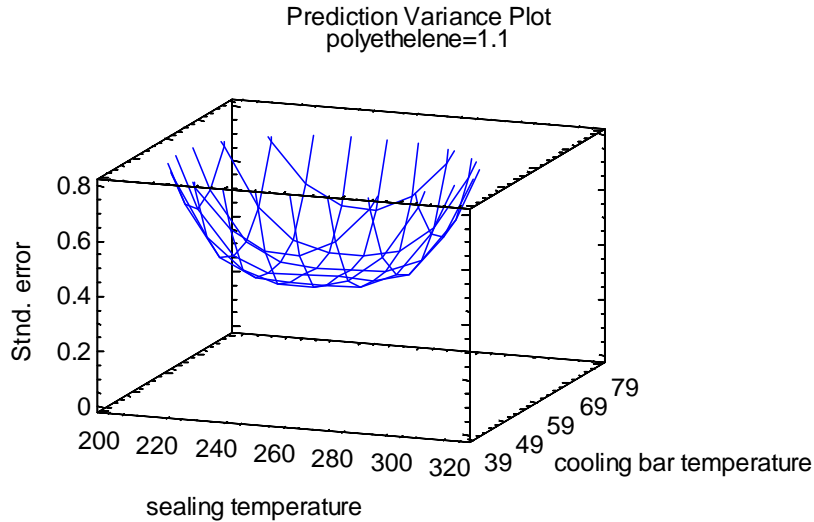
Myers and Montgomery p. 300



Note the 8 runs on the cube, the centerpoint, and the 6 star points.

Prediction Variance Plot

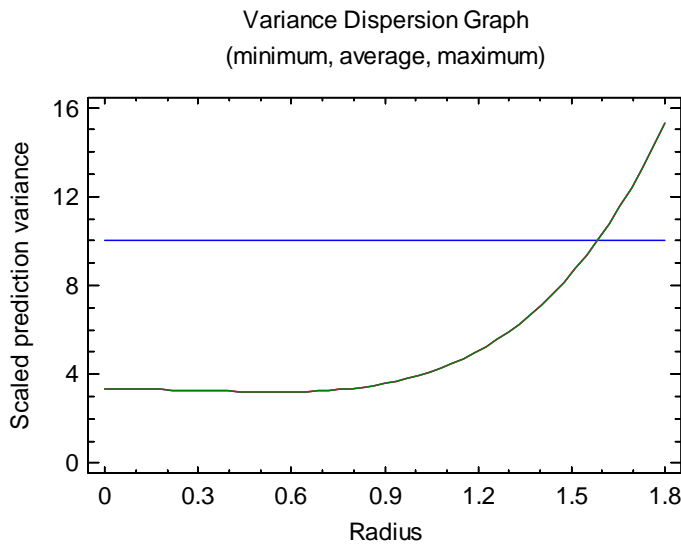
This plot shows how the standard error of the predicted response changes throughout the experimental region:



Note how the standard error increases symmetrically with distance from the center of the design.

Variance Dispersion Graph

The variance dispersion graph plots the minimum, maximum, and average scaled prediction as a function of distance from the center:

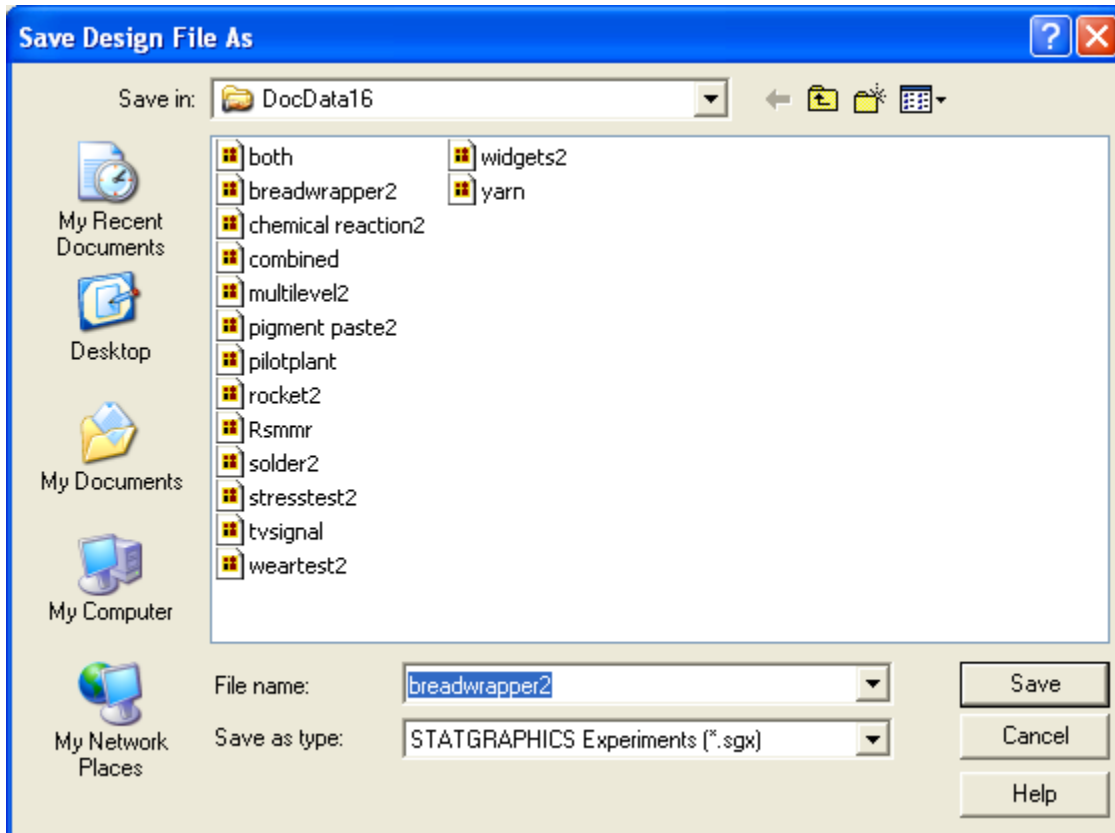


Only one line appears since for a rotatable design such as that selected, since the minimum and maximum variance at any given distance is the same in all directions.

Saving the Design File

Step #7: Save experiment

Once the experiment has been created and any additional runs entered, it must be saved on disk. Press the button labeled *Step 7* and select a name for the experiment file:



Design files are extended data files and have the extension *.sgx*. They include the data together with other information that was entered on the input dialog boxes.

To reopen an experiment file, select *Open Data File* from the *File* menu. The data will be loaded into the datasheet, and the *Experimental Design Wizard* window will be displayed.

Analyzing the Results

After the design file has been created and saved, the experiments would be performed. At a later date, once the results have been collected, the experimenter would return to STATGRAPHICS and reopen the saved design file using the *Open Data Source* selection on the main *File* menu. The results can then be typed into the response columns.

The results for the example are displayed below:

<i>run</i>	<i>sealing temperature</i> <i>(degrees F)</i>	<i>cooling bar temperature</i> <i>(degrees F)</i>	<i>polyethylene</i> <i>(%)</i>	<i>strength</i> <i>(grams per square inch)</i>
1	225.0	46.0	0.5	6.6
2	285.0	46.0	0.5	6.9
3	225.0	64.0	0.5	7.9
4	285.0	64.0	0.5	6.1
5	225.0	46.0	1.7	9.2
6	285.0	46.0	1.7	6.8
7	225.0	64.0	1.7	10.4
8	285.0	64.0	1.7	7.3
9	204.5	55.0	1.1	9.8
10	305.5	55.0	1.1	5.0
11	255.0	39.9	1.1	6.9
12	255.0	70.1	1.1	6.3
13	255.0	55.0	0.09	4.0
14	255.0	55.0	2.11	8.6
15	255.0	55.0	1.1	10.1
16	255.0	55.0	1.1	9.9
17	255.0	55.0	1.1	12.2
18	255.0	55.0	1.1	9.7
19	255.0	55.0	1.1	9.7
20	255.0	55.0	1.1	9.6

Note that the location of the star points has been rounded.

Step #8: Analyze data

Once the data have been entered, press the button labeled *Step #8* on the Experiment Design Wizard toolbar. This will display a dialog box listing each of the response variables:

Response	Transformation	Power	Addend
strength	None	1.0	0

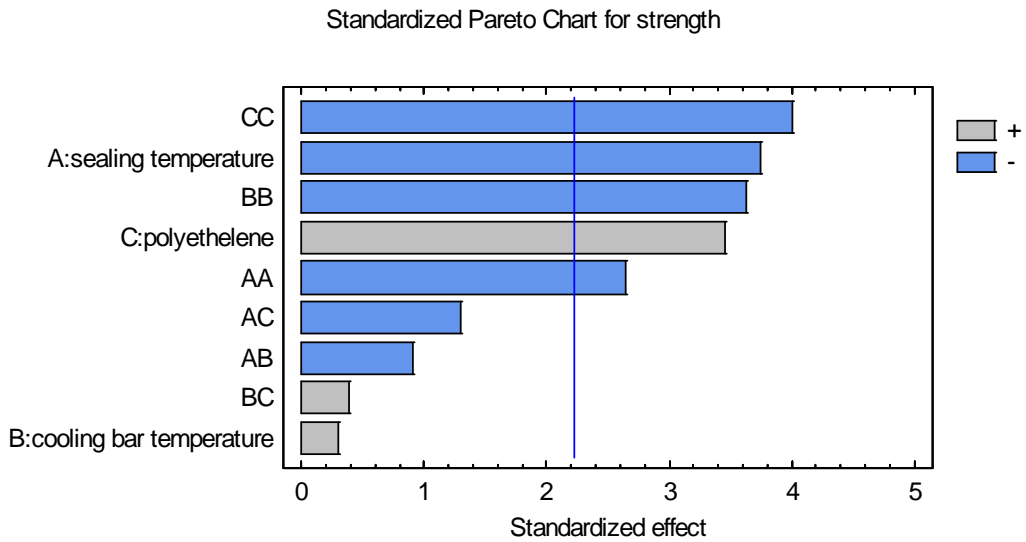
OK Cancel Help

- **Response:** column containing the response variable to be analyzed.
- **Transformation:** the desired transformation to be applied before the model is fit.
- **Power and addend:** the transformation parameters if a *Power* or *Box-Cox* transformation is selected.

If more than one response has been measured, you should repeat this step once for each response.

Pareto Chart

A useful summary of the results is given by the *Pareto Chart*:



The model shows 5 statistically significant effects: the main effects of factors A and C, and the quadratic effect of all 3 factors.

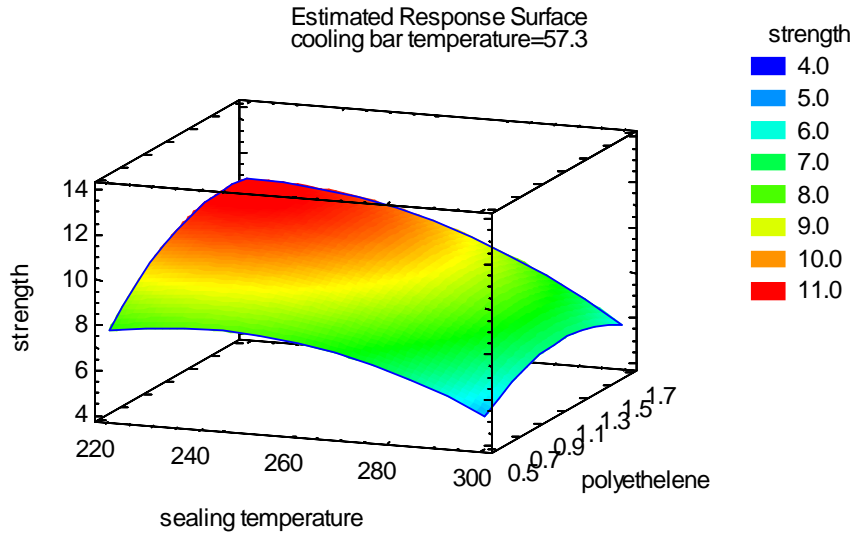
Optimization

The settings for the factors that maximize strength are shown below:

Optimize Response			
Goal: maximize strength			
Optimum value = 11.0829			
<i>Factor</i>	<i>Low</i>	<i>High</i>	<i>Optimum</i>
sealing temperature	204.5	305.5	224.612
cooling bar temperature	39.9	70.1	57.3425
polyethelene	0.09	2.11	1.5097

Response Surface Plot

The response surface plot, shown below with respect to factors A and C with factor B set at its optimum value, shows a rather flat peak:



The flat peak means that the response is not very sensitive to small deviations in the factor settings near the optimum. Such robust operating conditions are very desirable.