

# Section 11 – Statistical Details: Design Selection

This section of the Design-Expert<sup>®</sup> software manual provides details on design selection. You should complete the tutorials before wading into these details.

We will presume that you possess a working knowledge of the “standard” approach to design of experiments (DOE). If you need background on the subject, read *Design and Analysis of Experiments* by Douglas Montgomery. For advanced DOE techniques, we recommend *Response Surface Methodology* by Myers and Montgomery. You can buy either of these textbooks from Stat-Ease or direct from the publisher - John Wiley and Sons, Inc., New York.

If you need a quick education on the important statistics, consider attending one or more of Stat-Ease’s computer-intensive workshops. Call us to get details on course content and schedule. You will find contact information at the end of the Introduction.

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## Factorial Design Selection

Design-Expert offers six design types on the Factorial tab:

- Two-level factorial (2-15 factors)
- Irregular fractions (4-9 factors)
- General factorial (1-12 factors)
- D-optimal design (an option to the full general factorial)(2-14 factors)
- Plackett-Burman (11, 19, 23, 27 or 31 factors)
- Taguchi OA (Orthogonal Arrays for up to 63 factors)

We will discuss the design selection sub-menus separately for each general type of design.

### Standard Two-Level Factorials

The 2-Level Factorial selection offers standard two-level full factorial and fractional factorial designs. You can investigate from 2 to 15 factors in 4, 8, 16, 32, 64, 128 or 256 runs. This collection of designs provides an effective means for screening through many factors to find the critical few.

Full two-level factorial designs may be run for up to eight factors. These designs permit estimation of all main effects and all interaction effects (except those confounded with blocking). Design-Expert offers an option to completely replicate these designs up to 100 times. (Fractional factorials can be replicated also, but it would not make sense to do so.)

Design-Expert offers 50 fractional factorial designs, ranging from a 1/2 replicate for 3 to 9 factors to a 1/2048 replicate of 15 factors in 16 experiments. The program gives detailed information on the alias structure, which you can inspect to be sure that you get clean estimates of desired effects.

You will find the resolution of each fractional factorial by looking at the colors on the 2-Level Factorial design display. They're set up like a stoplight.

- Red: Resolution III design. Stop and think. One or more main effects will be aliased with at least one two-factor interaction. Resolution III designs can be misleading when two factor interactions significantly affect the response.
- Yellow: Resolution IV design. Proceed with caution. One or more two-factor interactions will be aliased with at least one other two-factor interaction. The main effects will be clear of two-factor interactions, so Resolution IV designs can be a good choice for a screening design.
- Green: Resolution V (or higher) designs. Go ahead. Assuming that no three-factor (and higher) interactions occur, all the main effects and two-factor interactions can be estimated. Resolution V designs work very well for screening. They're more efficient than full factorials.

The software picks the highest resolution design possible. When several designs of equivalent resolution are available, Design-Expert defaults to a choice with minimum aberration in the lengths of the words listed in the defining contrast.

Refer to part one of the Two-Level Factorial Tutorials for detailed illustrations of several choices from this design option.

## **Blocking**

Design-Expert provides various options for blocking standard two-level factorials, depending on how many runs you choose to perform, and the number of factors. For example, in the full factorial experiments with 16 runs, you may choose to carry out the experiment in 1, 2, 4 or 8 blocks. Keep the default selection of 1 for blocks if you want no blocking. A selection of 2 for blocks might be particularly helpful if, for some reason, you must do half the runs on one day and the other half on the next day. In this case, any day-to-day variation will be removed by blocking.

When you choose to block your design, one or more effects will no longer be estimable. Design-Expert will tell you which effects, if any, will be "lost to blocks." The software picks the highest resolution design possible. When several designs of equivalent resolution are available, Design-Expert defaults to a choice with minimum aberration in the lengths of the words listed in the blocking generator(s).

## Center Points

A useful extension of two-level factorial and fractional factorial designs incorporates center points into the factorial structure. If you have at least one numeric factor, you can choose to add center points to your design. Data from the center points provides:

- Estimates of pure error
- Estimates of curvature.

If there is curvature of the response surface in the region of the design, the center point will be either higher or lower than predicted by the factorial design points. Curvature of the surface may indicate that the design is in the region of an optimum.

Design-Expert automatically accounts for the presence of center points, constructing the estimate of pure error, as well as the test for curvature. For factorial designs, Design-Expert uses the average of the center point values, rather than the polynomial model, to predict the center point response. This excludes curvature from the Lack-of-Fit test and the residuals, thus providing more information about the fit of the model. (The software does a separate test for the curvature.) One benefit of this procedure is that the assumptions concerning normality and constant variance can be checked even in the presence of curvature. This allows you to identify problems in the data analysis that might be otherwise obscured by curvature inflating the residuals.

The effects of curvature and blocking do not appear in the predictive model. However, for purposes of computing residuals, these effects are included in the predicted values.

If you choose blocking in addition to center points, the number of center points entered during design selection will be multiplied by the number of blocks. For example, if you select a design with two blocks and three center points, six center points will be created, three in each block.

If you include categorical factors in your design, true center points cannot be constructed. For designs with both categorical and numeric factors, Design-Expert generates pseudo center points at the centers of the numeric factors for every combination of the categorical factors. Asking for center points in combination with categorical factors can produce large (but balanced) designs. For obvious reasons, Design-Expert will not allow center points if the design contains only categorical factors.

## Irregular fractions

Design-Expert offers a series of Resolution V designs with an irregular fraction of powers of two. The choices for factors and runs are: 4 in 12, 5 in 24, 6 in 48, 7 in 48, 8 in 48 and 9 in 96. The 4, 5 and 6-factor options are three-quarter replicates of full factorials. A smaller irregular fraction is provided for the 7 through 9 factor designs. The construction of these designs comes from Addelman, "Irregular Fractions of the 2<sup>n</sup> Factorial Experiments," *Technometrics*, 3, 479-496, and also John, "Three-Quarter Replicates of 24 and 25 Designs," *Biometrics*, 17, 319-321. With the exception of the five-factor option, the irregular fractions allow you to get by with fewer runs than the

Resolution V designs on the standard two-level factorial design builder. For example, you can study four factors in only 12 runs and detect all the two-factor interactions. A standard (regular) design of similar quality would require 16 runs.

## General Factorial Designs

The General Factorial option allows you to design for 1 to 12 categorical factors with varying numbers of levels of up to 20 each (maximum runs: 32766). For example, you can set up an experiment with three suppliers of four alternative materials to be processed in two different machines (3 by 4 by 2). If the factor(s) can be varied in a continuous manner, rather than categorical, consider doing a response surface design instead of a general factorial. You may replicate the entire design any number of times, limited only by the memory in your computer. Experiments can be run completely randomized or blocked. In the randomized block design each replicate is placed in a different block.

Refer to the General Factorial Tutorials for a detailed illustration of this option and its offshoots: split plot and nested designs.

## D-Optimal Factorial Designs

The D-Optimal Factorial design is designed for use with categorical factors as an alternative to the General Factorial design option. It offers the run-saving equivalent of fractional factorials. Based on the model that you specify, the D-Optimal algorithm chooses a desirable subset of runs generated from the full factorial array.

To use this design, first choose how many categorical factors you have. On the next screens, specify the names and number of levels for each factor. After completing those, you will reach a screen where you must specify the model that you want to be able to approximate. The default model is a 2-factor interaction model (2FI). Depending on the number of levels that each factor has, even a 2FI model may contain too many runs. In that case you will need to use your subject matter knowledge to decide if any of the two-factor interactions are unlikely to occur. If this is true, then these interactions can be individually eliminated from the model and the number of runs can be further reduced.

Create the design and carefully look it over to make sure that all the runs generated are possible to perform. Some runs will be replicated to be able to estimate pure error and lack of fit.

If you have any numeric factors, use the D-Optimal design on the Response Surface Tab. There you can specify both numeric and categorical factors.

## Plackett-Burman Designs

Plackett-Burman designs use a set of orthogonal contrasts with -1 and +1 coefficients. Some experimenters use Plackett-Burman designs to check if large effects exist in a process. But these designs are better suited for ruggedness testing, where you hope to

see little or no effect on the response due to any of the factors. In this latter case, a process or product that withstands the testing without any significant change would be declared to be robust. Design-Expert permits Plackett-Burman designs with 12, 20, 24, 28 or 32 experiments. The number of factors cannot exceed the number of runs minus one. For example, a design with 12 runs will enable you to estimate all main effects for up to 11 factors. This is called a “saturated design.” If you have less than the maximum allowable factors, the remainder become “dummy factors,” which will be used to estimate error.

Design-Expert provides alias patterns for all the Plackett-Burman designs. In the 12, 20, and 24-run designs each main effect gets partially confounded with several two-factor interactions. If any interactions are active in your system, their effect will be attributed to several main effects, thus creating potential confusion as to which factors are really important. In unsaturated designs, you may even see dummy factors generating apparently significant effects. This is not a good sign! Consider augmenting your design via a foldover, as shown in the last part of the Factorial Tutorials section.

## Taguchi Designs

Design-Expert provides a variety of Taguchi designs with differing numbers of factors and levels. See the Taguchi Design Tutorial for an example. If you aren't committed to the Taguchi approach, consider a standard two-level factorial design, which offers better alias structures.

To use the Taguchi designs, first pick the design you need from the pull-down list. Then click on Continue and check out the alias structure for this design. It is likely to be very complex. On the next screen, enter your response names. Then click on Continue and the design layout will be created.

Design-Expert software sets up saturated Taguchi designs. Use Taguchi's linear graphs (available in Taguchi textbooks) to determine which columns you want to use and which to eliminate. You can enter the names of the factors and the levels by right-clicking on each factor column header and selecting Edit Info.

## Order of Experiments

Design-Expert constructs designs in the standard order used in the referenced textbooks on design of experiments. To perform the experiments, a random order, called the “Run” is assigned by the program. Blocking affects this run order. The order will be randomized within each “Block.” You can change the assigned run numbers, as well as modify other aspects of the design, in the design layout.

## Factor Coding

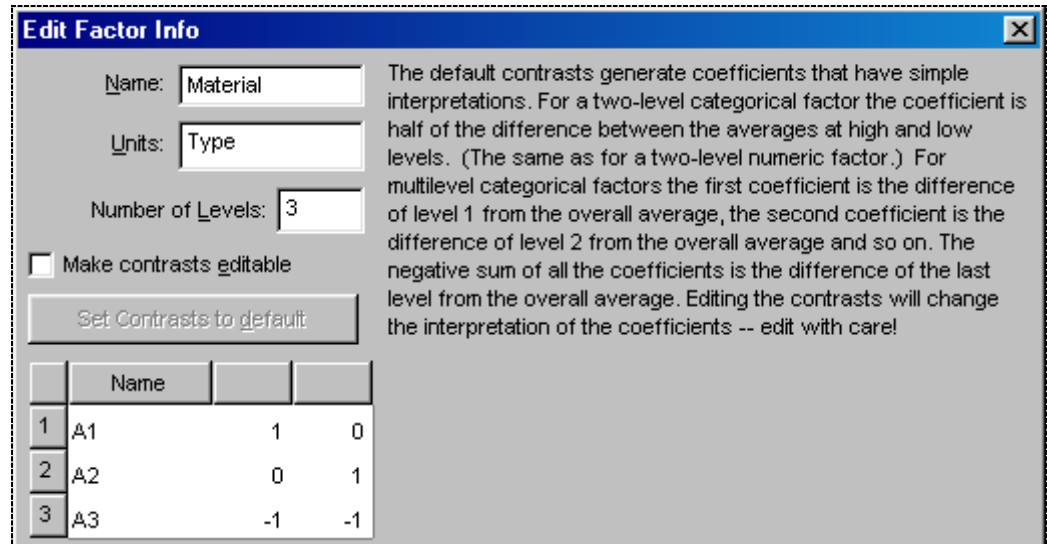
Design descriptions and analyses are done best with coded factors. Coding sets up factor levels that can be orthogonal or nearly so. Also, coding reduces the range of each factor to a common scale, and places the origin of the coordinate system in the center of the design space. It is easier to work with changes from low to high level for the factors

rather than their actual values, especially when computing squared terms and interactions. For example, one factor may vary from 100 to 200 while another varies from 0.1 to 0.5. This large discrepancy in the range of values makes interpretation of factor coefficients difficult. It is also important to remember that a regression coefficient tell us how the response changes relative to the intercept. The origin of the coordinate system (and therefore the intercept) is in the center of the design space in coded units, but can be far from our data in the actual units.

For non-mixtures, Design-Expert applies the standard coding of  $-1$  as the low level of a factor,  $+1$  as the high level, and  $0$  as the middle level.

The factor coding is defined by what you enter as the “Low” and “High” value during design building. These values can be changed by right-clicking on a factor column header and selecting Edit Info. *(Note: Do not attempt to change the low and/or high values by editing the numbers in the design layout. This will change the values on your screen, but not the low and high values used to define the coded values. It will result in non-orthogonal designs and ill-defined regression coefficients. Always use the Edit Info feature to change low and high values.)*

Design-Expert provides coding for categorical factors at as many as 20 levels. The general structure is illustrated by the following screen shot from the battery case described in Section 4.



*Coding for a Three-Level Categorical Factor*

Note the warning about editing the contrasts. This can be done only after clicking the “Make contrasts editable” option. The dialog box also presents a synopsis of how to interpret the model coefficients for the coded model. Other examples of coding for general factorials are shown below for four levels and five levels.

	Name			
1	A1	1	0	0
2	A2	0	1	0
3	A3	0	0	1
4	A4	-1	-1	-1

	Name				
1	A1	1	0	0	0
2	A2	0	1	0	0
3	A3	0	0	1	0
4	A4	0	0	0	1
5	A5	-1	-1	-1	-1

*Examples of Coding for Four-Level and Five-Level Categorical Factors*

To determine coding for greater numbers of levels, you can extrapolate from these examples, or actually set up such designs on Design-Expert and view the coding via a right-click on the factor column heading (choose Edit Info).

## Response Surface Design Selection

Response surface methodology (RSM) quantifies relationships among one or more measured responses and a number of input factors. It provides sophisticated maps from which you can identify peak performance. Design-Expert offers many RSM designs. The options depend on the number of design factors, which can range from one to ten. (You can also add up to ten additional categorical factors to any RSM design). Designs offered by the software under the Response Surface tab can be seen below. We highly recommend the central composite design (CCD) or Box-Behnken design. However, if you require multilinear constraints for the factors, we suggest you use the D-optimal design.

<b>Designs</b>	<b>Factors</b>
One-Factor	1
Pentagonal, Hexagonal	2
Three-Level Factorial	2 - 4
Central composite (Small composite)	2 - 10 (3 - 10)
Hybrid	3, 4, 6, 7
Box-Behnken	3, 4, 5, 6, 7, 9, 10
D-optimal, Distance-Based, Modified Distance	2 - 10
User-Defined	2 - 10

*Response Surface Designs*

## Central Composite Designs

The central composite design (CCD) is the most frequently used RSM design. Refer to the Response Surface Methods Tutorials for a detailed example of how to set up this type of design with Design-Expert. A CCD can be broken down into three parts:

1. Two-level full or fractional design (the core).
2. Axial points (outside the core).
3. Center points.

The two-level factorial part of the design consists of all possible combinations of the plus or minus one levels of the factors. Axial points, often represented by stars, emanate from the center point, with all but one of the factors set to 0. The coded distance of the axial points is represented as a plus or minus alpha ( $\alpha$ ). For a two-factor problem, the axial points are:  $(-\alpha, 0)$ ,  $(+\alpha, 0)$ ,  $(0, -\alpha)$  and  $(0, +\alpha)$ .

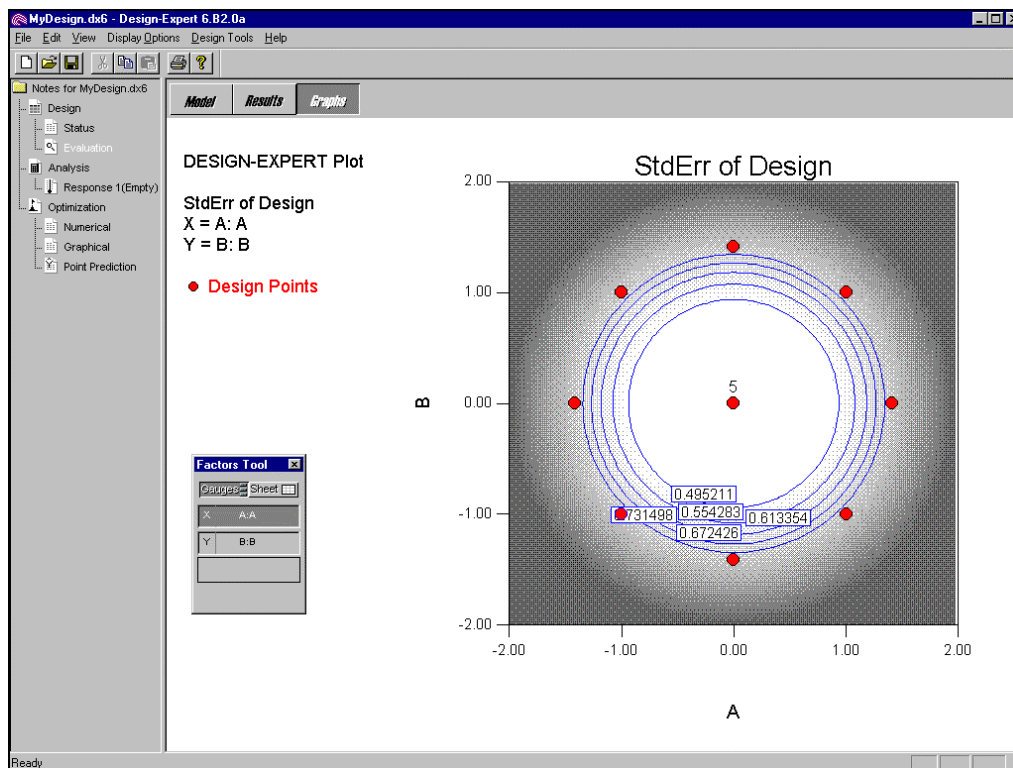
Center points are usually repeated to get an estimate of experimental error (pure error). These can be identified in the design layout by doing a right mouse click on the Block column and changing it to Display Point Type. (See screen shot below.)

	Std	Run	Type	Factor 1 A:A	Factor 2 B:B	Response 1 Response 1
	1	12	Fact		-1.00	
	2	11	Fact		-1.00	
	3	3	Fact		1.00	
	4	5	Fact		1.00	
	5	10	Axial	-1.41	0.00	
	6	2	Axial	1.41	0.00	
	7	7	Axial	0.00	-1.41	
	8	8	Axial	0.00	1.41	
	9	13	Center	0.00	0.00	
	10	9	Center	0.00	0.00	
	11	4	Center	0.00	0.00	
	12	6	Center	0.00	0.00	
	13	1	Center	0.00	0.00	

*Two-Factor Central Composite Design with Point Type Displayed*

Notice that the central composite design requires five coded levels of each factor: plus or minus one (factorial points), plus or minus alpha (axial points), and the all zero level (center point).

It's desirable to set alpha at a level that creates "rotatability" in the design. Designs with this property, such as the two-factor CCD with an alpha value of 1.414, exhibit circular contours on the standard error plot (see below). (You can generate these plots by going to the Evaluation node, Graphs option. For purposes of illustration, the one shown has the axes expanded well beyond the normal ranges.)



Standard Error Plot for Two-factor Central Composite Design (axes expanded)

## Blocking in Central Composite Designs

Central composite designs may be carried out in blocks. For example, blocking would be helpful if you couldn't conduct all of your experiments on one day or with one batch of material. The central composite design can always be divided into a factorial block and an axial point block. In designs with three or more factors, the factorial block can also be separated into two or more blocks.

The CCD structure lends itself to sequential design, a very desirable feature. For example, you could:

1. Perform a factorial design with center points to screen factors and determine if an optimum is within the design region.
2. If the optimum is contained within the region, but significant curvature prevents the factorial model from adequately representing the region, additional runs with star points and center points can be added via the augment design tool.
3. If the optimum does not appear to be within the design region, a new factorial design can be constructed in a different location where the possibility of an optimum is more likely.

Design-Expert offers various blocking patterns as options for the central composite designs. In addition, the block assignments can be changed in the design layout screen. When the experiment is blocked, there may be a choice of optimal alpha between the

value for rotatability and the value for orthogonal blocks. Design-Expert sets the default for alpha at the value for rotatability.

### Central Composite Design Options

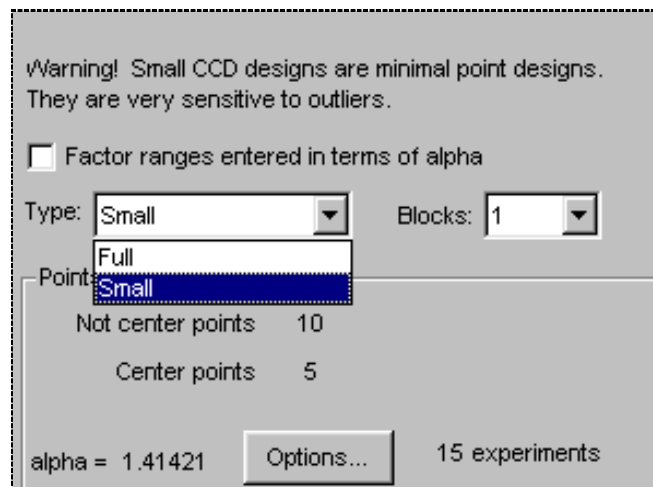
Full central composite designs include factorial points from a full factorial ( $2^k$ ), axial points and center points. Design-Expert makes the full CCD available for up to seven factors, above which the number of runs becomes excessive.

For RSM experiments with five or more factors, Design-Expert offers one or more options to do Resolution V fractional cores for the CCD. (A Resolution V fractional factorial allows estimates of all main effects and two-factor interactions, sufficient for a second order model.) You will find these designs to be much more efficient than full CCDs, with little or no loss of information.

### Small CCDs (Draper-Lin)

For the larger numbers of factors, you can also run a “small” CCD that makes use of a Resolution III Plackett-Burman core. (For details see “Small Response-Surface Designs,” Draper and Lin, *Technometrics*, May 1990, Vol. 32, No. 2.) The Draper-Lin small CCDs are near minimal point designs. However, they are not rotatable. Also, every run counts in terms of leverage on the model fitting, so outliers in the data cannot be tolerated. Another drawback to the small CCD is that model coefficients of the same order, such as those for the linear effects, may not be estimated with the same precision. In other words, the standard errors differ in an arbitrary fashion.

To run a small CCD in Design-Expert, select **File, New Design**. Then click on the **Response Surface** tab. In the **Central Composite** dialog box change **Numeric Factors** to **3**. Then, click on the list arrow for **Type** and select **Small**.



#### *Small Central Composite Design Option*

The program warns you that this is a minimal point design that’s very sensitive to outliers.

The choice of alpha values to ensure orthogonal blocking for 3, 4 and 6 factors in the small CCD are calculated in the usual manner. For 5, 7, 8, 9 and 10 factors there is no alpha that ensures orthogonal blocking. These designs have runs deleted, making the cube part of the design non-orthogonal, violating one of the requirements for orthogonal blocks. For these designs the alpha for blocks is chosen to minimize the average squared correlation of the block effect with all second order model coefficients, ignoring the constant.

## Box-Behnken Design

Design-Expert offers Box-Behnken designs for three to seven factors. These designs require only three levels, coded as  $-1$ ,  $0$ , and  $+1$ . Box and Behnken created this design by combining two-level factorial designs with incomplete block designs. This procedure creates designs with desirable statistical properties, but, most importantly, with only a fraction of the experiments needed for a full three-level factorial. These designs offer limited blocking options, except for the three-factor version. For more details on how to construct a Box-Behnken, see Myers and Montgomery, *Response Surface Methodology*.

## Three-Level Factorial Design

Design-Expert provides full factorial three-level designs for up to 4 factors. The number of experiments equals  $3^k$  plus some replicates of the center point. These designs will fit a quadratic model, but for more than two factors they require many more runs than needed to determine the coefficients in the model. We recommend the Box-Behnken designs instead.

## Hybrid Designs

Like the small CCD, hybrid designs allow experimenters to fit a quadratic model with a minimal number of runs. Design-Expert creates these designs from a  $k-1$  central composite. Then it assigns levels of the last factor ( $k$ ) to create a rotatable or nearly rotatable design. Therefore, the hybrid design will be a better choice than the small CCD. However, the hybrid design will be sensitive to outliers or missing data. It should be used only when budget considerations prohibit use of a regular CCD, Box-Behnken or full three-level factorial design. For more details on how to construct a hybrid design see Myers and Montgomery, *Response Surface Methodology*. The design as specified contains no replication. Therefore, we highly recommend you duplicate a point, preferably the center, at least three times to get an estimate of pure error.

## D-optimal Design

The D-optimal criteria, one of several “alphabetic” optimality, was developed to select design points to minimize the variance associated with the estimates of the coefficients in the model you specify. For details on optimality criteria see Myers and Montgomery, *Response Surface Methodology*.

The design space is defined by low and high level constraints on each factor. You can also add multiple linear constraints: See the Advanced Design Features section for an example.

To use D-optimality, you must choose a polynomial equation that you believe will adequately represent the response(s) in the region of interest. Often for RSM work experimenters specify the quadratic equation, a second order polynomial. Also, you must provide a candidate list of points to choose from. Design-Expert will do this part for you.

## **Candidate Points**

Design-Expert generates a candidate set of points based on the following geometric properties:

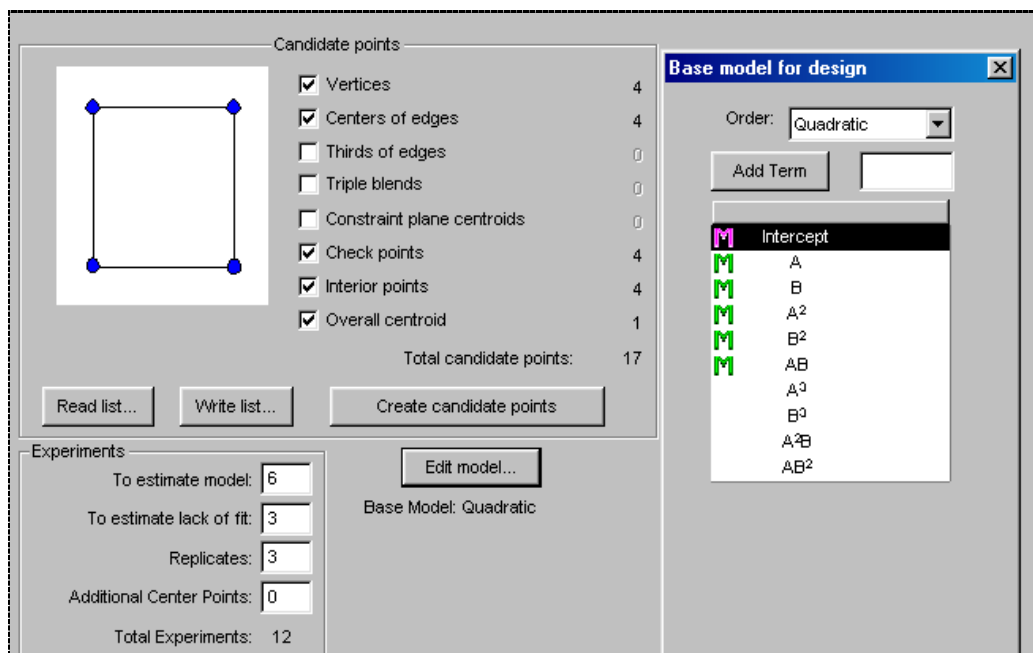
- Vertices - the corners of the design space
- Centers of edges - mid-points between adjacent vertices
- Thirds of edges - two points equally spaced between adjacent vertices
- Triple blends – averages of three adjacent vertices
- Constraint plane centroids – center points in the planar surfaces of the experimental region (the “convex hull”)
- Check points - average of centroid and vertices
- Interior points - average of centroid and (if the points are selected) “centers of edges,” “thirds of edges” and “constraint plane centroids”
- Overall centroid - center of design space.

The number of candidate points generated by Design-Expert depends on the model:

1. Linear: Vertices, check points, centroid.
2. 2FI (two-factor interaction) model: Same as linear.
3. Quadratic: Same as linear and 2FI models plus centers of edges, constraint plane centroids, and interior points.
4. Cubic: Same as quadratic plus thirds of edges and triple blends.

To keep the d-optimal exchange manageable, the algorithm limits the maximum number of any particular point type to 1500, and the total number of candidate points to 5000.

If you pick two factors, Design-Expert presents the options shown below. The screen shot shows a total of 17 candidate points for the default model (quadratic). To get this count, you must press the Create candidate points button. In large designs with many constraints it may take an appreciable amount of time to identify and count the candidate points. This will be done in any case, when you continue on and create the design, so don't bother creating the candidate points any earlier, unless it's absolutely necessary.



*D-Optimal Dialog Box for Two Factors, Quadratic Model*

In this illustration, the Edit Model button was pressed so you can see the polynomial. If you like, you can eliminate unwanted terms. This reduces the number of runs required to fit the model. It also changes the selection criterion.

If you like, you can generate your own candidate set. See the Advanced Design Features section for details. This section of the manual also shows how to create a candidate set based on multilevel full factorials.

### **Selection of Design Points**

Design-Expert gives you defaults for the minimum number of design points needed for “Model,” “Lack-of-Fit” and “Replicate.” As indicated below, the number of design points depends on the number of factors ( $k$ ) in the design and the number of coefficients in the model selected:

- “Model” points equal the number of coefficients. Points are selected using D-optimal criteria (see details on this below).
- “Lack-of-Fit” points by default will equal the number of factors plus one ( $k+1$ ) up to a maximum of five. You can add more if you like. Points are selected using the distance criterion.
- “Replicate” points by default will equal the number of factors plus one ( $k+1$ ) up to a maximum of five. You can add more if you like. The highest leverage points are replicated.

A D-optimal design minimizes the determinant of the  $(X'X)^{-1}$  matrix. This will minimize the volume of the confidence ellipsoid for the coefficients. Equivalently D-optimality maximizes the determinant  $(X'X)$ , which is called the “information” matrix.

The algorithm used to find an approximately D-optimal design is as follows:

1. Select a non-singular initial design of  $p$  points:
  - Pick the candidate point with the largest Euclidean norm as the first design point. This first point will be one of the perimeter design points, i.e., one of the points furthest from the center of the design space.
  - Pick each subsequent design point to give the maximum information about the estimable linear combinations of model coefficients and to increase the rank of the design matrix.
2. Select the remaining model points ( $\#$  model points  $- p$ ). Select the candidate point that adds the maximum amount of information about the model coefficients, i.e., the D-optimal candidate point.
3. Perform exchange steps:
  - A 1-point exchange step consists of adding to the current design the point in the candidate list that increases the determinant of the information matrix the most, and then deleting from the augmented design the point that decreases the determinant of the information matrix the least. A 2-point exchange step adds two points in sequence, and then deletes two points. Each step is taken to increase the determinant of the information matrix the most, or decrease it the least. An  $n$ -point exchange step adds and deletes  $n$  points.
  - Perform 1-point exchange steps until there is no improvement in the design. Then perform 2-point exchange steps, and so on until 5-point exchange steps show no improvement. If at any point there is improvement, start over with 1-point exchanges. (You can change the number of point exchanges from the default maximum of 5 in Design-Expert's Preference menu. The value can be set anywhere from 0 to 10. Going from 1 to 10 exchanges multiplies the time required to develop the design by about five.)

In the math design preferences you can select from zero to ten D-optimal random bootstraps - the default is four. After the first D-optimal design is built using the above algorithm, additional designs are built using the random bootstrap algorithm. Random bootstrap refers to the fact that steps one and two above are replaced by a random selection of points for the starting design. Then the point exchanges are carried out as above in step three. Since the design you end up with can depend on the starting design, using the random bootstrap improves the chances of finding a more D-optimal design. The best (as measured by D-optimality) design of those generated (by default five) is the one retained.

If the candidate list is large and/or the degree of the design is large, D-optimal point selection can be a lengthy process.

## Distance-Based Design

Distance-based designs consist of points, selected from a suitable candidate set, spread evenly over the feasible design region. The algorithm for selection starts with an extreme vertex. Then it chooses the point for which the minimum Euclidean distance to existing point(s) is at a maximum. It goes on from there until it adds a number of points that equals the number of coefficients in the model you select. The same approach is applied to picking additional lack-of-fit points. The points for pure error replicates get picked on the basis of leverage. We do not recommend the distance-based approach because it may create an aliased design where some model coefficients cannot be independently estimated. Use the modified distance-based method or, better yet, use a d-optimal design.

You will find more details on the modified-distance approach later in this section of the manual in the discussion on mixture design.

## Modified Distance Design

The modified distance-based algorithm ensures that each point selected will increase the rank of the design matrix. It ensures that the design will be able to estimate all the coefficients in the polynomial, even when the design space is highly constrained. Although this approach provides improvement over the unmodified distance-based algorithm, we recommend use of the d-optimal design.

You will find more details on the modified-distance approach later in this section of the manual in the discussion on mixture design.

## One-factor Design

Design-Expert will set up a design to fit the model of your choice to one numerical factor. (Categorical factors can be handled under the Factorial tab by the General Factorial selection.) The higher the order, the more points (shown in coded format) will be included in the one-factor design:

1. Linear: -1, 0, +1 (all points replicated).
2. Quadratic: -1, -0.5, 0, +0.5, +1 (outer and center points replicated).
3. Cubic: -1, -0.67, -0.33, 0, +0.33, +0.67, +1 (outer and center points replicated).

## Hexagon and Pentagon Designs

For two-factor designs, the hexagon and pentagon options provide geometrically-spaced designs. Some experimenters like them for their coverage of the experimental space.

We do not recommend the pentagon design. It contains minimal points for the quadratic model. Therefore, all of the points have a leverage of one, so the design is completely susceptible to outliers.

## User-Defined Design

The user-defined option allows you to put in all classes of candidate points that you want: vertices, centers of edges, thirds of edges, triple blends, constraint plane centroids, axial check blends and/or overall centroid.

## Adding Categorical Factors

Up to 10 categorical factors can be added to RSM designs, which will be multiplied accordingly. For example, if you choose a 13-run central composite design for two numerical factors, and then add two categorical factors at two levels each, you get a total of 52 runs ( $13 \times 2 \times 2$ ). See the Advanced Design Features section for more detail on adding categorical factors to RSM or any other type of design.

---

## Mixture Design Selection

Use mixture design when your response changes only as a function of the proportion of component ingredients. For example, the flavor of lemonade depends on the proportion of lemons to water, not the amounts. For an in-depth treatment of this subject we recommend Cornell's *Experiments with Mixtures*. This textbook can be obtained from Stat-Ease or direct from the publisher: John Wiley & Sons, Inc. If you only want an introductory-level review of mixture experiments, see Chapter 11 of Myers and Montgomery's *Response Surface Methodology*.

Design-Expert handles mixture problems with 2 to 24 components. The following table shows which designs you can choose, depending on the number of components and the order of the polynomial. In most cases, fewer components can be accommodated when you ask for a cubic (or special cubic) model.

Design	Number of components (q)
Simplex-lattice	$2 \leq q \leq 24$ (12 for cubic)
Simplex-centroid	$3 \leq q \leq 8$
Screening	$6 \leq q \leq 24$ (12 for cubic)
D-Optimal	$2 \leq q \leq 24$ (12 for cubic)
Distance based	$2 \leq q \leq 24$ (12 for cubic)
Modified distance	$2 \leq q \leq 24$ (12 for cubic)
User defined	$2 \leq q \leq 24$ (12 for cubic)

*Mixture Designs*

We will describe the design selection criteria separately for each general type of design.

## Constraints

You will often run up against constraints on mixture components. For example, you may need some minimal amount of sweetener to make your lemonade drinkable. The design builder feature allows you to enter names for each component, along with lower and upper limits for each, and/or multiple linear constraints (see the Advanced Features section). If you work in percentage units, then your lower and upper limits, as well as the total, will be expressed in percent. The program permits you to enter your limits and total in whatever scale is convenient for you.

## Components Coding

The actual units of measure, by weight or volume, used to blend a mixture, do not prove to be convenient for statistical calculations. Coding to the “Pseudo” scale, via the intermediary “Real” coded values, makes computations much simpler. The pseudo scale ranges from zero to one. It’s the equivalent of factorial coding for non-mixture DOE.

To get to pseudo scale, you first must convert your actual data to real scale, where components get expressed as fractions. For example, if you made 128 ounces (one gallon) of lemonade with 32 ounces of lemon juice, then the real lemon is 0.25 ( $=32/128$ ).

In the pseudo scale, each real component is rescaled to be a fraction of the active part of the mixture. It becomes important in the presence of individual constraints. To illustrate, suppose that a three-component nut mixture will always contain at least 50% peanuts, at least 15% pecans, and at least 5% cashews. Seventy percent of the mixture is predefined. We are going to do an experiment to determine the remaining 30%, the active part. In pseudo terms,

- Peanut pseudo component = ( % peanut - 50%) / 30%
- Pecan pseudo component = ( % pecan - 15%) / 30%
- Cashew pseudo component = ( % cashew - 5%) / 30%

If there are no lower-limit constraints, the real and pseudo scales are identical.

See the Mixture Design Tutorial for an example that uses actual, real and pseudo values.

## Simplex Designs

Design-Expert provides several different types of designs for mixture problems. The “lattice” and “centroid” simplex designs may only be used if there are no active upper limit constraints on the components. In such a case, the feasible design space in the pseudo-component scale is a simplex - the simplest shape with  $n+1$  vertices where  $n$  is the number of dimensions. The most common simplex is a triangle. A number of easy-to-compute symmetric designs are available in simplex space.

In general, the feasible simplex in the pseudo component scale consists of all points

$$(X_1, X_2, \dots, X_q)$$

with  $X_1 + X_2 + \dots + X_q = 1$ . For three components, this can be displayed as an equilateral triangle with the vertices of the triangle coded as: (1, 0, 0), (0, 1, 0), (0, 0, 1).

Points along the edges of the triangle represent mixtures of two components, and points in the interior represent mixtures of all three components.

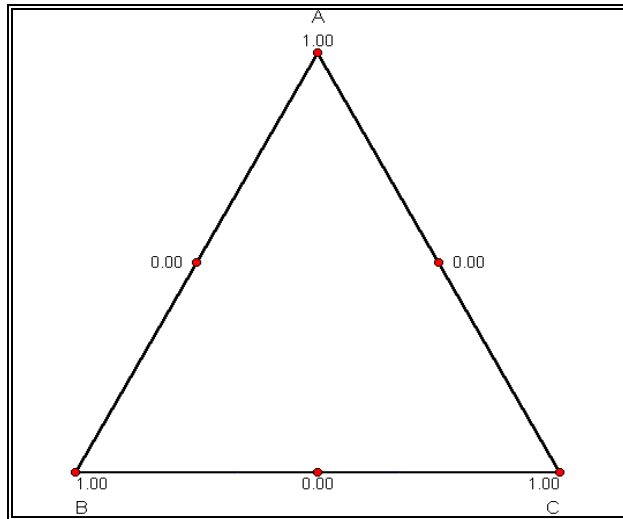
If there are active upper-limit constraints, the feasible design space may not be a simplex, so Design-Expert offers algorithmic designs, such as D-optimal.

### Simplex-Lattice Designs

A simplex-lattice design of degree  $m$  consists of all points in the simplex of the form

$$(i_1/m, i_2/m, \dots, i_q/m)$$

where  $i_1, i_2, \dots, i_q$  are integers in the set  $\{0, 1, 2, \dots, m\}$ . With Design-Expert you can specify the model you want: linear ( $m=1$ ), quadratic ( $m=2$ ), or cubic ( $m=3$ ). The program defaults the simplex lattice to the quadratic model. The second degree design can be seen below (for three components).



Simplex Lattice [  $q=3, m=2$  ]

### Augmenting Simplex-Lattice Designs

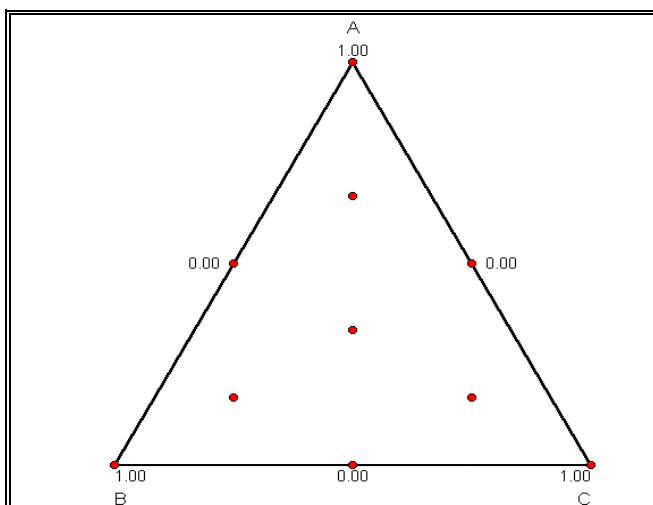
The second degree simplex-lattice designs provide only the minimum number of points to estimate the terms of a quadratic (second-degree) response surface. For that reason, you should augment the designs to provide some ability to detect lack-of-fit.

The simplex-lattice augmented design adds the following points to the simplex-lattice:

1. Overall center of the simplex, if not already in the design.

2. Axial check points, 50-50 combinations of the overall center and each vertex of the simplex.

The second degree augmented design is shown below (for three components).



*Augmented Simplex-Lattice [q=3, m=2]*

To get an estimate of the experimental error, some of the design points should be replicated. The points that are replicated are those with the highest leverage for the model on which the design is based.

### **Simplex-Centroid Designs**

A simplex-centroid design consists of all points that are equally weighted mixtures of one to q components. For instance, for four components, you get 15 points: (1,0,0,0), (0,1,0,0), (0,0,1,0), (0,0,0,1), (1/2,1/2,0,0), (1/2,0,1/2,0), (1/2,0,0,1/2), (0,1/2,1/2,0), (0,1/2,0,1/2), (0,0,1/2,1/2), (1/3,1/3,1/3,0), (1/3,1/3,0,1/3), (1/3,0,1/3,1/3), (0,1/3,1/3,1/3), (1/4,1/4,1/4,1/4). The last point is the overall centroid.

Augmenting the simplex-centroid design adds check points (50-50 combinations of the overall center and each vertex) to the design.

Unlike the simplex-lattice, the simplex-centroid design does not require specification of a model. However, Design-Expert provides the model selection option for picking the replicates you need to estimate the experimental error. It will use the model you pick to duplicate the highest leverage points. You can choose whether or not to augment, and how many replicates you want, if any.

### **Screening Designs**

Screening designs for mixtures allow you to look at a large number of components in a minimal number of blends. They won't give much information, if any, about interactions (synergisms or antagonisms), but they will tell you about the big hitters -

positive or negative. Design-Expert offers different screening options depending on whether or not you've created a simplex experimental region.

For a simplex space, the program requires the vertices, but you can optionally add axial check points and constraint plane centroids. Replicates of the overall centroid provide an estimate of the pure error. The program recommends five centroid replicates, but you can change this if you like. The centroid also provides an estimate of curvature. If the response curves up or down in the middle of the space, it will be captured in the form of the quadratic terms. These may be aliased, but if significant, the quadratic terms indicate the need to do a more sophisticated design the next time around. Ideally, the screening study leads to a reduction in components so you can afford to do an in-depth experiment.

For non-simplex space, you must decide how many vertices to put in the screening design. The program recommends a number equal to two times the number of components, but you may want to scale this back somewhat. The desired number of vertices are selected d-optimally from the available set. You also should run a number of overall centroid replicates - the program recommends five.

## D-optimal Design

Given a candidate set, the D-optimal design process for mixture designs works exactly the same way as that described for RSM designs. For details on point selection, refer to the appropriate heading in the description of RSM given earlier.

### **Construction of Candidate Set**

The number of candidate points generated by Design-Expert depends on the model:

1. Linear: Vertices, axial check blends, centroid.
2. Quadratic: Same as linear plus centers of edges, constraint plane centroids, and interior blends.
4. Special Cubic: Same as quadratic.
4. Cubic: Same as special cubic plus thirds of edges and triple blends.

To keep the d-optimal exchange manageable, the algorithm limits the maximum number of any particular point type to 1500, and the total number of candidate points to 5000.

Design-Expert uses the CONVERT algorithm to find vertices (see Piepel, *Journal of Quality Technology*, pp125-133, April, 1988.) We believe the algorithm finds all vertices of the simplex, but in higher dimensions with complex constraints, it is possible that an extra point or two may be in the vertex list. This does no real harm, since the candidate list is merely expanded.

### **Model Reduction**

For the algorithmic designs (distance, modified distance and D-optimal) the mixture polynomials can be reduced prior to point selection. Terms that are not of interest can be eliminated. Reducing the number of coefficients reduces the number of model points

required and changes the selection criterion (which is based upon minimizing the generalized variance of the coefficients in the model). If you select model reduction (the Edit model button on the dialog box) a list of model terms appears. Highlight and right click on any term you wish to select or clear from the model.

## Canonical (Scheffe) Form

By default, Design-Expert uses a canonical polynomial for fitting data collected from mixture experiments. These polynomials can be recognized by their lack of an intercept term. They can be derived from the usual RSM models by substitution of the overall constraint that all components add to one. The program labels the canonical model “Scheffe,” after a pioneering author.

You cannot eliminate the main effect terms, because they incorporate information on the overall average response. For details see Cornell’s *Experiments with Mixtures*, page 23, or Myers and Montgomery’s *Response Surface Methodology*, page 539. Design-Expert shows a padlock symbol by the locked terms. They will be forced into the model.

## Slack Variable Form

In some cases of constrained mixtures, it becomes difficult to get a good regression fit of the Scheffe model. This occurs when you introduce a wide disparity in the constraint ranges. For example, you might make a juice blend with one ingredient that’s very powerful, so you constrain it to fractions of volume percent, while all other ingredients can be varied over wide volumes. The resulting space will be a narrow sliver with very poor design properties. If it’s really bad, then Design-Expert will recommend you try the “slack variable” mixture model. This model resembles the usual RSM models except that one component must be removed, because it will be a linear combination of all the others. Design-Expert recommends a term to remove (the one with the widest range). You can change this if you like.

You cannot eliminate any of the other main effect terms, because they incorporate information on other terms. They will be forced into the model.

Because it excludes at least one component and all its interactions, we recommend that you not use the slack variable form if at all possible. Instead consider changing the metric of your mixture to a form that results in more even ranges. For example, you might convert from weight percent to mole percent in a chemical mixture. In any case, if it works, the design you get with the Scheffe model will likely be nearly as good as the slack form. You will still be able to analyze your data with the slack form should you feel it necessary.

We advise that you always evaluate your mixture design before you run it. (See “Design Evaluation” in the Advanced Design Features section.) Any special problems with the design may then be discovered before it’s too late.

## Distance-Based Design

Distance-based designs consist of points, selected from a suitable candidate set, spread evenly over the feasible design region. You specify the candidate list (see section above on d-optimal design for details).

### *Design-Point Selection*

After Design-Expert prepares the candidate point set, you will be asked to specify the number of points you want in your design. If you select too few, the design cannot estimate the desired number of coefficients. Default settings are:

- “Model” points equal the number of coefficients. Points are selected using distance criteria as outlined below.
  1. Choose an initial point from the candidate list that is as close to a pure component as possible.
  2. Find a point as far away as possible from all the others already chosen. Add this to the design. (In geometric terms, “far away” means the point whose minimum Euclidean distance to other points already in the design is as large as possible.)
  3. Repeat step (2) until the desired number of points are in the design. The distance-based procedure spreads points fairly evenly over the design region. However, the computational algorithm may not select enough points to ensure that the chosen polynomial can be estimated. Therefore, after selecting the design, Design-Expert tests the design matrix to see if it is non-singular for the desired polynomial model (in other words, whether all the coefficients can be estimated). If the test fails, you are given the option of adding design points to correct the problem. Then Design-Expert adds design points, using the distance selection method, until the design is non-singular, or the number of design points uses up the available memory. If the design matrix remains singular, no replicates are added.
- “Lack-of-Fit” points by default equal the number of components plus one ( $q+1$ ) up to a maximum of five. You can add more if you like. Points are selected using the distance criterion (see steps listed above).
- “Replicate” points by default equal the number of components plus one ( $q+1$ ) up to a maximum of five. You can add more if you like. The highest leverage points are replicated. If the design is singular, no replicates are selected.

## Modified Distance-Based Design

As discussed above, the distance-based selection process may not pick appropriate design points to estimate the chosen model. The choice of “modified” distance-based design triggers a different point selection algorithm within Design-Expert that overcomes this deficiency.

The candidate list will be the same as shown above under “pure” distance-based design. From this list, the modified distance-based point selection algorithm selects model points (and lack-of-fit points) as described below.

1. First  $p$  points ( $p$  in this case meaning the number of terms in polynomial):
  - a. Choose an initial point that is as close to a pure component as possible.
  - b. Rank the points in decreasing order of minimum Euclidean distance to other points already in the design. If the first point (the point whose minimum Euclidean distance to other points already in the design is as large as possible) increases the rank of the design matrix, add it to the design. If the rank is not increased, try the second point, and so on. Select the first point that increases the rank of the matrix.
  - c. Repeat step (b) until  $p$  number of points are in the design.
2. The remainder of the model plus lack-of-fit points:
  - a. Add to the design the point whose minimum Euclidean distance to other points already in the design is as large as possible.
  - b. Repeat step (a) until the desired number of points are in the design.

Replicate points will be chosen in the same way as described for “pure” distance-based design. From the design points chosen, Design-Expert selects those with the highest leverage to replicate.

Modified distance-based point selection provides a set of points spread (approximately) evenly over the feasible design region, while ensuring the points chosen are adequate to estimate the polynomial selected.

## User-Defined Point Selection

The user-defined method simply puts all candidate points in the design. You can then use the design layout to add, delete, or duplicate points in the design.

## Crossed Design Options

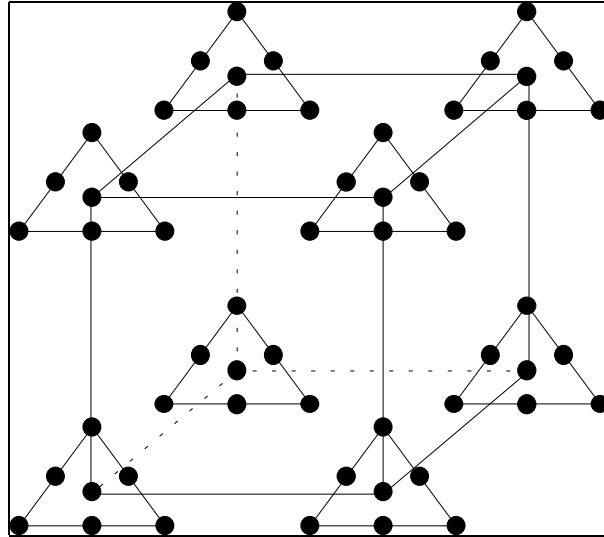
### Adding Process Factors

Crossed designs allow us to study mixture components and process factors in the same design. They are built as follows:

1. Choose a mixture design that supports the mixture polynomial you wish to fit.
2. Select a standard process design such as a two-level factorial.
3. Run the mixture design for every run in the process design.

To analyze, cross the mixture model with the ordinary polynomial.

For example, in the “Mixture-Process Tutorials” three mixture components are studied in conjunction with three process factors. The mixture design has seven blends and supports up to a special cubic polynomial and the process design is a  $2^3$  factorial (eight runs) supporting up to a two-factor interaction polynomial. The crossed design is shown below.



*Seven Blends(on Triangles) at Eight Process Combinations (Cube)*

A drawback to the crossed design is that the designs grow large quite quickly. Most often the complete crossed design is used as a candidate points set and a subset is selected using D-optimal selection. See “The Experiment as D-Optimal Design” the second part of the “Mixture-Process Tutorials” section of this manual.

## Adding Categorical Factors

Categorical factors can be added to mixture designs in the same fashion as process factors. See “Adding Categorical Factors” in the “Advanced Design Features” section of this manual.

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## Design Editing

The design layout can be used to change virtually any aspect of your design. You can change levels; add, delete or duplicate runs; or modify blocking assignments. Factor names can be edited. You can also name blocks. The following section gives you the highlights of these and other design editor features, but to really get a feel for what can be done, there’s no substitute for experimentation. Build your own design and check it out. Try right mouse clicks on column headings and explore the options.

## Order of Experiments

The design layout defaults to run order. You can switch to standard order by right clicking on either of the column headings or using the **View** menu. The standard order labels can be changed and sorted to identification (“ID”) order by right clicking on the column headings. The ID for replicate runs will be identical, whereas both standard and run orders must be unique.

## Point Type

The various parts of your design, for example, factorial versus axial points versus center points in a CCD, can be identified by doing a right click on the **Block** column. This is especially helpful for constrained mixtures to determine which blends are extreme vertices, the overall centroid, and all other types.

## Actual vs. Coded Values

The design layout works in coded or actual (pseudo, real and actuals for mixtures) values, as you wish. Changes made in one scale are automatically applied to the other scales. All analyses are done in the coded scale for response surface problems. You can switch between coded and actual values by using the **Options** menu.

## Botched Design

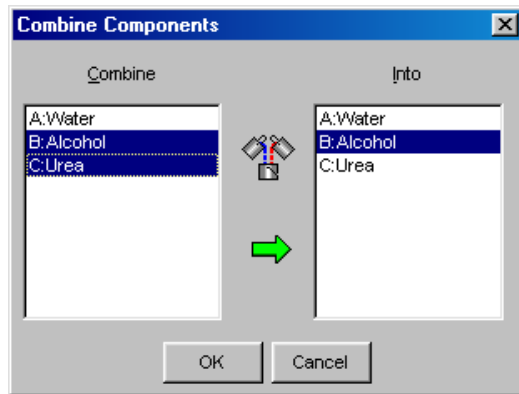
You can use the design layout to correct badly missed factor levels from a “botched” design. This feature should not be used to adjust for normal variation of the factors around their design levels. Make changes only when significant deviations from the desired factor levels occur. Ideally, you will be able to assign a special cause to the deviation. In most cases you will be interested in predicting the response as a function of the designed factor levels, so adjustment will not be desirable. Box, Hunter, and Hunter provide an interesting case study of a botched factorial in Appendix 14C, page 503, of their book *Statistics for Experimenters*.

## Delete Factors

In most cases, when you run a factorial screening design, some factors will not be significant. If you want to augment such a design, for example to a CCD, then it will be desirable to include only the significant factors. You can delete the insignificant factors by doing a right click on the unwanted columns and selecting **Delete**.

## Combine Components

You may decide after setting up a mixture design, that several components belong together, for example various forms of sugar in a food formulation. To check this out, open the **Mix-a.dx6** data file. Right click on any component column heading and select **Combine Components** to bring up the following dialog box.



*Combine Component Dialog Box*

In this example, you will get a modified design with the last two components combined as one.

## Response Editing

Use the design layout to enter responses after completing your experiments. To make entry simple, sort the experiment in run order, the random order assigned when Design-Expert sets up the experiment. Right clicking on the response column headings brings up added options for formatting, changing names, units, etc.

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## Power Calculations

The Design Evaluation feature in Design-Expert now calculates “power”, which tells you the probability of finding an effect of a given size (either  $\frac{1}{2}$ , 1 or 2 standard deviations) for any specific design. (For other details on design evaluation refer back to the last part of the section on Advanced Design Features.) In general, power increases as you add more runs. The sweet spot for power is from .8 to .95 probability. At lower than .8 power you risk missing effects of interest. On the other hand, it’s wasteful to invest in more runs than needed for power of .95.

If you are not sure what power can do for you, refer to the short primer on this topic in the “Handbook for Experiments,” which we send to all registered software users. For the statistical details, see “Sizing Fixed Effects for Computing Power in Experimental Designs,” Fall Technical Conference, 2000, by Oehlert and Whitcomb. The following discussion provides some guidance on how to generate data on power, and how the program does the calculations, which depends on the chosen design: factorial, response surface, mixture, or crossed.

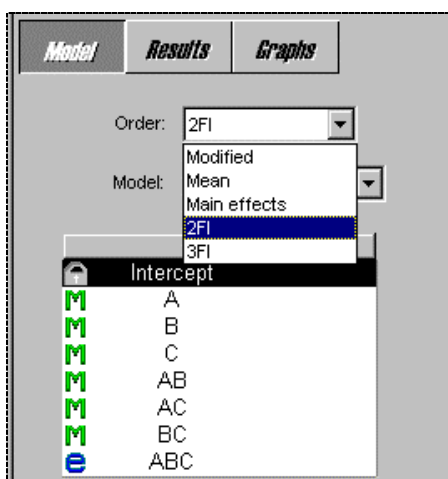
The power calculations for two-level factorial designs focus on the effects - the difference in response means at the high (coded +1) versus low (coded -1). The model term equals one-half the effect. Power for unreplicated factorials can only be estimated if you designate at least one term for error. For example, if you set up a full two-level factorial on three factors and do a design evaluation on the default model, you will see the following error message for power.

Term	StdErr**	VIF	Ri-Squared	Power at 5 % alpha level for effect of		
				1/2 Std. Dev.	1 Std. Dev.	2 Std. Dev.
A	0.35	1.00	0.0000	Not Defined when the Residual Degrees of Freedom is 0.		
B	0.35	1.00	0.0000			
C	0.35	1.00	0.0000			
AB	0.35	1.00	0.0000			
AC	0.35	1.00	0.0000			
BC	0.35	1.00	0.0000			
ABC	0.35	1.00	0.0000			

\*\*Basis Std. Dev. = 1.0

*Error Message When Analyzing Unreplicated Factorial for Default Model*

In this case you must go back to the Model screen and designate individual terms as error, or select a lesser model as shown below.



*Selecting a Different Model with Term(s) Left for Error*

Now when you press the Results button you get the following results for power at the 5% alpha level. (Note: go to Edit Preferences if you want to change the significance threshold from 5% to either 1% or 10%.)

Term	StdErr**	VIF	Ri-Squared	Power at 5 % alpha level for effect of		
				1/2 Std. Dev.	1 Std. Dev.	2 Std. Dev.
A	0.35	1.00	0.0000	6.2 %	9.3 %	17.6 %
B	0.35	1.00	0.0000	6.2 %	9.3 %	17.6 %
C	0.35	1.00	0.0000	6.2 %	9.3 %	17.6 %
AB	0.35	1.00	0.0000	6.2 %	9.3 %	17.6 %
AC	0.35	1.00	0.0000	6.2 %	9.3 %	17.6 %
BC	0.35	1.00	0.0000	6.2 %	9.3 %	17.6 %

\*\*Basis Std. Dev. = 1.0

*Power Calculated for Two-Level Factorial (Three Factors, ABC as Error)*

This design, because it's so small, is not very powerful. For example, the report shows only a 17.6% probability (for power) of detecting a two standard deviation change in any given term. As shown below, the power increases dramatically if you replicate the design (accomplished by entering 2 in the associated field when re-building the design).

Term	StdErr**	VIF	Ri-Squared	Power at 5 % alpha level for effect of		
				1/2 Std. Dev.	1 Std. Dev.	2 Std. Dev.
A	0.25	1.00	0.0000	14.6 %	43.1 %	94.4 %
B	0.25	1.00	0.0000	14.6 %	43.1 %	94.4 %
C	0.25	1.00	0.0000	14.6 %	43.1 %	94.4 %
AB	0.25	1.00	0.0000	14.6 %	43.1 %	94.4 %
AC	0.25	1.00	0.0000	14.6 %	43.1 %	94.4 %
BC	0.25	1.00	0.0000	14.6 %	43.1 %	94.4 %

\*\*Basis Std. Dev. = 1.0

*Power Increased by Replication (ABC designated as an error term)*

If you try to reproduce this output, remember to designate ABC as error. It's not necessary to do this, due to the pure error obtained from replication, but it makes comparison of the power results fairer.

For general factorial designs, power is defined as the probability of finding a difference separating the two most extreme terms in a group of terms. For example, see the output below, where factor A has three levels. (Factors B and C are at two levels. The evaluation is done for the two-factor interaction (2FI) model, so the ABC term is being used for error.)

Term	StdErr**	VIF	Ri-Squared	Power at 5 % alpha level for effect of		
				1/2 Std. Dev.	1 Std. Dev.	2 Std. Dev.
A[1]	0.41			6.2 %	9.6 %	22.2 %
A[2]	0.41					
B	0.29	1.00	0.0000	8.4 %	17.9 %	47.1 %
C	0.29	1.00	0.0000	8.4 %	17.9 %	47.1 %
A[1]B	0.41			6.2 %	9.6 %	22.2 %
A[2]B	0.41					
A[1]C	0.41			6.2 %	9.6 %	22.2 %
A[2]C	0.41					
BC	0.29	1.00	0.0000	8.4 %	17.9 %	47.1 %

\*\*Basis Std. Dev. = 1.0

*Power Calculation for General Factorial Design*

For response surface (RSM) designs, Design-Expert defines power as the probability of finding an effect of a given size (either 1/2, 1 or 2 standard deviations) for a polynomial model. Linear effects are calculated in the usual way, by taking the difference between factor highs (coded +1) and lows (coded -1). These limits on the linear effects define

the range for all higher order effects. As shown in the table below, the range for a pure quadratic (squared) effect then becomes 0 to +1. As you can see, this same range applies to other terms that are even powers, while the odd-powered terms (such as A<sup>3</sup>) revert back to the -1 to +1 range.

Effect	Low	High
Linear	-1	+1
2FI	-1	+1
Quadratic	0	+1
Cubic A <sup>3</sup>	-1	+1
Cubic A <sup>2</sup> B	-1	+1
Cubic ABC	-1	+1
Quartic A <sup>4</sup>	0	+1
Quartic A <sup>3</sup> B	-1	+1
Quartic A <sup>2</sup> B <sup>2</sup>	0	+1
Quartic A <sup>2</sup> BC	-1	+1
Quartic ABCD	-1	+1

*Effect Ranges for Calculating Power of RSM Design*

The basis for the power calculations for mixture designs is the difference between the value at 0 and the value at +1 for a linear effect. These limits define the range for all higher order effects. Therefore the range for a quadratic effect is from 0 to +1/4 (the maximum product of A\*B). Similar rules apply to the higher order mixture effects as shown in the table below. An effect of either 1/2, 1 or 2 standard deviations implies that there is a difference of that many standard deviations separating the high and low values of that effect in the model.

Effect	Low	High
Linear A	0	+1
Quadratic AB	0	+1/4
Special cubic ABC	0	+1/27
Cubic AB(A-B)	-3/32	+3/32
Special quartic A <sup>2</sup> BC	0	1/64

*Effect Ranges for Calculating Power of a Mixture Design*

The power calculations for crossed mixture-process effects are complicated. For example, the range for a linear mixture by linear process effect is calculated by multiplying (0, 1) from the mixture by (-1, +1) from process, which yields four cross products: (0 times -1 = 0), (0 times +1 = 0), (1 times -1 = -1) and (1 times +1 = +1). Similar rules apply to the higher order crossed effects. The following table provides the resulting ranges.

<b>[Mixture]* Process</b>	<b>Low</b>	<b>High</b>	<b>[Mixture]* Process</b>	<b>Low</b>	<b>High</b>
[A]*Mean	0	+1	[ABC]*efg	-1/27	+1/27
[A]*e	-1	+1	[ABC]*e <sup>4</sup>	0	+1/27
[A]*ef	-1	+1	[ABC]*e <sup>3</sup> f	-1/27	+1/27
[A]*e <sup>2</sup>	0	+1	[ABC]*e <sup>2</sup> f <sup>2</sup>	0	+1/27
[A]*e <sup>3</sup>	-1	+1	[ABC]*e <sup>2</sup> fg	-1/27	+1/27
[A]*e <sup>2</sup> f	-1	+1	[ABC]*efgh	-1/27	+1/27
[A]*efg	-1	+1	[AB(A-B)]*Mean	-3/32	+3/32
[A]*e <sup>4</sup>	0	+1	[AB(A-B)]*e	-3/32	+3/32
[A]*e <sup>3</sup> f	-1	+1	[AB(A-B)]*ef	-3/32	+3/32
[A]*e <sup>2</sup> f <sup>2</sup>	0	+1	[AB(A-B)]*e <sup>2</sup>	-3/32	+3/32
[A]*e <sup>2</sup> fg	-1	+1	[AB(A-B)]*e <sup>3</sup>	-3/32	+3/32
[A]*efgh	-1	+1	[AB(A-B)]*e <sup>2</sup> f	-3/32	+3/32
[AB]*Mean	0	+1/4	[AB(A-B)]*efg	-3/32	+3/32
[AB]*e	-1/4	+1/4	[AB(A-B)]*e <sup>4</sup>	-3/32	+3/32
[AB]*ef	-1/4	+1/4	[AB(A-B)]*e <sup>3</sup> f	-3/32	+3/32
[AB]*e <sup>2</sup>	0	+1/4	[AB(A-B)]*e <sup>2</sup> f <sup>2</sup>	-3/32	+3/32
[AB]*e <sup>3</sup>	-1/4	+1/4	[AB(A-B)]*e <sup>2</sup> fg	-3/32	+3/32
[AB]*e <sup>2</sup> f	-1/4	+1/4	[AB(A-B)]*efgh	-3/32	+3/32
[AB]*efg	-1/4	+1/4	[A <sup>2</sup> BC]*Mean	0	1/64
[AB]*e <sup>4</sup>	0	+1/4	[A <sup>2</sup> BC]*e	-1/64	+1/64
[AB]*e <sup>3</sup> f	-1/4	+1/4	[A <sup>2</sup> BC]*ef	-1/64	+1/64
[AB]*e <sup>2</sup> f <sup>2</sup>	0	+1/4	[A <sup>2</sup> BC]*e <sup>2</sup>	0	+1/64
[AB]*e <sup>2</sup> fg	-1/4	+1/4	[A <sup>2</sup> BC]*e <sup>3</sup>	-1/64	+1/64
[AB]*efgh	-1/4	+1/4	[A <sup>2</sup> BC]*e <sup>2</sup> f	-1/64	+1/64
[ABC]*Mean	0	+1/27	[A <sup>2</sup> BC]*efg	-1/64	+1/64
[ABC]*e	-1/27	+1/27	[A <sup>2</sup> BC]*e <sup>4</sup>	0	+1/64
[ABC]*ef	-1/27	+1/27	[A <sup>2</sup> BC]*e <sup>3</sup> f	-1/64	+1/64
[ABC]*e <sup>2</sup>	0	+1/27	[A <sup>2</sup> BC]*e <sup>2</sup> f <sup>2</sup>	0	+1/64
[ABC]*e <sup>3</sup>	-1/27	+1/27	[A <sup>2</sup> BC]*e <sup>2</sup> fg	-1/64	+1/64
[ABC]*e <sup>2</sup> f	-1/27	+1/27	[A <sup>2</sup> BC]*efgh	-1/64	+1/64

*Effect Ranges for Calculating Power of Combined Mixture-Process Designs*