

Section 9 – Advanced Design Features

This section discusses advanced design topics. Be prepared to give your software a session of vigorous exercise. You will discover many new program muscles that were not used in the preceding tutorials. Don't be afraid to take some side-tracks along the way. In fact, you will be encouraged to explore various features encountered as you work through this section.

You will find more information in the Statistical Details: Design Selection section of this manual. Also, check out the on-line help system in the Design-Expert program. If you still need help, then give Stat-Ease a call. Our telephone number is at the end of the Introduction.

Custom Generators for Fractional Factorials

Design-Expert version 6 automatically generates two-level designs that provide maximum resolution of effects, taking into account the degree of fractionation and/or blocking. The software now allows users to over-ride the design selection criteria by entering custom generators. Before showing how this is done, we will provide a short review of fractional factorial design, introducing a relatively new concept called “abberation.”

A standard two-level fractional factorial can be represented as a 2^{k-p} design, where

- “k” is the number of factors studied,
- 2^{k-p} is the number of experiments run,
- and 2^{-p} is the fraction.

A 2^{k-p} fractional factorial is uniquely defined by the (2^p-1) words in the defining contrast. (See “Design and Analysis of Experiments” by Montgomery for background.)

For example, consider a 2^{7-2} fractional factorial. There are seven factors in a total of thirty-two experiments. It is a 2^{-2} , or a one-quarter fraction of a full 2^7 factorial. The defining contrast contains three (2^2-1) words. Using the default factor generators the defining contrast is:

$$I = DEFG = ABCDF = ABCEG$$

The number of letters in a word is called its “word-length.” The shortest word-length in the defining contrast is called the “resolution” of the design. In our example the shortest word has four letters (DEFG), so the resolution is IV.

Design-Expert created the 2^{7-2} fractional factorial design by taking the standard effect matrix for thirty-two runs (2^5) and generating the extra two factors as follows:

$$F = ABCD$$
$$G = ABCE$$

However, other choices of factor generators could create an equally good design in terms of resolution, but not as good for estimating factor interactions. For example, you change the factor generators to:

$$F = ABD$$
$$G = ACE$$

Which makes the defining contrast:

$$I = ABDF = ACEG = BCDEFG$$

The design is still resolution IV, i.e., the shortest word in the defining contrast is four letters, but now there are two words of length four, rather than the one word that occurred using the default generators. This causes more two-factor interactions to be aliased with each other. Not good! All else being equal in terms of resolution, the design with the smallest number of shortest word-length words is said to exhibit “minimum aberration”, i.e., the least confusion among the lower order interactions.

Design-Expert version 6 automatically chooses designs of minimum aberration, not only for the fraction itself, but also for the blocking schemes. For details see:

1. D. X. Sun, C. F. J. Wu and Y Chen, “Optimal Blocking Schemes for 2^n and 2^{n-p} Designs,” *Technometrics*, August 1997, Vol. 39, No. 3.
2. R. R. Sitter, J Chen and M. Feder, “Fractional Resolution and Minimum Aberration in Blocked 2^{n-k} Designs,” *Technometrics*, Nov. 1997, Vol. 39, No. 4.

Note that the designs chosen by Design-Expert’s minimum aberration criteria may differ from those in standard textbooks. However, as illustrated by the following mini-tutorial, version 6 of Design-Expert offers the option to define your own generators, thus providing a mechanism to match textbook designs.

In Example 9-6 of his text, Montgomery reports an experiment on a five-axis CNC (computer numeric control) machine used to machine a jet turbine impeller. The engineers varied eight factors in 32 experiments (a 2^{8-3} design) in four blocks (spindles). They desired minimum deviation between the actual versus specified blade profile.

To reproduce this DOE, choose **File, New Design** (or click the “blank page” icon at the left of the toolbar). On the **Factorial** tab, with default design of **2 Level Factorial**, click on the square where 8 factors intersects with 32 experiments ($1/8^{\text{th}}$ fraction). Change the number of **Blocks** from 1 to **4**.

2 Level Factorial Design
 Design for 2 to 15 factors where each factor is varied over 2 levels. Useful for estimating main effects and interactions. Fractional factorials can be used for screening many factors to find the significant few. The color coding represents the design resolution: Green = Res V, Yellow = Res IV, and Red = Res III.

		Number of Factors													
		2	3	4	5	6	7	8	9	10	11	12	13	14	15
Experiments	4	Full	1/2 Fract.												
	8		Full	1/2 Fract.	1/4 Fract.	1/8 Fract.	1/16 Fract.								
	16			Full	1/2 Fract.	1/4 Fract.	1/8 Fract.	1/16 Fract.	1/32 Fract.	1/64 Fract.	1/128 Fract.	1/256 Fract.	1/512 Fract.	1/1024 Fract.	1/2048 Fract.
	32				Full	1/2 Fract.	1/4 Fract.	1/8 Fract.	1/16 Fract.	1/32 Fract.	1/64 Fract.	1/128 Fract.	1/256 Fract.	1/512 Fract.	1/1024 Fract.
	64					Full	1/2 Fract.	1/4 Fract.	1/8 Fract.	1/16 Fract.	1/32 Fract.	1/64 Fract.	1/128 Fract.	1/256 Fract.	1/512 Fract.
	128						Full	1/2 Fract.	1/4 Fract.	1/8 Fract.	1/16 Fract.	1/32 Fract.	1/64 Fract.	1/128 Fract.	1/256 Fract.
	256							Full	1/2 Fract.	1/4 Fract.	1/8 Fract.	1/16 Fract.	1/32 Fract.	1/64 Fract.	1/128 Fract.
	512								Full	1/2 Fract.	1/4 Fract.	1/8 Fract.	1/16 Fract.	1/32 Fract.	1/64 Fract.

Replicates: 1 Blocks: 1 Center points per block: 0

Buttons: Cancel Continue >>

Selecting the Fractional Factorial Design for Turbine Case Study

Click on the **Continue** button. Montgomery uses different (but equivalent) factor and block generators. Click on **Make generators editable** to make it possible to change the generators to match those used by Montgomery. Enter on your screen what's shown below.

Factor Generators

F = ABC

G = ABD

H = BCDE

Blocking Generators

1 = ABE

2 = BCD

Make generators editable Set generators to defaults

The default generators give a minimum aberration (the highest possible resolution) design. Editing the generators will change the aliasing patterns and may degrade the design's resolution -- edit with care!

Entering Custom Generators

Click on the **Continue** button. Examine the aliases.

8 Factors: A, B, C, D, E, F, G, H

Design Matrix Evaluation for Factorial Reduced 3FI Model

Factorial Effects Aliases

Est. Terms] Aliased Terms

[Intercept] = Intercept

[Block 1] = Block 1 - EH - ABE + ABH - ACG - ADF - BCD - BFG - CEF + CFH
- DEG + DGH

[Block 2] = Block 2 - EH + ABE - ABH - ACG - ADF - BCD - BFG + CEF - CFH
+ DEG - DGH

[Block 3] = Block 3 + EH - ABE - ABH + ACG + ADF + BCD + BFG - CEF - CFH
- DEG - DGH

[Block 4] = Block 4 + EH + ABE + ABH + ACG + ADF + BCD + BFG + CEF + CFH
+ DEG + DGH

[A] = A + BCF + BDG

[B] = B + ACF + ADG

[C] = C + ABF + DFG

[D] = D + ABG + CFG

[E] = E

[F] = F + ABC + CDG

[G] = G + ABD + CDF

[H] = H

Alias Structure for Blocks and Main Effects

Notice that the EH interaction is aliased with blocks. The experimenters decided to assign the factors least likely to interact to this combination. This completes the tutorial portion of this case study, which demonstrates how to create your own generators. Press Cancel several times if you'd like to quit now. However, if you'd like to complete the study, click **Continue**. Then, enter the eight factors as shown on the screen shot below.

	Name	Units	Type	Low	High
A:	x-axis shift	mils	Numeric	0	15
B:	y-axis shift	mils	Numeric	0	15
C:	z-axis shift	mils	Numeric	0	15
D:	Vendor		Categorical	vendor 1	vendor 2
E:	a-axis shift	mils	Numeric	0	30
F:	Speed	%	Numeric	90	110
G:	Height	mils	Numeric	0	15
H:	Rate	%	Numeric	90	110

Factor Entry

Click **Continue** to enter the response - the standard deviation (**Std Dev**) of the difference in **mils** between the actual versus specified blade profile.

	Name	Units
	Std Dev	mils

Response Entry

Click **Continue** to bring up the design layout. (Optional step: double-check the alias structure by going to the Evaluation node and click the Results button.) Simulate the response by right clicking on the response column heading, choosing **Simulate response** and selecting the **Turbine.sim** file. Click **OK** to generate the data.

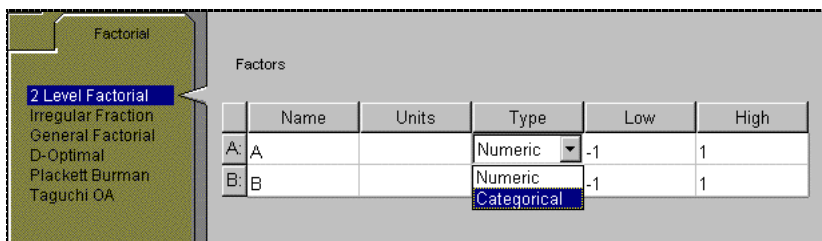
Analyze the data if you like. Here's a few hints:

- Since the response is standard deviation, try a log transformation. On the half-normal plot, don't overlook smaller, but significant effects of G, D and BE.
- There is an outlier, which should be made obvious by the outlier-t diagnostic plot provided by Design-Expert. Find the offending run in the design layout and Toggle Ignore Status. Then re-analyze the data without the outlier.
- Choose the factor levels to minimize standard deviation. Do the end results depend on the transformation and/or whether you ignore the outlier?

To learn more about the final outcome of the turbine case, see the Montgomery text.

Adding Categorical Factors

Version 6 of Design-Expert software offers lots of flexibility for including categorical factors. For example, in the standard two-level designs, or irregular fractions, you can change any factor from numerical to categorical as shown below.



Changing Factor from Numeric to Categorical

This allows you to enter alpha-numeric lows and highs such as “Cheap” versus “Costly.” Also, the program now recognizes that the factor cannot be continuously varied, so it would make no sense to allow a centerpoint.

The general factorial, d-optimal (under Factorial tab) and Taguchi designs in Design-Expert default to the categorical type for factors. However, as demonstrated in part two

of the General Factorial Tutorials, you can change this by right-clicking the factor column header in the design layout column and selecting Make Numeric. See the tutorial for details on how the program handles this change when it does the analysis.


If you choose any of the other design tabs (Response Surface, Mixture, or Crossed), you will see the option to add categorical factors. This will be demonstrated via the following case study.

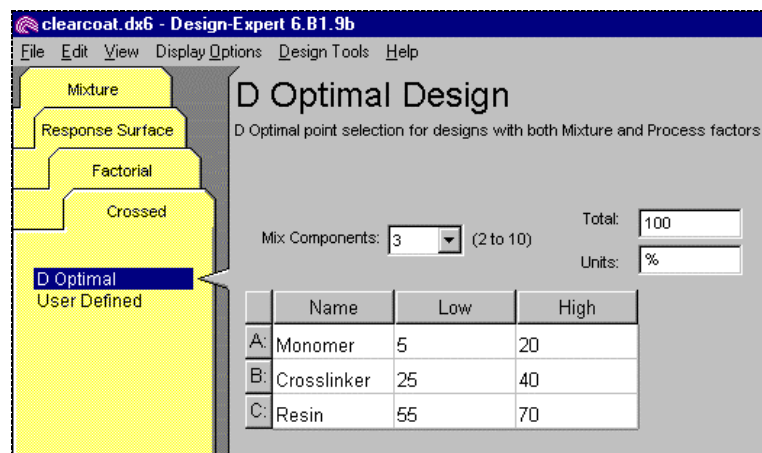
Formulators of an automotive clear coat explored the impact of three components: monomer, crosslinker and resin on two key responses: hardness and solids. Based on knowledge of the chemistry, they restricted the component levels as shown in Table 1.

Component	Supplier(s)	Low	High
A. Monomer	M1 or M2	5 %	20 %
B. Crosslinker	X1, X2, X3	25 %	40 %
C. Resin	Fixed	55 %	70 %

Mixture Components for Case Study on Coating

Note the categorical choices for supplier of the monomer and crosslinker. To keep things simple, suppliers must not be mixed. For example, monomer M1 cannot be blended with M2. The same rule applies to the three possible crosslinker suppliers (X1, X2, X3). The formulators decided not to vary supplier of the resin.

To set this up with Design-Expert, click on the blank-sheet icon  at the left end of the toolbar (or select File, New Design) and choose the **Crossed** tab. Go with the default design choice of **D-Optimal**. Then, change **Mix Components** to **3**. Enter the component names, units and constraints as shown on the screen shot below.



Entry Screen for Mixture Components

Press the **Continue** button. Change the **Categorical Factors** to **2**. There are no numerical process factors so the remainder of the screen is blank.

Numeric Factors:	<input type="text" value="0"/>	(0 to 10)		
Categorical Factors:	<input type="text" value="2"/>	(0 to 10)		
	Name	Units	Low	High

Specifying the Number of Categorical Factors

You must press **Continue** to enter the details for the first categorical factor. Leave the **Factor Levels** at its default value of **2**. Then type in the factor and treatment information shown on the following screen shot.

Factor Name:	<input type="text" value="Vendor"/>
Factor Units:	<input type="text" value="monomer"/>
Factor Levels:	<input type="text" value="2"/> (2 to 20)
	Treatments
	M1
	M2

Entering Details on First Categorical Factor

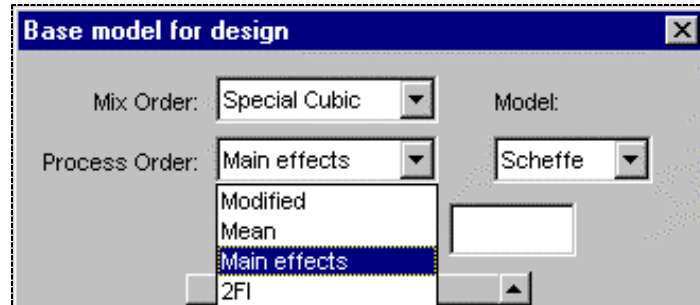
Press **Continue**. Change the **Factor Levels** for this categorical factor to **3**. Then enter the information shown below for the factor name and treatments.

Factor Name:	<input type="text" value="Type"/>
Factor Units:	<input type="text" value="crosslinker"/>
Factor Levels:	<input type="text" value="3"/> (2 to 20)
	Treatments
	CL1
	CL2
	CL3

Entering Details on Second Categorical Factor

Press **Continue** again. Design-Expert now displays options for the d-optimal candidate set. The experimenters believe that all three mixture components will interact, so click

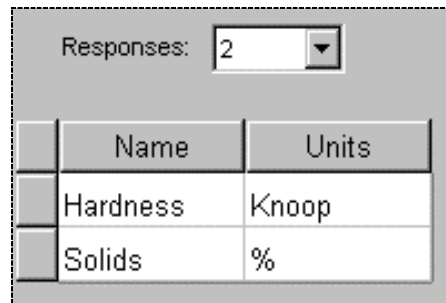
on **Edit model** and change the **Mix Order** to **Special Cubic**. On the other hand, they want to simplify matters by not trying to estimate interactions between the categorical suppliers, so change the **Process Order** to **Main effects** as shown below. Then click **OK**.



Changing the Base Model for D-Optimal Design

Click **Create Candidate Points**. A total of 78 points will be generated by the crossing of the six combinations (2 x 3) of the two sets of suppliers for monomer and crosslinker, crossed with the 13 candidate blends suggested for the special cubic model. From this candidate set, the software will apply d-optimal criteria to select the best 28 points needed for the desired (crossed) model. To add statistical power, the software will replicate the five points with highest leverage, a statistical measure of relative influence. It also will add five additional unique points to fill gaps and test for lack of fit.

Press **Continue** and change the number of **Responses** to **2**. Enter the names and units as shown below.



Response Names and Units

Press **Continue** to create the design.

This concludes the design portion of the coatings case, which demonstrates Design-Expert's ability to add categorical factors to a crossed mixture-process design. In a similar fashion, categorical factors can also be added to mixture or response surface (process) designs. You can see the results of the experiment by opening up a file named "**Clearcoat.dx6**." Go ahead and analyze this data if you like. To get our spin on the outcome, see the November 1999 issue of Paint and Coatings Industry (*Computer-Aided Tools for Optimal Mixture Design*, by Mark J. Anderson and Patrick J. Whitcomb). Reprints of this article can be obtained via the Stat-Ease web site (www.statease.com).

Establishing Multiple Linear Constraints

In some cases, simple lower and upper bounds will not properly define your feasible region. For example, metallurgists find that crossing compositional or processing boundaries lead to dramatic changes in properties. In this case, the experimenter would want to stay within known constraints for a given alloy.

Design-Expert software allows you to impose multivariable constraints in linear form:

$$C_j \leq \beta_{1j}X_1 + \beta_{2j}X_2 + \dots + \beta_{qj}X_q \leq D_j, j = 1, 2, \dots, m$$

where the β_{ij} are scalar constants (some of the β_{ij} may be negative or zero) and m is the number of constraint equations you impose on the design.

This feature can be employed either for response surface or mixture design. It provides considerable flexibility for defining your experimental region. To see for yourself, use Design-Expert to analyze data presented by Ronald Snee in his article “Experimental Designs for Mixture Systems with Multicomponent Constraints” from *Communications in Statistics, Theory and Methods*, 1979, A8, pp. 303-326.

First build a mixture design using the **File, New Design** option off the main menu. Then on the **Mixture** tab select a **D-optimal** design for **3** mix components. Enter the simple upper and lower constraints as shown on the following screen.

	Name	Low	High
A:	A	0.1	0.5
B:	B	0.1	0.7
C:	C	0.1	0.7

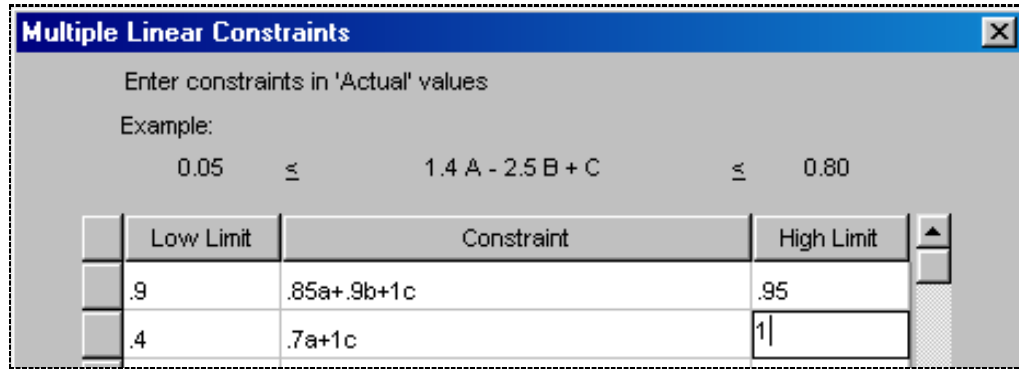
Simple Constraints for Snee Case

Click on **Edit Constraints**. Add the following multiple linear constraints:

$$.90 \leq 0.85A + 0.90B + 1.0C \leq 0.95$$

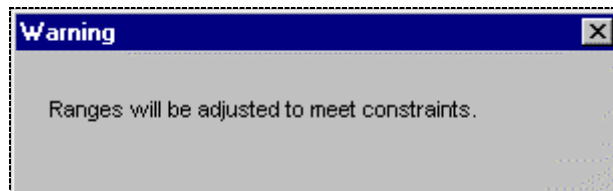
$$0.4 \leq 0.7A + 1.0C \leq 1.0$$

Enter the low and high limits and the equations. (Tip: use the tab key to move from field to field after each entry.) Your screen should now look like the following figure.



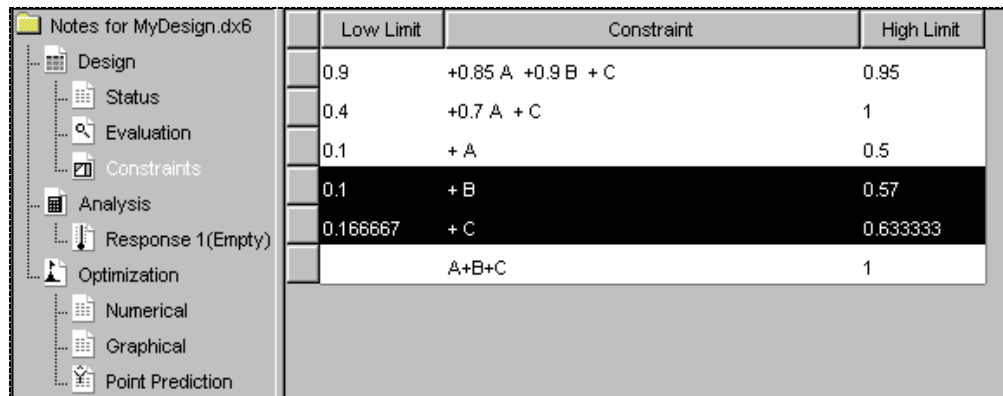
Edit Constraints

Press **OK**. Then press **Continue** repeatedly until the design layout is visible. The software will warn you that it must modify the component ranges based on the linear constraints you just entered.



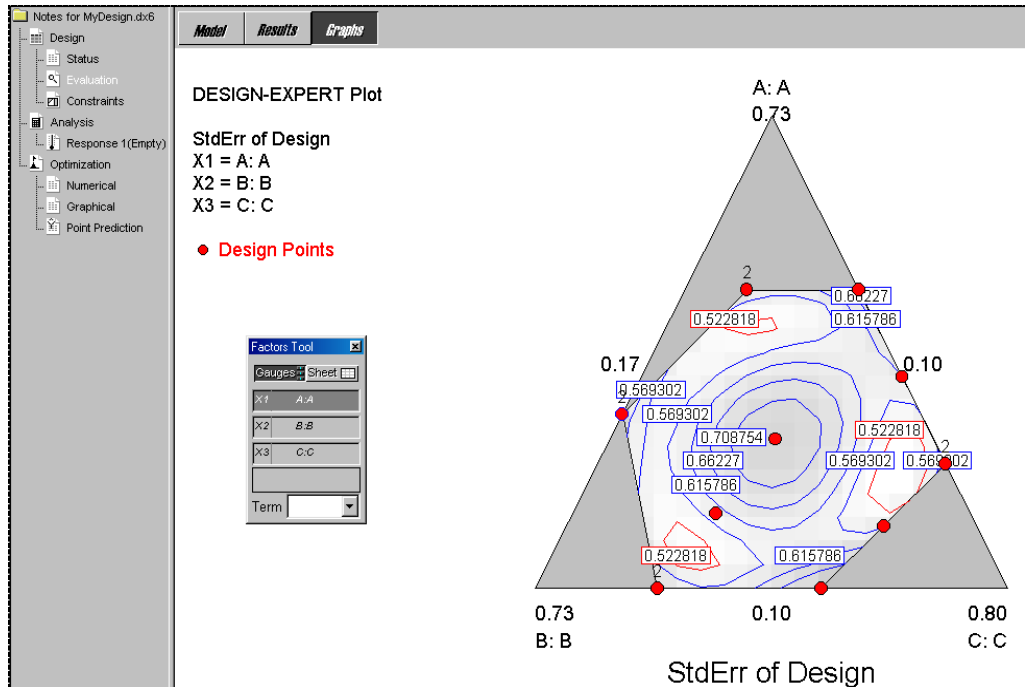
Warning When Software Must Adjust Ranges of Simple Constraints

Press **OK** to let the software do its thing. Press the **Constraints** node to see how the program adjusted the linear constraints to make them feasible.



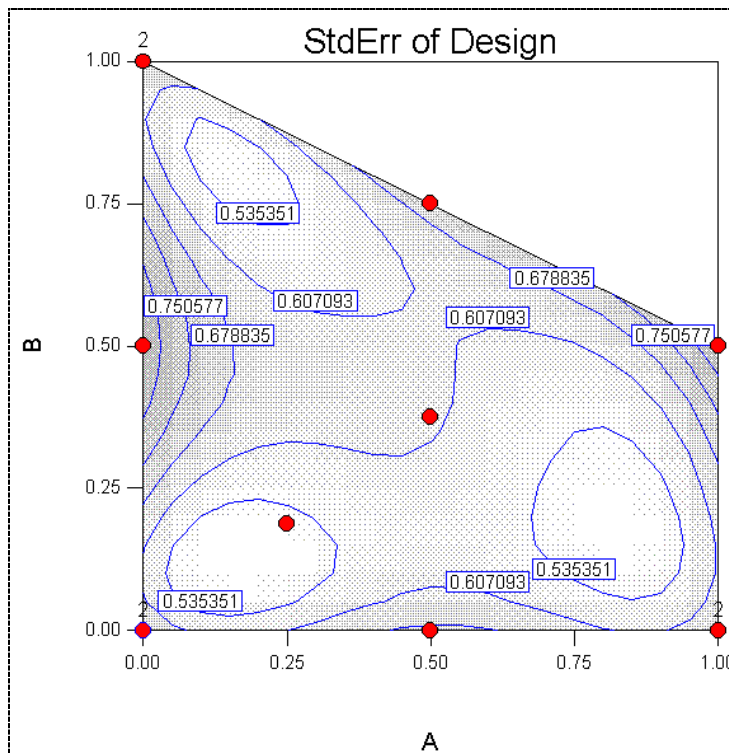
Constraints Node (adjusted constraints highlighted)

Click the **Evaluation** node and the **Graphs** button to plot the standard error with the modified constraints. The results can be seen below.



Mixture Space for Snee Case: Including Multiple Linear Constraints

Multiple linear constraints can also be applied to process situations. The following output comes from a simple example where equipment limitations precluded runs with both factors at their high levels.



Linear Constraint on Response Surface Design

The experimenter went to the **Response Surface** tab, set up a **D-Optimal** design for **2** factors ranging from **0** to **1**, and clicked on **Edit Constraint** to enter the following multiple linear constraint: $1A + 2B \leq 2$. He then pressed **OK** to accept the equation. Then he repeatedly pressed **Continue** to create the design. The experimental region was revealed by going to the **Evaluation** node and clicking on the **Graphs** button.

The multiple linear constraints option allows you great flexibility to restrict your experiments within specific regions.

Creating Your Own Candidate List


Any design can be saved as a candidate list for generating new designs using the d-optimal process. You may add your own points, create your own subsets of large design spaces, etc.

For example, a client of Stat-Ease collected a library of 39 raw material lots with varying physical properties as shown in the table below.

Factor	Low level	High level
A – Molecular weight	14,240	24,200
B – Weight % Alcohol	2.84	3.26
C – Monomer	2.13	3.90

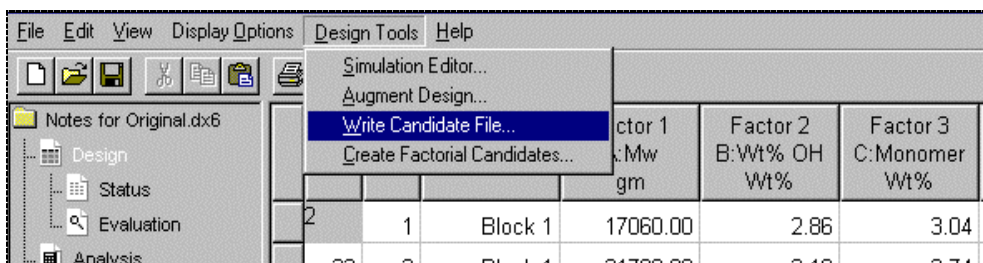
Actual Factor Ranges for Critical Properties of a Product

The client wanted to determine the combination of properties that would make the best finished product. However, it would be wasteful to process every sample in the library, especially since many of them exhibited nearly identical properties. This proved to be an ideal application for the candidate list feature of Design-Expert software. The program determined that only 18 out of the 39 samples, a reduction of more than 50%, would be needed to generate a quadratic model of the response. The following procedure leads you through the design construction for this unique case.

Click on the blank-sheet icon  at the left end of the toolbar (or select File, New Design) and select any design off the **Response Surface** tab. (This design will be replaced with the actual properties for the 39 samples, so it doesn't matter which you pick.) Change the number of **Numeric Factors** to **3**.

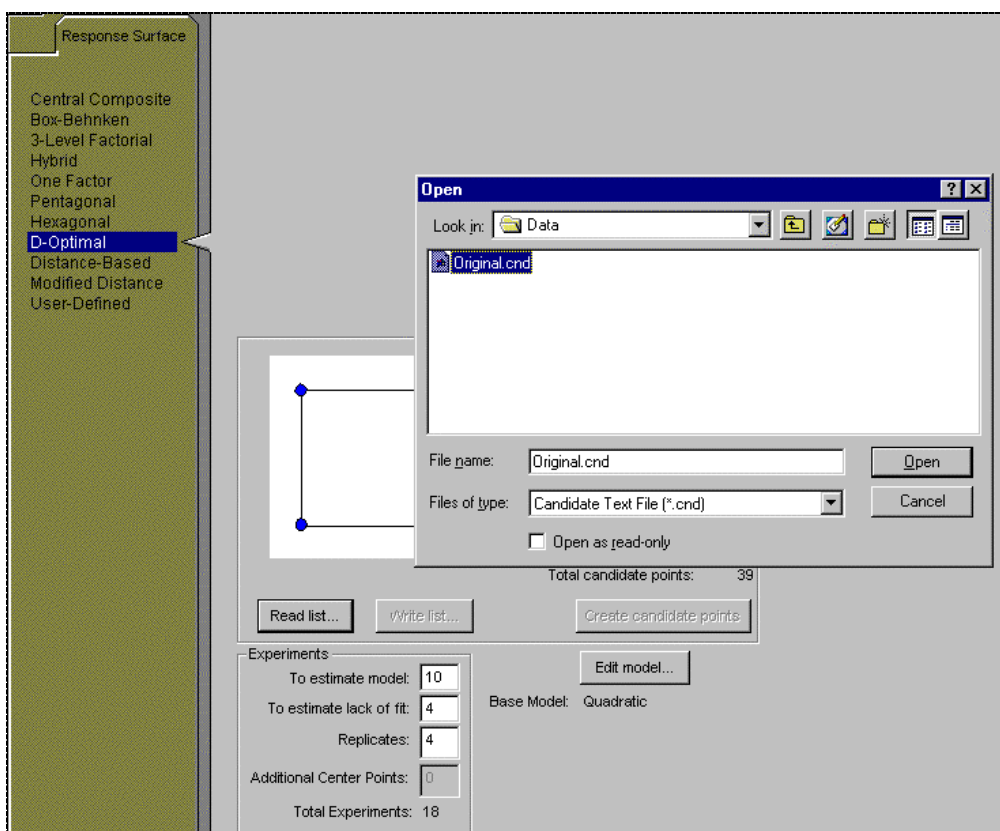
Set the extreme factor levels to the actual minimum and maximum values shown in the table above. The press **Continue** repeatedly until you get to the design layout. Don't worry about entering the response name.

At this point the client edited the design to match the actual samples. To see the raw material library data, open the file named "**Original.dx6**." Then write this to a candidate set file by clicking **Design Tools, Write Candidate File**.



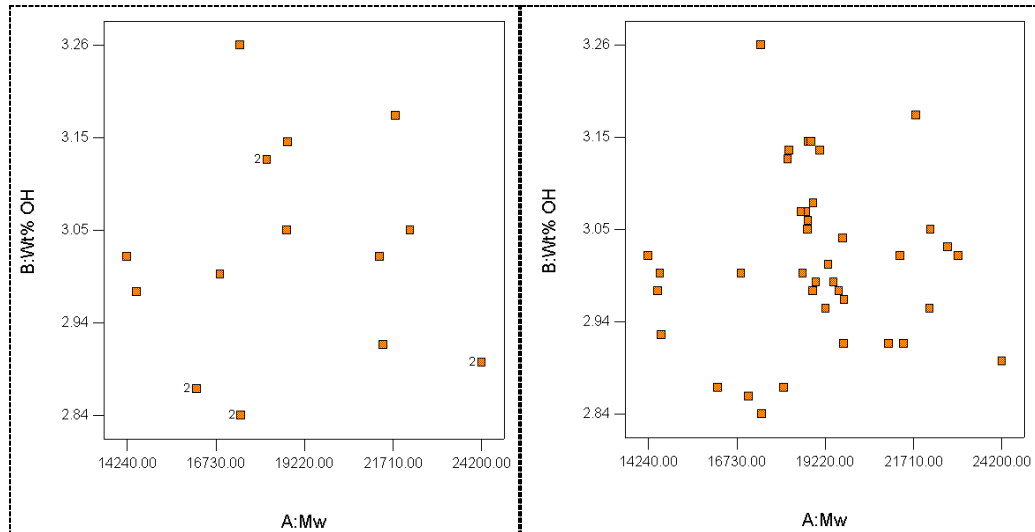
Writing Candidate File

When the **Save as** menu appears, change the **File name** to “**Original**” and click **Save**. It will be saved with the extension “.cnd.” Now you are ready to choose the optimal subset of samples for further study. Select **File, New Design** and say **Yes** to use the previous design information. The Response Surface tab will then be displayed. Select the **D-Optimal** design and click **Continue**. Click on **Read List**. Highlight the **Original.cnd** file you created earlier and press **Open**.



The Read List Option for D-Optimal Candidate Set

Press **Continue** to see the response entry screen. Accept the defaults by again pressing **Continue**. Design-Expert now selects the subset of candidate points needed to fit a quadratic model. By selecting **View, Graph Columns** and changing the **Y-Axis** to factor **B**, you can see a cross-section of properties. Compare this to a similar plot made from the complete library of data contained in the “Original.dx6” file.

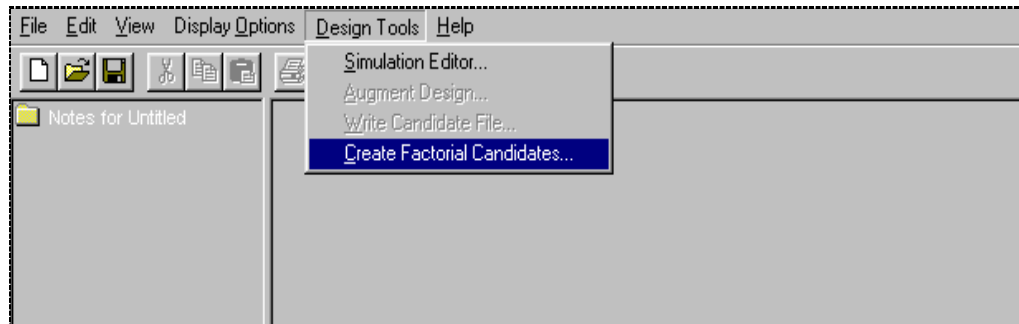


Properties of D-Optimal Subset (left) Versus Entire Library (right)

Notice how samples with very similar properties did not get chosen to be processed into the final product, thus avoiding duplication of effort.

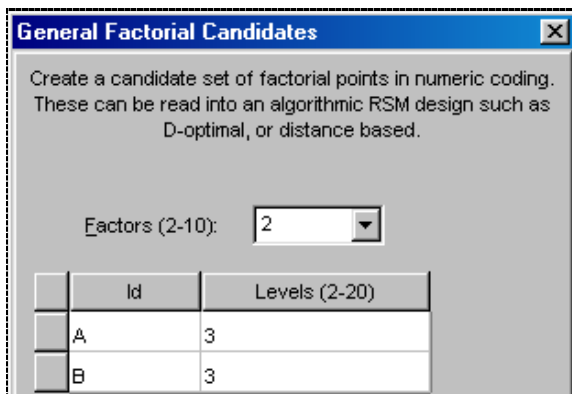
Factorial Candidate Points

The case described above illustrates a relatively unique application of the option provided by Design-Expert to create your own candidate set. A more common reason to do this is to create a grid of points that differs from what the software offers. This can be done by creating a dummy design and editing it as described above. Another way to create a grid of points is via the **Design Tools, Create Factorial Candidates** option under on the main menu. You don't need to create or open a design to access this feature.



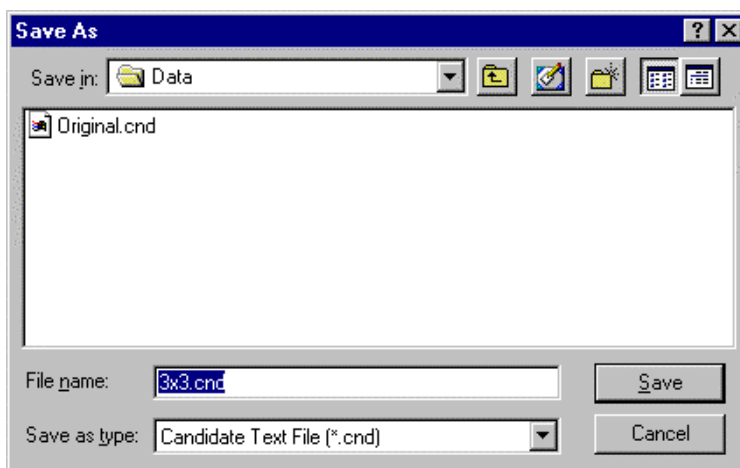
Creating Factorial Candidates

The program then presents options for creating a candidate set with two to ten factors at up to 20 levels each.



Specifying Factors and Levels for Candidate Set

Press **OK**. The program then prompts you to save your factorial candidate set as a file with a “.cnd” extension. Notice that the default name relates to the levels selected.



Saving the Factorial Candidate Set

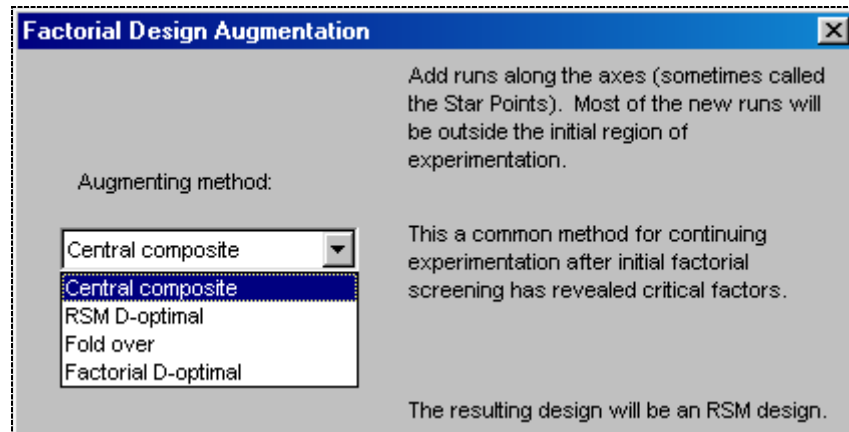
You can read this candidate set when you create a d-optimal, distance-based, or modified distance-based design. The program creates a grid of candidate points based on the levels specified and the lows and highs entered for the factor levels. Stat-Ease presents an interesting application of a factorial candidate set in its Response Surface Methods for Process Optimization workshop. The case involves a machine that offers only fixed settings for continuous factors such as RPM on the motor. After performing a response surface design using fixed levels from the specially created candidate set, the experimenters are able to recommend an optimal level that presumably can be accomplished with some mechanical work.

Design Augmentation

Design-Expert software offers very powerful tools for augmenting an existing collection of experimental data. You can access this feature by clicking the Design node and selecting Design Tools, Augment Design from the menu.

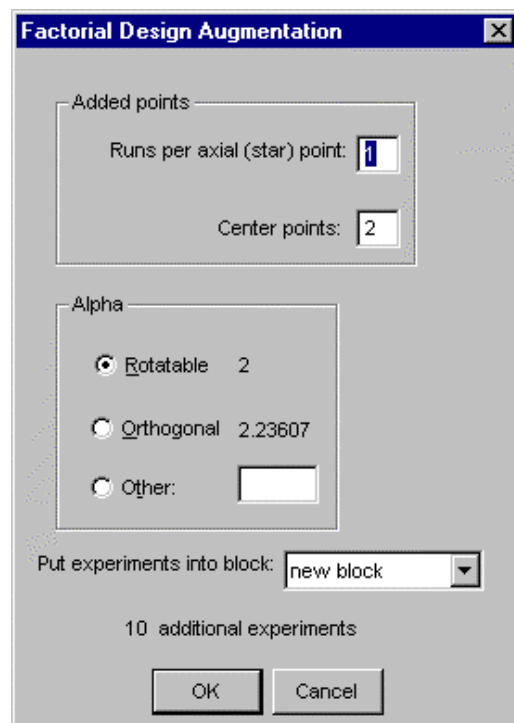
Two-level Factorial to Central Composite Design

Often, augmentation will be needed to expand upon two-level factorial designs. To see what Design-Expert can do at this stage, re-open the design you saved from the Factorial Design Tutorial, or just create a new two-level design with 4 factors. Assume that you see indications of significant curvature. This leads you to believe that you're near the optimum. Therefore augmentation to a central composite design would be very helpful. Select **Design Tools, Augment Design**.



Factorial Design Augmentation Screen

Press **OK** to get a screen for specifying the parameters of the central composite design created via augmentation of the pre-existing factorial design.

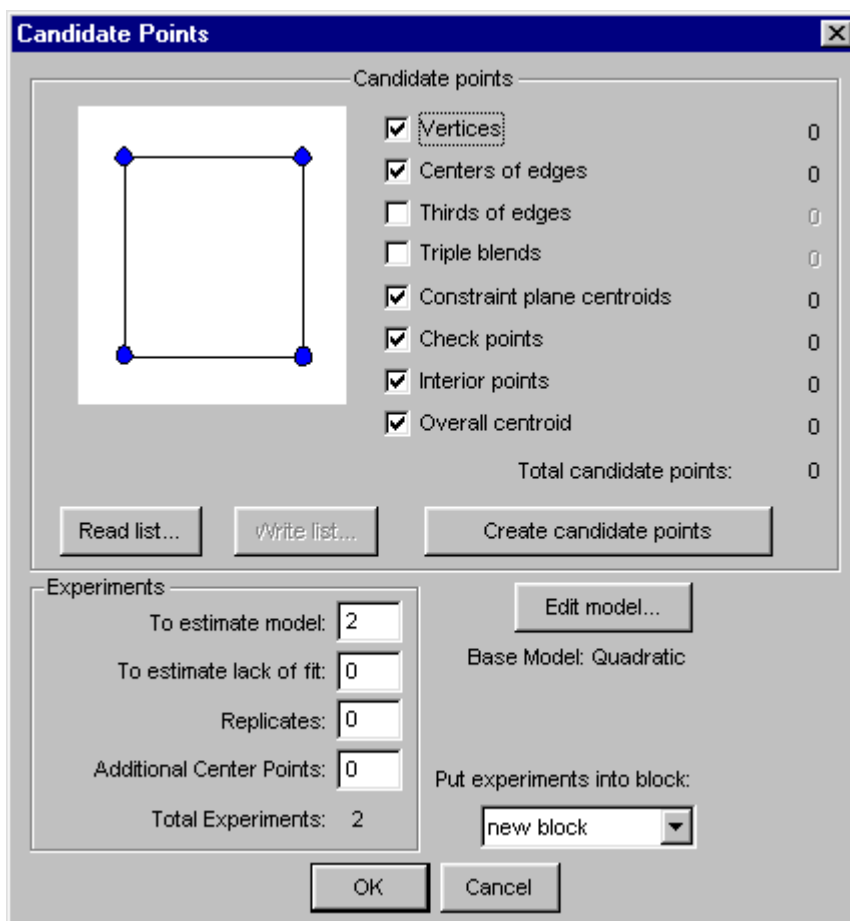


Specifying the Parameters for Augmentation

Refer to the first part of the Response Surface Tutorials for background on creating a central composite design (CCD). Press **OK** to create the CCD. Design-Expert will provide an additional block of 10 runs: two of which are centerpoints as specified. The other eight points are the axial points that fall two coded units from the centerpoint (outside the original plus or minus levels of the four factors).

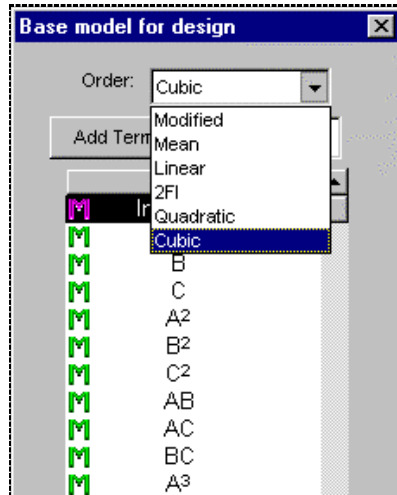
D-Optimal

With the aid of d-optimal selection, the program can give you additional experiments needed to fit a higher order model, above and beyond what would be mathematically possible from your original set of design points. Check this out for yourself by opening the **Rsm-a.dx6** file. Then select **Design Tools, Augment Design**.



Augmenting a Central Composite Design

Then you can click **Edit Model** and select a **Cubic** model.



Selecting a Cubic Model for Augmentation

Click **OK** a few times and Design-Expert will give you an additional 14 runs in a new block of experiments. Check it out. By doing these additional runs you could then fit the higher order model. The same approach will work for mixtures as well. You could also use this feature to augment a fractional factorial design and de-alias specific terms. In fact, you can augment any set of data, even one collected in a happenstance manner, and create a design that will fit up to a full cubic model. This is a marvelous feature that allows you to do design repair. Check it out!

Design Evaluation

With Design-Expert's design layout features, you can modify virtually any aspect of your design. Before undertaking your design of experiments, you may change factor levels; add, delete or duplicate experimental runs; or modify block assignments. See the last part of the One Factor Tutorials for a demonstration of design editing.

Whenever you modify a design, we advise that you make use of Design-Expert's unique evaluation capability. Focus on these properties:

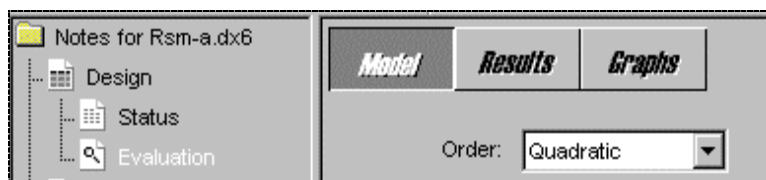
- Aliased effects due to lack of unique design points
- Absence of lack of fit test due to absence of replicates
- Absence of curvature test due to lack of center points.
- High leverage points (near one). (The leverage can be reduced by replication of the offending points.)

For a handy checklist with more details on the properties listed above, see the *Handbook for Experimenters* published by Stat-Ease (given free of charge to all registered software users). You can further modify your design if the evaluation looks poor.

To explore the design evaluation features option, take a look at the response surface tutorial data. It's a central composite design for three process variables. To load the

file, select **File, Open Design** from the menu bar. Find the correct drive and highlight **Rsm-a.dx6**. Then press **OK**. Then, if you like, click at the top of each response column to highlight all the data, and then with your mouse over the highlighted area, right-click it and select **Edit, Clear**. Whether data is present or not, it makes no difference so far as the evaluation is concerned. All that matters is the design itself.

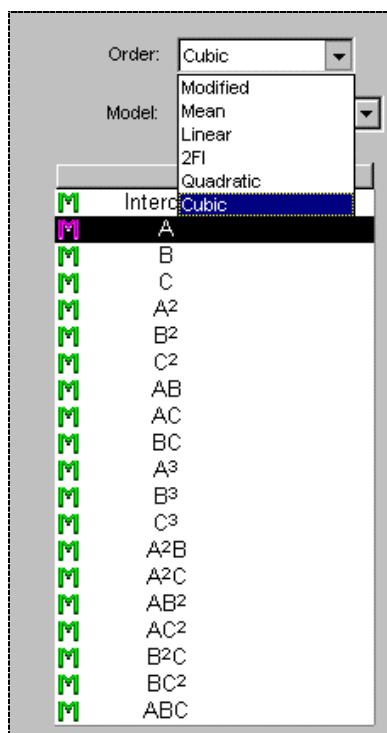
Begin the evaluation process by clicking on the **Evaluation** node. You have a choice of models, full or reduced, for design evaluation. The model you originally selected during design setup is the default. In this case, it's a quadratic.



Model Selection Dialog Box

When evaluating a design, Design-Expert first determines whether or not the selected design adequately estimates coefficients for the desired model. If the design provides too few points or picks the wrong points, the estimated model terms will be aliased, which means that they cannot be separated during the analysis.

To see what happens with an aliased design, select **Cubic** model order.



Evaluating Cubic Model

Notice that all the third order terms change to “M” (for model). The “M” indicates currently selected terms. Double-click to toggle any term in and out of the model. Another way to do this is to right click and choose Ignore (status “X”) or Error. Check it out! Use this feature if you want to modify the model to be evaluated.

Now click on the **Results** icon. The design provides too few points for a cubic model, so the program displays a table of aliases. The equations show the relationships between the aliased and unaliased terms. For example, the coefficient for A comes from the combination of A and the higher order interactions AB^2 and AC^2 .

Model	Results	Graphs
3 Factors: A, B, C		
Design Matrix Evaluation for Response Surface Cubic Model		
Alias Matrix		
[Est. Terms]	Aliased Terms	
[Intercept]	= Intercept	
[Block 1]	= Block 1	
[Block 2]	= Block 2	
[A]	= A + 1.55 * AB ² + 1.55 * AC ²	
[B]	= B + 1.55 * A ² B + 1.55 * BC ²	
[C]	= C + 1.55 * A ² C + 1.55 * B ² C	

Alias Matrix for Cubic Model from Central Composite Design

It’s clear from the alias matrix that you won’t get a cubic model from a central composite design. However, this exercise provides a flavor of the software’s capability to calculate aliases. This is especially handy for evaluating fractional factorials, including Plackett-Burman and Taguchi designs.

Re-evaluate the response surface design by clicking on the **Model** icon, selecting a **Quadratic** order and clicking on **Results** icon. Your screen should now look like that below, displaying the message that “No aliases found” (that’s good!).

Design Matrix Evaluation for Response Surface Quadratic Model	
No aliases found	
Degrees of Freedom for Evaluation	
Blocks	1
Model	9
Residuals	9
Lack Of Fit	5
Pure Error	4
Corr Total	19

Degrees of Freedom for Evaluation of Quadratic Model

A good design for an in-depth study, or outright optimization, provides at least three lack-of-fit degrees of freedom and four pure error degrees of freedom. Larger degrees of freedom increase the discrimination between adequate and inadequate models. (Exception to the rule: if you are doing a screening study, an unreplicated fractional two-level is a good design choice. Obviously this provides no pure error estimates.)

Scroll down to evaluate how well the central composite design estimates each term in the quadratic model.

Term	StdErr**	VIF	Ri-Squared	Power at 5 % alpha level for effect of		
				1/2 Std. Dev.	1 Std. Dev.	2 Std. Dev.
Block 1	0.23					
A	0.27	1.00	0.0000	13.2 %	37.9 %	90.7 %
B	0.27	1.00	0.0000	13.2 %	37.9 %	90.7 %
C	0.27	1.00	0.0000	13.2 %	37.9 %	90.7 %
A ²	0.26	1.02	0.0187	39.6 %	92.0 %	99.9 %
B ²	0.26	1.02	0.0187	39.6 %	92.0 %	99.9 %
C ²	0.26	1.02	0.0187	39.6 %	92.0 %	99.9 %
AB	0.35	1.00	0.0000	9.7 %	24.5 %	71.2 %
AC	0.35	1.00	0.0000	9.7 %	24.5 %	71.2 %
BC	0.35	1.00	0.0000	9.7 %	24.5 %	71.2 %

**Basis Std. Dev. = 1.0

Evaluation of Model Terms

The software reports the standard error of each term. Notice that in this case, they remain the same within each class of terms. The next column in this table reports the variance inflation factor (“VIF”), which measures how much the variance of that model coefficient increases due to the lack of orthogonality in the design. The standard error of a model coefficient increases in proportion to the square root of the VIF. If a coefficient is orthogonal to the remaining model terms, its VIF is one. One or more large VIFs indicate multicollinearity. VIFs exceeding ten indicate problems due to multicollinearity. (For example: if a coefficient has a VIF of sixteen, its standard error is four times as large as it would be in an orthogonal design.)

The next column, labeled “Ri-Squared,” shows how each term correlates with all the others. These values relate to VIF as shown in the following formula:

$$\text{VIF} = \frac{1.0}{(1 - R_i^2)}$$

The last three columns report the power to estimate each term, assuming effects of up to two standard deviations. For example, in this case, the probability of detecting a shift of one-half standard deviation in the effect of A is very low, only 13.2 percent. On the other hand, a much greater shift of two standard deviations in A will almost certainly be detected, as indicated by the probability value of 90.7 percent. The actual calculation for power depends on the nature of the design. For details, see the last part of the Statistical Details: Design Selection, or go to program Help and search for “power calculation.” The power increases when you replicate runs. For example, if you

repeated the entire design, you would see a marked increase in the reported probabilities, particularly at the one-half standard deviation level. (A quick way to check this is to click back on the Design node. Then click on the first run and shift-click the last run to highlight the entire design. Right-click on any of the buttons on the left and select Duplicate to replicate the entire design. Evaluate this for power. When done, go back and delete the added rows, or just re-open the “Rsm-a” file.)

Scroll down to look at the leverages of the design points.

Measures Derived From the $(X'X)^{-1}$ Matrix		
Std	Leverage	Point Type
1	0.7058	Fact
2	0.7058	Fact
3	0.7058	Fact
4	0.7058	Fact
5	0.7058	Fact
6	0.7058	Fact
7	0.7058	Fact
8	0.7058	Fact
9	0.1944	Center
10	0.1944	Center
11	0.1944	Center
12	0.1944	Center
13	0.6793	Axial
14	0.6793	Axial
15	0.6793	Axial
16	0.6793	Axial
17	0.6793	Axial
18	0.6793	Axial
19	0.2500	Center
20	0.2500	Center
Average =	0.5500	

Report on Leverages

High leverage points, those with values twice that of the average, will unduly influence the model fit. The average leverage equals the number of model terms, including constant and block coefficients, divided by the number of experiments. In this example the average leverage is 0.55 (11 terms divided by 20 runs).

At the extreme, a leverage of one indicates that the model will fit that particular point no matter what its value. Obviously this should be avoided. You can reduce the leverage of a design point by replicating it, or by adding design points.

Scroll down to look at various measures of the design matrix.

Maximum Prediction Variance (at a design point) = 0.706

Average Prediction Variance = 0.550

Condition Number of Coefficient Matrix = 1.345

G Efficiency (calculated from the design points) = 77.9 %

Scaled D-optimality Criterion = 1.560

Determinant of $(X'X)^{-1} = 6.500E-13$

Trace of $(X'X)^{-1} = 1.025$

Design Evaluation Output: Matrix Measures

The average prediction variance as a percentage of the maximum prediction variance is expressed as “G Efficiency”. (Note that the prediction variances are based on the actual design points.) If possible, try to get a G efficiency of at least 50%.

The “condition number of the coefficient matrix” indicates the degree of multicollinearity present in the design matrix, where $\kappa = \lambda_{\max}/\lambda_{\min}$, the maximum and minimum eigenvalues of the $X'X$ matrix.

- $\kappa = 1$ no multicollinearity, i.e. orthogonal
- $\kappa < 100$ multicollinearity not a serious problem
- $100 < \kappa < 1000$ moderate to severe multicollinearity
- $\kappa > 1000$ severe multicollinearity

The scaled d-optimal criterion is calculated by:

$$N((\text{determinant of } (X'X)^{-1})^{1/p})$$

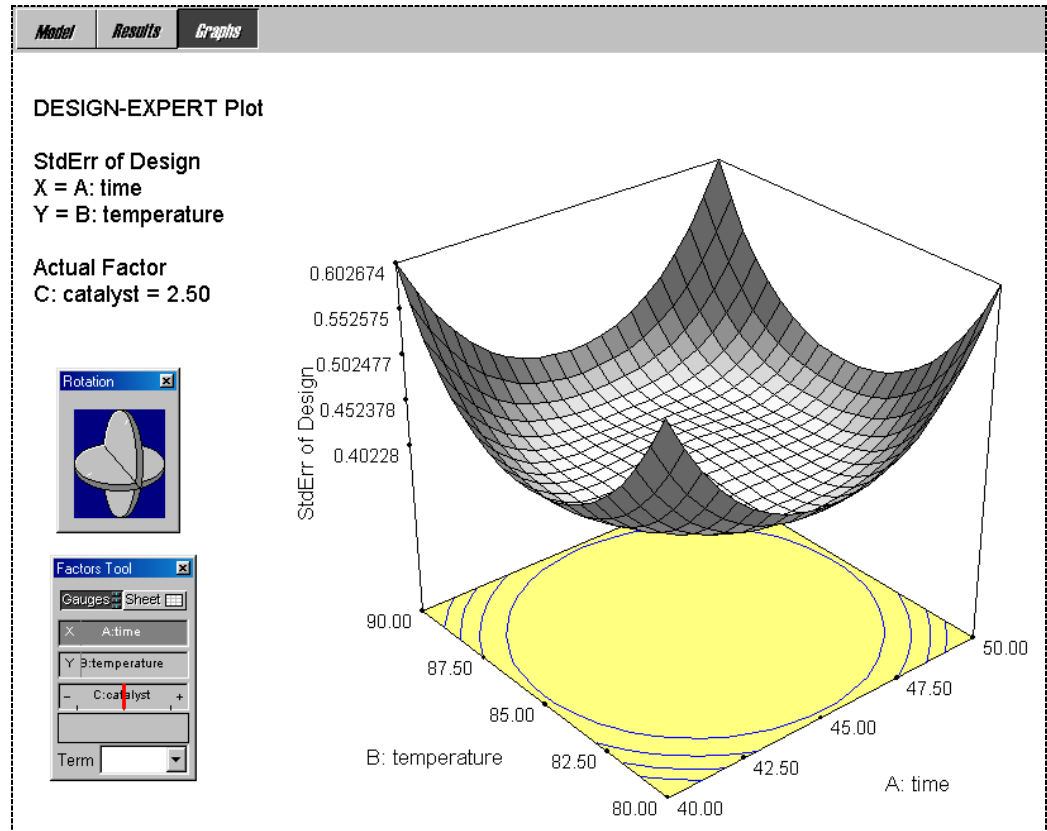
where N is the number of experiments and p is the number of model terms (including the intercept and any block coefficients). The scaling allows comparison of designs with different number of runs. The smaller the scaled d-optimal criterion the smaller the volume of joint confidence interval of the model coefficients. That’s good!

The determinant and trace are relative measures used to compare designs having the same number of experiments. They are primarily used for algorithmic point selection. Check the *Handbook for Experimenters* for specific guidelines on these measures and all others reported in the design evaluation.

Scroll down to see all details on correlation of the coefficients and the factors themselves. In the ideal orthogonal design, none of the coefficients will be correlated (all non-diagonal values in the matrix equal zero). In this case you see just a few terms that are partially correlated, thus creating minor inflation in the variance associated with specific coefficient estimates. Similar problems can be observed on the correlation

matrix of factors (“Pearson’s r”), the last part of the design evaluation output. This matrix was created to reveal mistakes in coding. For example, if you changed a low level to a high level (or vice-versa) in the factorial portion of the design, it would be difficult to see in the correlation matrix of coefficients, but easy to see in the correlation matrix of factors. (If you’d like to see this for yourself, go back to the design layout and for standard order number one change the level of A from 40 to 50. Then go back to the Evaluation, Results and in both matrices (for coefficients and factors) observe the correlations shown under column A versus those reported for B and C. Remember to correct the changed factor level before you move on to the next stage of evaluation.)

After reviewing all the statistical outputs for design evaluation, you should look at plots of the standard error over the design space. Click on the **Graphs** icon, and then select **View, 3D Surface** to see the following plot.



Standard Error Plot: 3D View

The shape of the standard error plot depends only on the design points and the polynomial being fit. (The actual magnitude of the plot will be a function of the process standard deviation, which depends upon the response data. A standard deviation of 1 is used to generate the standard error plot for design evaluation.) Rotatable designs like this one exhibit circular contours and a symmetrical 3D shape. This is ideal. Another desirable feature is the relatively low and flat error around the centerpoint. It doesn’t get much better than this!