21 Mixture Designs

See also,

- Chapter 22, *Optimal Designs*
- Chapter 23, *Response Optimization*

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Mixture Designs Overview

Mixture experiments are a special class of response surface experiments in which the product under investigation is made up of several components or ingredients. Designs for these experiments are useful because many product design and development activities in industrial situations involve formulations or mixtures. In these situations, the response is a function of the proportions of the different ingredients in the mixture. For example, you may be developing a pancake mix that is made of flour, baking powder, milk, eggs, and oil. Or, you may be developing an insecticide that blends four chemical ingredients.

In the simplest mixture experiment, the response (the quality or performance of the product based on some criterion) depends on the *relative proportions* of the components (ingredients). The quantities of components, measured in weights, volumes, or some other units, add up to a common total. In contrast, in a factorial design, the response varies depending on the *amount* of each factor (input variable).

MINITAB can create designs and analyze data from three types of experiments:

- mixture experiments
- mixture-amounts (MA) experiments (page 21-11)
- mixture-process variable (MPV) experiments (21-14)

The difference in these experiments is summarized below:

Type	Response depends on…	Example
mixture	the relative proportions of the components *only*.	the taste of lemonade depends *only* on the proportions of lemon juice, sugar, and water
mixture-amounts	the relative proportions of the components *and* the total amount of the mixture.	the yield of a crop depends on the amount of an insecticide applied *and* the proportions of the insecticide ingredients
mixture-process variable	the relative proportions of the components *and* process variables. Process variables are factors that are not part of the mixture but may affect the blending properties of the mixture.	the taste of a cake depends on the cooking time and cooking temperature, *and* the proportions of cake mix ingredients

Mixture experiments in MINITAB

The design and subsequent analysis of a mixture experiment might consist of the following steps:

1 Choose a mixture design for the experiment. Before you begin using MINITAB, you need to determine what design is appropriate for your problem. See *Choosing a Design* on page 21-3.

2 Use **Create Mixture Design** to generate a simplex centroid, simplex lattice, or extreme vertices mixture design (page 21-5). In addition, you can include amounts or process variables in your design to create mixture-amounts designs (page 21-11) and mixture-process variable designs (page 21-14).

   Use **Define Custom Mixture Design** to create a design from data you already have in the worksheet. Define Custom Mixture Design allows you to specify which columns contain your components and other design characteristics. You can then easily fit a model to the design. See *Defining Custom Designs* on page 21-28.

3 Use **Modify Design** to rename the components, replicate the design, randomize the design, and renumber the design. See *Modifying Designs* on page 21-30.

4 Use **Display Design** to change the display order of the runs and to change the units in which MINITAB expresses the components or process variables in the worksheet. See *Displaying Designs* on page 21-35.

5 Perform the mixture experiment and collect the response data. Then, enter the data in your MINITAB worksheet. See *Collecting and Entering Data* on page 21-37.

6 Use **Analyze Mixture Design** to fit a model to the experimental data. See *Analyzing Mixture Designs* on page 21-38.

7 Use plots to visualize the design space or response surface patterns. Use **Simplex Design Plot** (page 21-24) to view the design space, or **Response Trace Plot** (page 21-45) and **Contour/ Surface (Wireframe) Plots** to visualize response surface patterns (21-49).

8 If you are trying to optimize responses, use **Response Optimizer** (page 23-2) or **Overlaid Contour Plot** (page 23-19) to obtain a numerical and graphical analysis.

Depending on your experiment, you may do some of the steps in a different order, perform a given step more than once, or eliminate a step.

Choosing a Design

Before you use MINITAB, you need to determine what design is most appropriate for your experiment. MINITAB provides simplex centroid, simplex lattice, and extreme vertices designs.

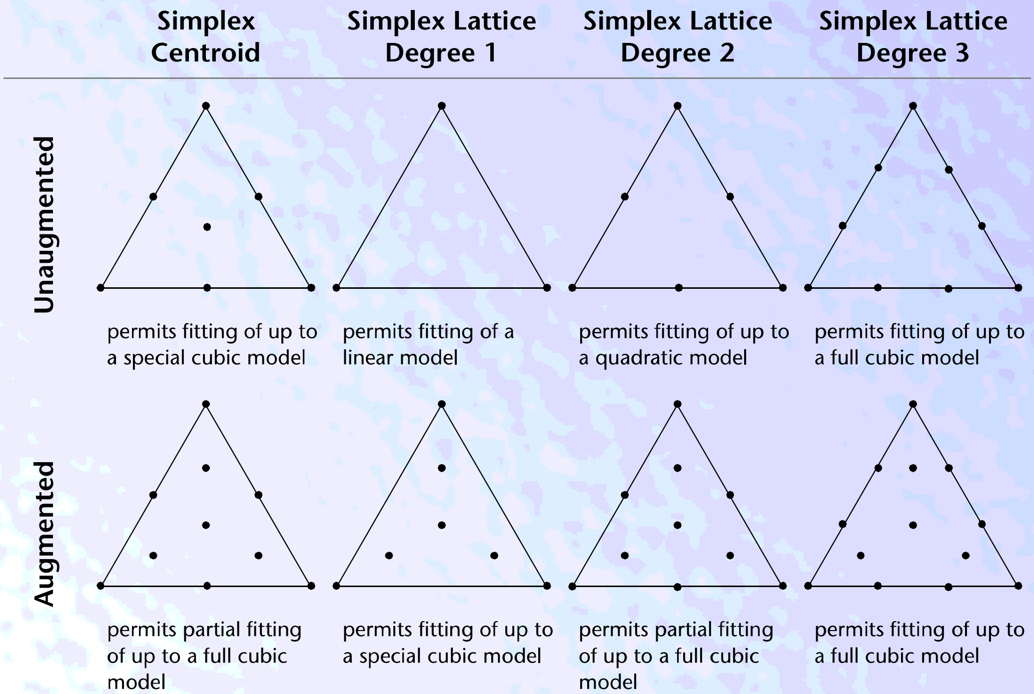
When you are choosing a design you need to

- identify the components, process variables, and mixture amounts that are of interest
- determine the model you want to fit—see *Selecting model terms* on page 21-41

- ensure adequate coverage of the region of interest on the response surface
- determine the impact that other considerations (such as cost, time, availability of facilities, or lower and upper bound constraints) have on your choice of a design

For a complete discussion of choosing a design, see [1].

To help you visualize a mixture design, the following illustrations show design points using triangular coordinates. Each point on the triangle represents a particular blend of components that you would use in your experiment. For simplicity, the illustrations show three component designs. The diagrams below only show a few of the mixture designs you can create. MINITAB can also create simplex lattice designs up to degree 10 and extreme vertices designs. For an explanation of triangular coordinates, see page 21-54.



Note When selecting a design, it is important to consider the maximum order of the fitted model required to adequately model the response surface. Mixture experiments frequently require a higher-order model than is initially planned. Therefore, it is usually a good idea, whenever possible, to perform additional runs beyond the minimum required to fit the model. For guidelines, see [1].

Creating Mixture Designs

You can create simplex centroid, simplex lattice, or extreme vertices designs.

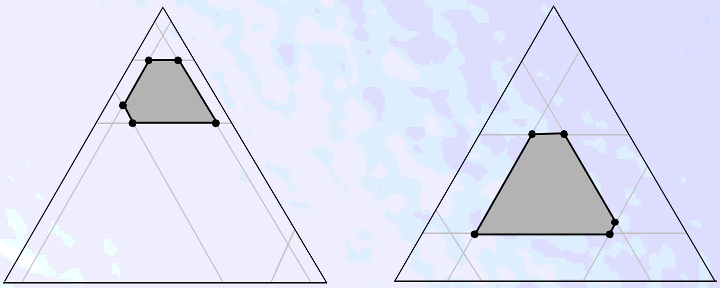
Simplex centroid and simplex lattice designs

In the simplex designs, the points are arranged in a uniform manner (or lattice) over an L-simplex. An L-simplex is similar to and has sides parallel to the 0□1 triangle shown on page 21-4.

For both simplex centroid and simplex lattice designs, you can add points to the interior of the design space. These points provide information on the interior of the response surface thereby improving coverage of the design space. See *Augmenting the design* on page 21-8.

Extreme vertices designs

In extreme vertices designs, MINITAB employs an algorithm that generates extreme vertices and their blends up to the specified degree. These designs must be used when your chosen design space is not an L-simplex. The presence of both lower and upper bound constraints on the components often create this condition. The goal of an extreme vertices design is to choose design points that adequately cover the design space. The illustration below shows the extreme vertices for two three-component designs with both upper and lower constraints:



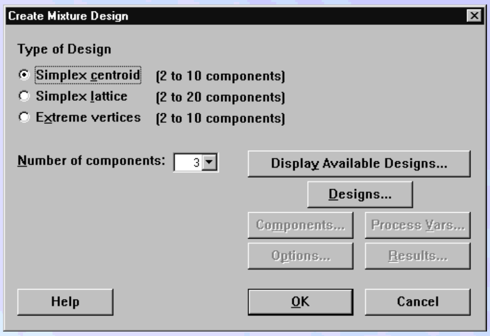
The light gray lines represent the lower and upper bound constraints on the components. The dark gray area represents the design space. The points are placed at the extreme vertices of design space.

More For a discussion of upper and lower bound constraints, see *Setting lower and upper bounds* on page 21-12.

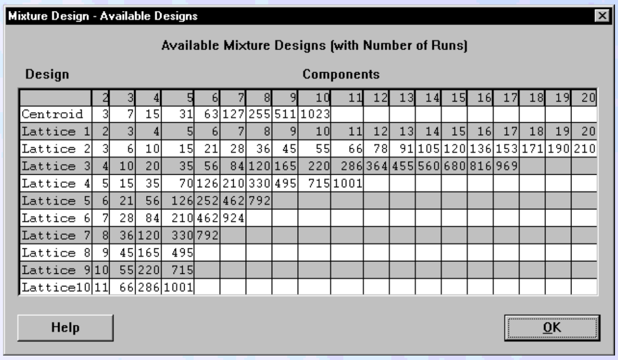
Note To create a design from data that you already have in the worksheet, see *Defining Custom Designs* on page 21-28.

▶ To create a mixture design

1 Choose **Stat ▸ DOE ▸ Mixture ▸ Create Mixture Design**.



2 If you want to see a summary of the simplex designs, click **Display Available Designs**. Use this table to compare design features. Click **OK**.


Mixture Design - Available Designs

Available Mixture Designs (with Number of Runs)

Design	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
Centroid	3	7	15	31	63	127	255	511	1023										
Lattice 1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
Lattice 2	3	6	10	15	21	28	36	45	55	66	78	91	105	120	136	153	171	190	210
Lattice 3	4	10	20	35	56	84	120	165	220	286	364	455	560	680	816	969			
Lattice 4	5	15	35	70	126	210	330	495	715	1001									
Lattice 5	6	21	56	126	252	462	792												
Lattice 6	7	28	84	210	462	924													
Lattice 7	8	36	120	330	792														
Lattice 8	9	45	165	495															
Lattice 9	10	55	220	715															
Lattice10	11	66	286	1001															

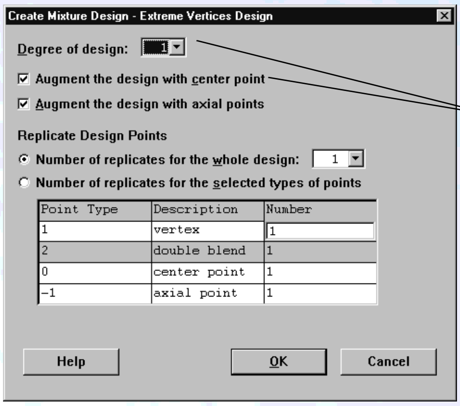
(Components: 2–20)

Help OK

3 Under **Type of Design**, choose **Simplex centroid**, **Simplex lattice**, or **Extreme vertices**.

4 From **Number of components**, choose a number.

5 Click **Designs**.



These two options are for simplex lattice and extreme vertices designs only.

6 If you like, use any of the options listed under *Design subdialog box* on page 21-7.

7 Click **OK** even if you do not change any of the options. This selects the design and brings you back to the main dialog box.

8 If you like, click **Components**, **Process Vars**, **Options**, or **Results** to use any of the options listed below, then click **OK** to create your design.

Options

Design subdialog box

- choose the degree of a simplex lattice or extreme vertices design—see *Choosing a Design* on page 21-3 and *Calculation of design points* on page 21-56
- add a center point (simplex lattice and extreme vertices designs only) or add axial points to the interior of the design (by default, MINITAB adds these points to the design)—see *Augmenting the design* on page 21-8
- replicate the design—see *Replicating the design* on page 21-9

Components subdialog box

- generate the design in units of the actual measurements rather than the proportions of the components—see *Generating the design in actual measurements* on page 21-10
- perform a mixture amounts experiment with up to five amount totals—see *Mixture-amounts designs* on page 21-11
- name components—see *Naming components* on page 21-12
- set lower and upper bounds for constrained designs—see *Setting lower and upper bounds* on page 21-12
- for extreme vertices designs, set linear constraints for the set of components—see *Setting linear constraints for extreme vertices designs* on page 21-13

Process variables subdialog box

- include up to seven process variables (factors) in your design—see *Mixture-process variable designs* on page 21-14
- specify the type of design (full or fractional factorial designs) and the fraction number to use for fractional factorial designs—see *Fractionating a mixture-process variable design* on page 21-15
- name the process variables—see *Naming process variables* on page 21-16
- set the high and low levels for the process variables—see *Setting process variable levels* on page 21-17

Options subdialog box

- randomize the design—see *Randomizing the design* on page 21-19

- store the design—see *Storing the design* on page 21-19
- store the design parameters (amounts, upper and lower bounds of the components, and linear constraints) in separate columns in the worksheet—see *Storing the design* on page 21-19

Results subdialog box

- display the following in the Session window:
  - no results
  - a summary of the design
  - the default results, which includes a detailed description of the design
  - the default results, plus the data table

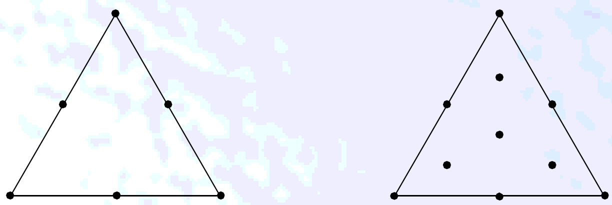
Augmenting the design

In order to adequately cover the response surface, you want to use a design that has interior points. By default, MINITAB augments a design by adding interior points to the design. MINITAB adds axial points and a center point if it is not already in the base design. Each of these additional points is a complete mixture—that is, a mixture in which all components are simultaneously present. A design with these interior points would provide information on the inner portion of the response surface and allow you to model more complicated curvature.

These points are primarily used to examine the lack-of-fit of a model. In addition, a design with these interior points would provide information on the inner portion of the response surface and allow you to model more complicated curvature.

Each axial point is added halfway between a vertex and the center of the design. See *Appendix for Mixture Designs* on page 21-54 and Help for details.

The illustrations below show the points that are added when you augment a second-degree three-component simplex lattice design with both axial points and a center point.



Unaugmented **Augmented**

To compare some other three-component designs, see the table under *Choosing a Design* on page 21-3. To view any design in MINITAB, use Simplex Design Plot.

Note If you do not want to augment your design, uncheck **Augment the design with a center point** and/or **Augment the design with axial points** in the Designs subdialog box.

Replicating the design

You can replicate your design in one of two ways. You can replicate

- the whole design up to 50 times
- only certain types of points as many times as you want

When you replicate the whole design, you duplicate the complete set of design points from the base design. The design points that would be added to a first-degree three-component simplex lattice design are as follows:

Base design			One replicate added (total of two replicates)			Two replicates added (total of three replicates)		
A	B	C	A	B	C	A	B	C
1	0	0	1	0	0	1	0	0
0	1	0	0	1	0	0	1	0
0	0	1	0	0	1	0	0	1
			1	**0**	**0**	**1**	**0**	**0**
			0	**1**	**0**	**0**	**1**	**0**
			0	**0**	**1**	**0**	**0**	**1**
						1	**0**	**0**
						0	**1**	**0**
						0	**0**	**1**

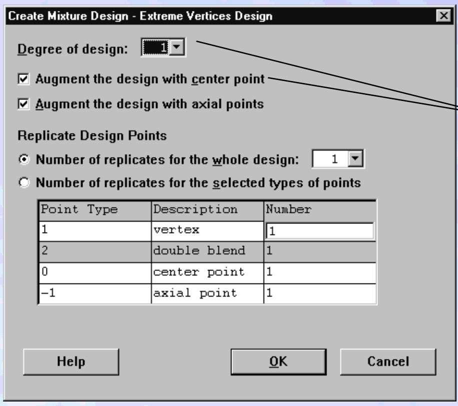
When you choose which types of points to replicate, you duplicate only the design points of the specified types of points from the base design. For example, the design points for a replicated second-degree three-component simplex lattice design are as follows:

Base design			One replicate of each vertex and two replicates of each double blend			Two replicates of each vertex and two replicates of each double blend		
A	B	C	A	B	C	A	B	C
1	0	0	1	0	0	1	0	0
.5	.5	0	.5	.5	0	.5	.5	0
.5	0	.5	.5	0	.5	.5	0	.5
0	1	0	0	1	0	0	1	0
0	.5	.5	0	.5	.5	0	.5	.5
0	0	1	0	0	1	0	0	1
			.5	**.5**	**0**	**1**	**0**	**0**
			.5	**0**	**.5**	**0**	**1**	**0**
			0	**.5**	**.5**	**0**	**0**	**1**
						.5	**.5**	**0**
						.5	**0**	**.5**
						0	**.5**	**.5**

True replication provides an estimate of the error or noise in your process and may allow for more precise estimates of effects.

▶ To replicate the design

1 In the Create Mixture Design dialog box, click **Designs**.



These two options are for simplex lattice and extreme vertices designs only.

1 Under **Replicate design points**, do one of the following:

- To replicate the entire base design, choose **Number of replicates for the whole design** and choose a number up to 50.
- To replicate only certain types of points, choose **Number of replicates for the selected types of points** and enter the number of replicates for each point type in the **Number** column of the table.

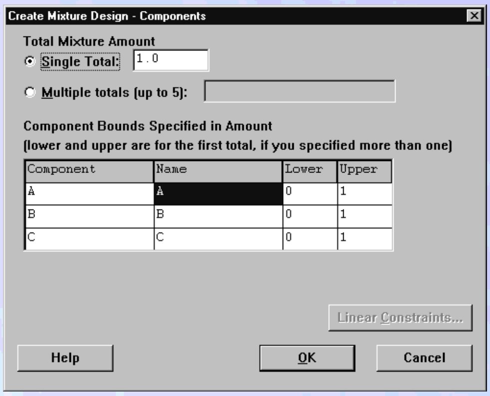
2 Click **OK**.

Generating the design in actual measurements

By default, MINITAB expresses the design points in terms of the proportions of all components, where the sum of the proportions is one. This is equivalent to an amount total equal to one.

▶ To express a design in actual measurements

1 In the Create Mixture Design dialog box, click **Components**.



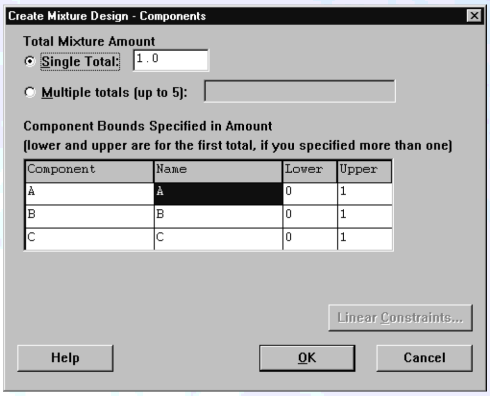
2 Under **Total Mixture Amount**, choose **Single total** and enter the sum of all the component measurements. Suppose you measure all the components of your mixture in liters. If the measurements add up to a total of 5.2 liters, you would enter 5.2. Click **OK**.

Mixture-amounts designs

In the simplest mixture experiment, the response is assumed to only depend on the proportions of the components in the mixture. In the mixture-amounts experiment, the response is assumed to depend on the proportions of the components *and* the amount of the mixture. For example, the amount applied *and* the proportions of the ingredients of a plant food may affect the growth of a house plant. When a mixture experiment is performed at two or more levels of the total mixture amount, it is called a *mixture-amounts experiment*.

▶ To create a mixture-amounts design

1 In the Create Mixture Design dialog box, click **Components**.



2 Under **Total Mixture Amount**, choose **Multiple totals** and enter up to five mixture totals. Suppose you are testing plant food and would like evaluate plant growth when one gram versus two grams of food are applied. You would enter *1 2*. Click **OK**.

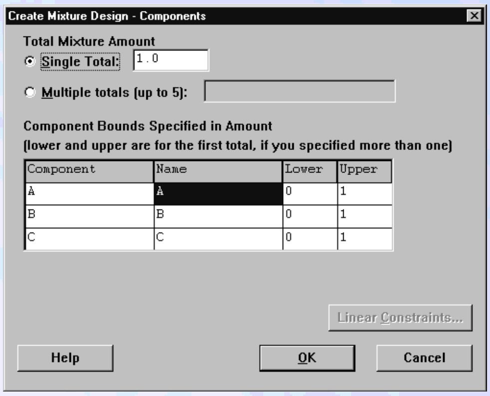
More | For a complete discussion of mixture-amounts experiments, see [1] and [2].

Naming components

By default, MINITAB names the components alphabetically, skipping the letter T.

▶ To name components

1 In the Create Mixture Design dialog box, click **Components**.



2 Under **Name**, click in the first row and type the name of the first component. Then, use the ↓ key to move down the column and enter the remaining names.

More | After you have created the design, you can change the component names by typing new names in the Data window, or with Modify Design (page 21-30).

Setting lower and upper bounds

By default, MINITAB generates settings for an unconstrained design, that is, the lower bound is zero and the upper bound is one for all the components. However, in some mixture experimentation, it is necessary to set a lower bound and/or an upper bound on some or all of the components.

- Lower bounds are necessary when any of the components must be present in the mixture. For example, lemonade must contain lemon juice.
- Upper bounds are necessary when the mixture cannot contain more than a given proportion of an ingredient. For example, a cake mix cannot contain more than 5% baking powder.

Constrained designs (those in which you specify lower or upper bounds) produce coefficients that are highly correlated. Generally, you can reduce the correlations among the coefficients by

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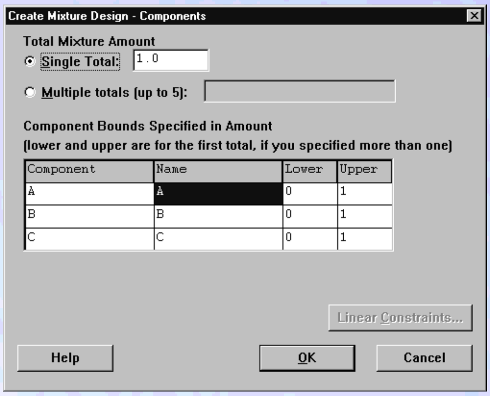
transforming the components to pseudocomponents. For information on displaying or analyzing the design in pseudocomponents, see *Specifying the units for components* on page 21-35 and *Analyzing Mixture Designs* on page 21-38. For a complete discussion, see [1] and [3].

▶ To set lower and upper bounds

1 In the Create Mixture Design dialog box, click **Components**.



2 Under **Lower**, click in the component row for which you want set a lower bound, and type a positive number.

Each lower bound must be less than the corresponding upper bound. The sum of the lower bounds for all the components must be less than the value of **Single total** or the first value in **Multiple totals**.

3 Use the → key to move to **Upper** and enter a positive number.

Each upper bound must be greater than the corresponding lower bound. Each upper bound must be less than the value of **Single total** or the first value in **Multiple totals**. The sum of the upper bounds for all the components must be greater than the value of **Single total** or the first value in **Multiple totals**.

4 Repeat steps 2 and 3 to assign bounds for other components. Click **OK**.

When you change the default lower or upper bounds of a component, the achievable bounds on the other components may need to be adjusted. See Help for calculations.

Setting linear constraints for extreme vertices designs

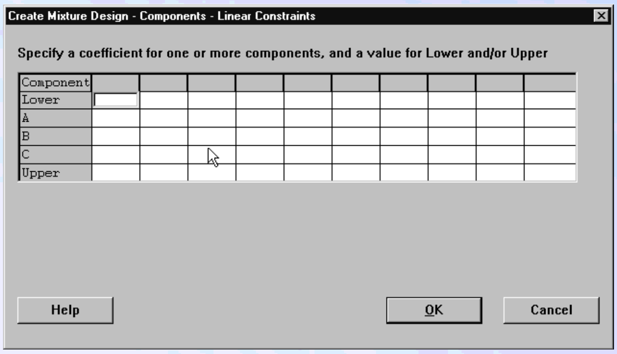
In addition to the individual bounds on the components, you may have up to ten linear constraints on the set of components. Suppose the wet ingredients (eggs, milk, oil) of a cake mix cannot be less 40% or greater than 60% of the total mixture. If you are willing to allow equal amounts of these three ingredients, the lower value is 0.4, the upper value is 0.6, and the component coefficients are all 1. Examples for a four-component blend are shown in the table below:

Condition	Lower Value	Coefficients A	B	C	D	Upper Value
A + B ≥ 10 and A + B ≤ 20	10	1	1			20
5A + 3B + 8D ≤ 0.1		5	3		8	0.1
0.5B + 0.8D ≥ 0.9	0.9		0.5	0.8		

▶ To set linear constraints for a set of components

1 In the Create Mixture Design dialog box, click **Components**.

2 Click **Linear Constraints**.



3 In the first column of the table, enter a coefficient for one or more of the components and a lower and/or upper value. Use the ↓ key to move down the column and enter desired values. The lower and upper values that you enter must be consistent with value of **Single total** or the first value in **Multiple totals**.

You must enter at least one coefficient and an upper or lower value. If you do not enter a coefficient for a component, MINITAB assumes it to be zero.

4 Repeat step 3 to enter up to ten different linear constraints on the set of components. Click **OK**.

Mixture-process variable designs

Process variables are factors in an experiment that are not part of the mixture but may affect the blending properties of the mixture. For example, the adhesive properties of a paint may depend on the temperature at which it is applied.

You can include up to seven two-level process variables in the mixture design. The process variables may be included as full or fractional factorial designs. The mixture design will be generated at each combination of levels of the process variables or at a fraction of the level combinations.

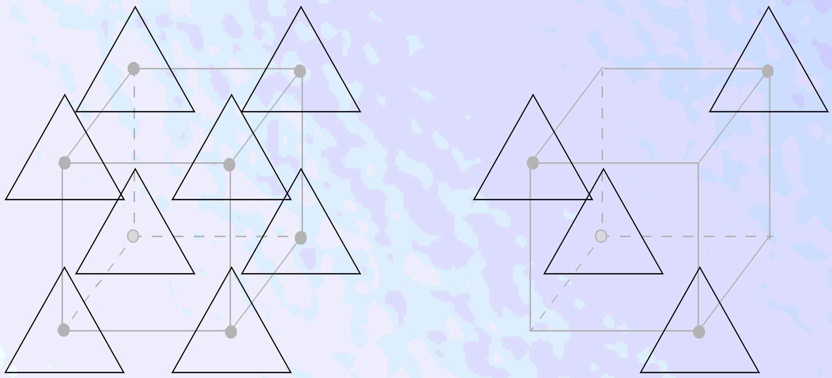
Fractionating a mixture-process variable design

When you generate a "complete" mixture-process variable design, the mixture design is generated at each combination of levels of the process variables. This may result in a prohibitive number of runs because the number of design points in the complete design increases quickly as the number of process variables increase. For example, a complete simplex centroid design with 3 mixture components and 2 process variables has 28 runs. The same 3-component design with three process variables has 56 runs; this design with 4 process variables has 112 runs.

Tip You can also use an optimal design to reduce the number of runs—see Chapter 22, *Optimal Designs*.

The illustrations below show a 3-component mixture with 3 process variables:

Full Factorial **½ Fraction**



Notice that the full factorial design contains twice as many design points as the ½ fraction design. The response is only measured at four of the possible eight corner points of the factorial portion of the design.

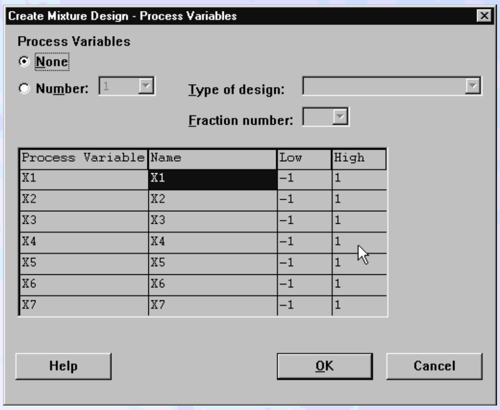
The types of factorial designs that are available depend on the number of process variables. Factorial design availability is summarized in the table below:

Number of process variables	Type of factorial design				
	full	1/2 fraction	1/4 fraction	1/8 fraction	1/16 fraction
one	▯				
two	▯				
three	▯	▯			

Number of process variables	Type of factorial design: full	1/2 fraction	1/4 fraction	1/8 fraction	1/16 fraction
four	▯	▯			
five	▯	▯	▯		
six	▯	▯	▯	▯	
seven	▯	▯	▯	▯	▯

▶ To add process variables to a design

1 In the Create Mixture Design dialog box, click **Process Vars**.



2 Under **Process Variables**, choose **Number**, then choose a value from 1 to 7.

3 From **Type of design**, choose a full or fractional factorial design. The available designs depend on the number of process variables chosen.

4 If you like, you can select the fraction number you want to use. By default, MINITAB uses the principal fraction. See *Choosing a fraction* on page 19-15.

5 If you like, you can name the process variables (described below) and set the process variable levels (described on page 21-17).

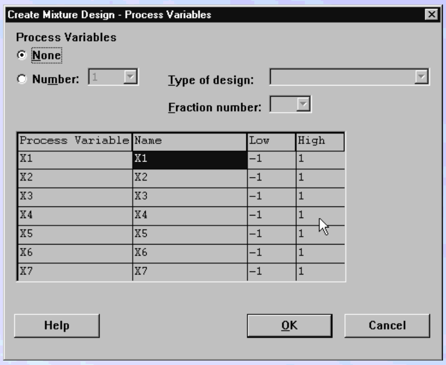
6 Click **OK**.

Naming process variables

By default, MINITAB names the process variables as X1,…,Xn, where n is the number of process variables.

▶ To name process variables

1 In the Create Mixture Design dialog box, click **Process Vars**.



2 Under **Name**, click in the first row and type the name of the first process variable. Then, use the ↓ key to move down the column and enter the remaining names.

3 Click **OK**.

More | After you have created the design, you can change the process variable names by typing new names in the Data window or with Modify Design (page 21-30).

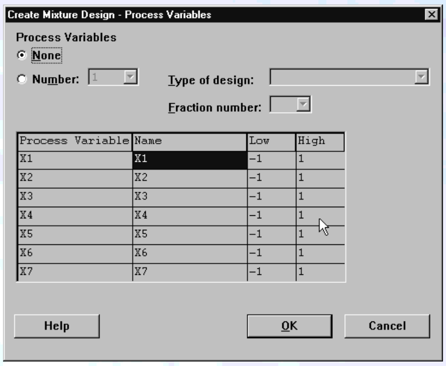
Setting process variable levels

You can enter process variable levels as numeric or text. If your process variables could be *continuous*, use numeric levels; if your process variables are *categorical*, use text levels. Continuous variables can take on any value on the measurement scale being used (for example, length of reaction time). In contrast, categorical variables can only assume a limited number of possible values (for example, type of catalyst).

By default, MINITAB sets the low level of all factors to □1 and the high level to +1.

▶ To assign process variable levels

1 In the Create Mixture Design dialog box, click **Process Vars**.



2 Under **Low**, click in the process variable row to which you would like to assign values and enter any value. Use the ⇥ key to move to **High** and enter a value. If you use numeric levels, the value you enter in **High** must be larger than the value you enter in **Low**.

3 Repeat step 2 to assign levels for other process variables. Click **OK**.

More To change the process variable levels after you have created the design, use **Stat ▸ DOE ▸ Modify Design**.

Randomizing the design

By default, MINITAB randomizes the run order of the design. The ordered sequence of the design points is called the *run order*. It is usually a good idea to randomize the run order to lessen the effects of factors that are not included in the study, particularly effects that are time-dependent.

However, there may be situations when randomization leads to an undesirable run order. For instance, in industrial applications, it may be difficult or expensive to change component levels. Or, after component levels have been changed, it may take a long time for the system to return to steady state. Under these conditions, you may not want to randomize the design in order to minimize the level changes.

Every time you create a design, MINITAB reserves and names C1 (StdOrder) and C2 (RunOrder) to store the standard order and run order, respectively.

- StdOrder shows what the order of the runs in the experiment would be if the experiment was done in standard order.
- RunOrder shows what the order of the runs in the experiment would be if the experiment was run in random order.

If you did not randomize, the run order and standard order are the same.

If you want to re-create a design with the same ordering of the runs (that is, the same design order), you can choose a base for the random data generator. Then, when you want to re-create the design, you just use the same base.

More You can use **Stat ➤ DOE ➤ Display Design** (page 21-35) to switch back and forth between a random and standard order display in the worksheet.

Storing the design

If you want to analyze a design, you *must* store it in the worksheet. By default, MINITAB stores the design. If you want to see the properties of various designs before selecting the design you want to store, uncheck **Store design in worksheet** in the Options subdialog box.

Every time you create a design, MINITAB reserves and names the following columns:

- C1 (StdOrder) stores the standard order.
- C2 (RunOrder) stores run order.
- C3 (PtType) stores a numerical representation of the type of design point.
- C4 (Blocks) stores the blocking variable. When a design is not blocked, as with mixture designs, MINITAB sets all column values to one.
- C5,…,$C_{number\ of\ components\ +\ 4}$ stores the components. MINITAB stores each component in your design in a separate column.
- In addition, depending on your design and storage options, MINITAB may store the following:

- each process variable in a separate column (named X1,…,Xn)
- an amount variable (named Amount)
- the design parameters (named Totals, Lower, Upper, Linear)

If you named the components or process variables, these names display in the worksheet. After you create the design, you can change the component names directly in the Data window or with **Stat ➤ DOE ➤ Modify Design** (page 21-30).

If you did not change the total for the mixture from the default value of one, MINITAB uses proportions to store your data. If you did change the total for the mixture, MINITAB uses amounts—what you actually measure—to express your data. After you create the design, you can specify one of three scales (described on page 21-35) to represent the data: amounts, proportions, or pseudocomponents. To change which of the three scales is displayed in the worksheet, use **Stat ➤ DOE ➤ Display Design** (page 21-35).

Caution When you create a design using Create Mixture Design, MINITAB stores the appropriate design information in the worksheet. MINITAB needs this stored information to analyze the data properly. If you want to use Analyze Mixture Design, you must follow certain rules when modifying the worksheet data. See *Modifying and Using Worksheet Data* on page 18-4.

If you make changes that corrupt your design, you may still be able to analyze it with Analyze Mixture Design after you use Define Custom Mixture Design (page 21-28).

▶ Example of a simplex centroid design

Suppose you want to study how the proportions of three ingredients in an herbal blend household deodorizer affect the acceptance of the product based on scent. The three components are neroli oil, rose oil, and tangerine oil.

1 Choose **Stat ➤ DOE ➤ Mixture ➤ Create Mixture Design**.

2 Under **Type of Design**, choose **Simplex centroid**.

3 From **Number of components**, choose 3.

4 Click **Designs**. Make sure **Augment the design with axial points** is checked. Click **OK**.

5 Click **Components**. In **Name**, enter *Neroli*, *Rose*, and *Tangerine* in rows 1 to 3, respectively. Click **OK**.

6 Click **Results**. Choose **Detailed description and data table**.

7 Click **OK** in each dialog box.

Session window output

Simplex Centroid Design

```
Components:         3     Design points:    10
Process variables: 0     Design degree:     3

Mixture total: 1

Number of Boundaries for Each Dimension

Point Type        1      2      0
Dimension         0      1      2
Number            3      3      1

Number of Design Points for Each Type

Point Type        1      2      3      0     -1
Distinct          3      3      0      1      3
Replicates        1      1      0      1      1
Total Number      3      3      0      1      3

Bounds of Mixture Components

               Amount              Proportion          Pseudocomponent
Comp      Lower     Upper     Lower     Upper     Lower     Upper
   A     0.0000    1.0000    0.0000    1.0000    0.0000    1.0000
   B     0.0000    1.0000    0.0000    1.0000    0.0000    1.0000
   C     0.0000    1.0000    0.0000    1.0000    0.0000    1.0000

Data Matrix (randomized)

   Run  Type          A          B          C
     1    -1     0.1667     0.1667     0.6667
     2    -1     0.6667     0.1667     0.1667
     3     2     0.5000     0.5000     0.0000
     4     2     0.5000     0.0000     0.5000
     5    -1     0.1667     0.6667     0.1667
     6     2     0.0000     0.5000     0.5000
     7     1     0.0000     0.0000     1.0000
     8     1     0.0000     1.0000     0.0000
     9     0     0.3333     0.3333     0.3333
    10     1     1.0000     0.0000     0.0000
```

Interpreting the results

MINITAB creates an augmented three-component simplex centroid design. The base design provides seven runs; augmentation adds three runs for a total of ten runs.

Because you chose to display the detailed description and data tables, MINITAB shows the component proportions you will use to create ten blends of your mixture. When you perform the experiment, use the blends in the run order that is shown. (Because you did not change the mixture total from the default of one, MINITAB expresses each component in proportions.) For example, the first blend you will test will be made up of equal amounts of neroli (0.1667) and rose oils (0.1667), and tangerine oil will make up the remaining 0.6667.

Note MINITAB randomizes the design by default, so if you try to replicate this example, your runs may not match the order shown.

▶ Example of an extreme vertices design

Suppose you need to determine the proportions of flour, milk, baking powder, eggs, and oil in a pancake mix that would produce an optimal product based on taste. Because previous experimentation suggests that a mix that does not contain all of the ingredients or has too much baking powder will not meet the taste requirements, you decide to constrain the design by setting lower bounds and upper bounds.

You decide that quadratic model will sufficiently model the response surface, so you decide to create a second-degree design.

1 Choose **Stat** ▸ **DOE** ▸ **Mixture** ▸ **Create Mixture Design**.

2 Under **Type of Design**, choose **Extreme vertices**.

3 From **Number of components**, choose 5.

4 Click **Designs**. From **Degree of design**, choose 2.

5 Make sure **Augment the design with center point** and **Augment the design with axial points** are checked. Click **OK**.

6 Click **Components**. Complete the **Name**, **Lower**, and **Upper** columns of the table as shown below, then click **OK**.

Component	Name	Lower	Upper
A	Flour	.425	1
B	Milk	.30	1
C	Baking powder	.025	.05
D	Eggs	.10	1
E	Oil	.10	1

7 Click **Results**. Choose **Detailed description and data table**. Click **OK** in each dialog box.

Session window output

Extreme Vertices Design

```
Components:         5     Design points:    33
Process variables: 0     Design degree:     2

Mixture total: 1

Number of Boundaries for Each Dimension

Point Type         1      2      3      4      0
Dimension          0      1      2      3      4
Number             8     16     14      6      1

Number of Design Points for Each Type

Point Type         1      2      3      4      5      0     -1
Distinct           8     16      0      0      0      1      8
Replicates         1      1      0      0      0      1      1
Total Number       8     16      0      0      0      1      8

Bounds of Mixture Components

               Amount               Proportion          Pseudocomponent
Comp       Lower      Upper      Lower      Upper      Lower      Upper
   A    0.425000   0.475000   0.425000   0.475000   0.000000   1.000000
   B    0.300000   0.350000   0.300000   0.350000   0.000000   1.000000
   C    0.025000   0.050000   0.025000   0.050000   0.000000   0.500000
   D    0.100000   0.150000   0.100000   0.150000   0.000000   1.000000
   E    0.100000   0.150000   0.100000   0.150000   0.000000   1.000000

* NOTE * Bounds were adjusted to accommodate specified constraints.

Data Matrix (randomized)

   Run  Type          A          B          C          D          E
     1     2   0.462500   0.300000   0.037500   0.100000   0.100000
     2    -1   0.429687   0.304688   0.043750   0.104688   0.117188
     3     2   0.425000   0.300000   0.037500   0.100000   0.137500
     4    -1   0.454687   0.304688   0.031250   0.104688   0.104688
     5     2   0.425000   0.300000   0.037500   0.137500   0.100000
     6     1   0.475000   0.300000   0.025000   0.100000   0.100000
     7     2   0.425000   0.312500   0.050000   0.112500   0.100000
     8    -1   0.429687   0.304688   0.031250   0.129688   0.104688
     9     2   0.437500   0.312500   0.050000   0.100000   0.100000
    10     2   0.450000   0.300000   0.025000   0.100000   0.125000
    11     2   0.437500   0.300000   0.050000   0.112500   0.100000
    12     2   0.425000   0.325000   0.025000   0.125000   0.100000
    13    -1   0.429687   0.304688   0.043750   0.117188   0.104688
    14     1   0.425000   0.300000   0.025000   0.150000   0.100000
    15     2   0.450000   0.325000   0.025000   0.100000   0.100000
    16    -1   0.429687   0.304688   0.031250   0.104688   0.129688
    17    -1   0.429687   0.317188   0.043750   0.104688   0.104688
    18     1   0.425000   0.300000   0.025000   0.100000   0.150000
    19     1   0.425000   0.350000   0.025000   0.100000   0.100000
    20    -1   0.442187   0.304688   0.043750   0.104688   0.104688
```

21	-1	0.429687	0.329687	0.031250	0.104688	0.104688
22	0	0.434375	0.309375	0.037500	0.109375	0.109375
23	2	0.425000	0.337500	0.037500	0.100000	0.100000
24	2	0.437500	0.300000	0.050000	0.100000	0.112500
25	2	0.425000	0.325000	0.025000	0.100000	0.125000
26	2	0.425000	0.312500	0.050000	0.100000	0.112500
27	2	0.425000	0.300000	0.025000	0.125000	0.125000
28	1	0.425000	0.300000	0.050000	0.100000	0.125000
29	1	0.425000	0.325000	0.050000	0.100000	0.100000
30	2	0.450000	0.300000	0.025000	0.125000	0.100000
31	1	0.450000	0.300000	0.050000	0.100000	0.100000
32	2	0.425000	0.300000	0.050000	0.112500	0.112500
33	1	0.425000	0.300000	0.050000	0.125000	0.100000

Interpreting the results

MINITAB creates an augmented five-component extreme vertices design. The base design provides 24 design points; augmentation adds 9 design points for a total of 33 runs. Augmenting this design adds 8 axial points and 1 center point to the design.

Because you chose to display the summary and data tables, MINITAB shows the component proportions you will use to create 33 blends of your mixture. When you perform the experiment, use the blends in the run order that is shown. (Because you did not change the mixture total from the default of one, MINITAB expresses each component in proportions.)

Note MINITAB randomizes the design by default, so if you try to replicate this example, your runs may not match the order shown.

Displaying Simplex Design Plots

You can use a simplex design plot to visualize the mixture design space (or a slice of the design space if you have more than three components). MINITAB plots the design points on triangular axes. You can plot the following:

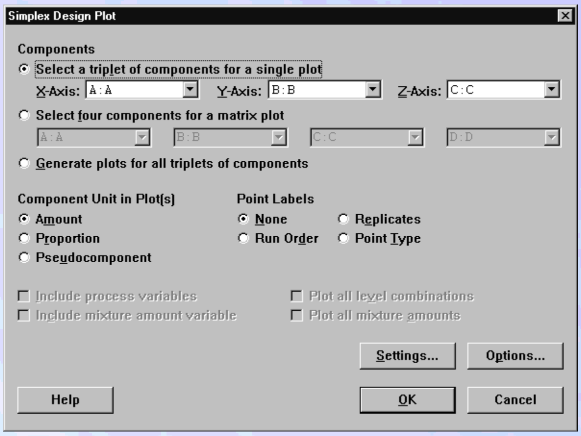
- components only
- components and process variables
- components and an amount variable

Data

You must create and store a design using Create Mixture Design.

▶ To display a simplex design plot

1 Choose **Stat ➤ DOE ➤ Mixture ➤ Simplex Design Plot**.



2 Do one of the following to select the number of plots to display:

- To display a single simplex design plot for any three components, choose **Select a triplet of components for a single plot**. Then, choose any three components that are in your design.
- To display a layout with four simplex design plots (each plot displays three components), choose **Select four components for a matrix plot**. Then, choose any four components that are in your design.
- To display a simplex design plot for all combinations of components, each in a separate window, choose **Generate plots for all triplets of components**.

3 If you like, use any of the options listed below, then click **OK**.

Options

Simplex Design Plot dialog box

- display four simplex design plots in a single page layout
- generate plots for all triplets of components
- display the plot in amounts, proportions, or pseudocomponents
- use the run order, number of replicates, or point type for design point labels on the plot
- include process variables, and for a single simplex design plot include all the levels of the process variables in a single layout
- include an amount variable (by default, MINITAB will plot the amount variable at its first defined value), and for a single simplex design plot include all the levels of the amount variable in a single layout

Settings subdialog box

- specify values for design variables that are not included in the plot—see *Settings for extra components, process variables, and an amount variable* below

Options subdialog box

- define minimum and maximum values for the x-axis, y-axis, and z-axis
- define the background grid or suppress grid lines
- replace the default title with your own title

Settings for extra components, process variables, and an amount variable

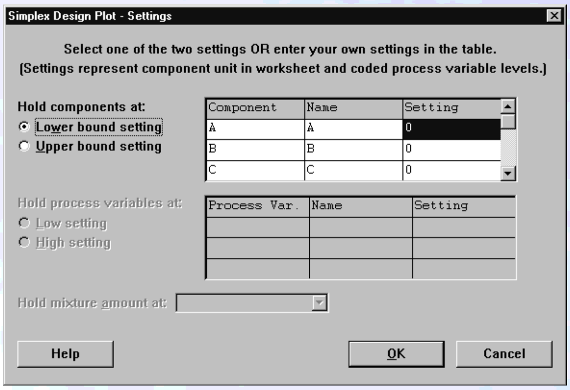
You can set the holding level for components and process variables that are not in the plot at their highest or lowest settings, or you can set specific levels to hold each. For an amount variable, you can set the hold value at any of the totals. The hold values must be expressed in the following units:

- components in the *units displayed in the worksheet*
- process variables in *coded units*

Note If you have text process variables in your design, you can only set their holding values at one of the text levels.

▶ To set the holding level for design variables not in the plot

1 In the Simplex Design Plot dialog box, click **Settings**.



2 Do one or more of the following to set the holding values:

- For components (only available for design with more than three components):

- To use the preset values for components, choose **Lower bound setting** or **Upper bound setting** under **Hold components at**. When you use a preset value, *all* components not in the plot will be held at their lower bound or upper bound.
- To specify the value at which to hold the components, enter a number in **Setting** for each component that you want to control. This option allows you to set a different holding value for each component.

- For process variables:
  - To use the preset values for process variables, choose **High setting** or **Low setting** under **Hold process variables at**. When you use a preset value, *all* variables not in the plot will be held at their high or low settings.
  - To specify the value at which to hold the process variables, enter a number in **Setting** for each of the process variables you want to control. This option allows you to set a different holding value for each process variable.

- For an amount variable:
  - In **Hold mixture amount at**, choose one of the mixture totals. MINITAB displays the multiple totals that you entered in the Components subdialog box when you were creating the design.

3 Click **OK**.

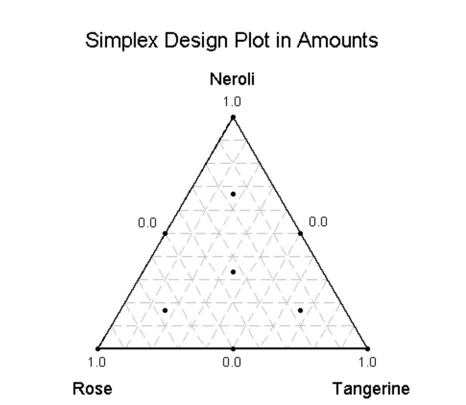
▶ Example of simplex design plot

In the *Example of a simplex centroid design* on page 21-20, you created a design to study how the proportions of three ingredients in an herbal blend household deodorizer affect the acceptance of the product based on scent. The three components are neroli oil, rose oil, and tangerine oil. To help you visualize the design space, you want to display a simplex design plot.

1 Open the worksheet DEODORIZ.MTW.

2 Choose **Stat** ▶ **DOE** ▶ **Mixture** ▶ **Simplex Design Plot**. Click **OK**.

Graph window output



Interpreting the results

The simplex design plot shows that there are ten points in the design space. The points are as follows:

- three pure mixtures, one for each component (Neroli, Rose, and Tangerine). These points are found at the vertices of the triangle.
- three binary blends, one for each possible two-component blend (Neroli-Rose, Rose-Tangerine, and Tangerine-Neroli). These design points are found at the midpoint of each edge of the triangle.
- three complete blends. All three components are included in these blends, but not in equal proportions.
- one center point (or centroid). Equal proportions of all three components are included in this blend.

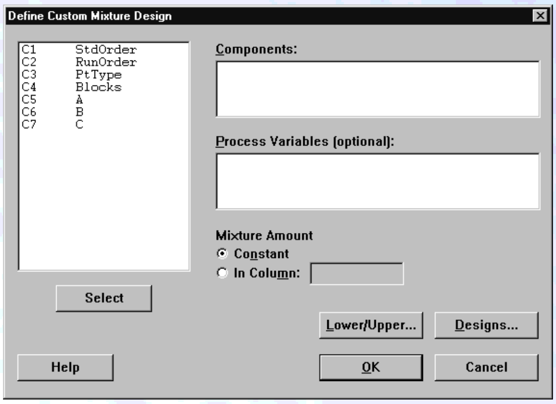
Defining Custom Designs

Use Define Custom Mixture Design to create a design from data you already have in the worksheet. For example, you may have a design that you created using MINITAB session commands, entered directly into the Data window, imported from a data file, or created with earlier releases of MINITAB. You can also use Define Custom Mixture Design to redefine a design that you created with Create Mixture Design and then modified directly in the worksheet.

Custom designs allow you to specify which columns contain your components and other design characteristics. After you define your design, you can use Modify Design (page 21-30), Display Design (page 21-35), and Analyze Mixture Design (page 21-38).

▶ To define a custom mixture design

1 Choose **Stat > DOE > Mixture > Define Custom Mixture Design**.

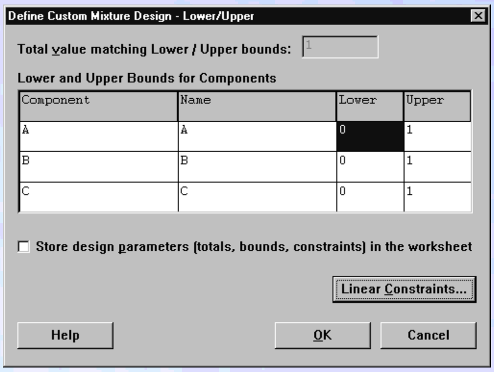


2 In **Components**, enter the columns that contain the component data. Data must be in the form of amounts. (When the mixture total is one, amounts and proportions are equivalent.) For information the data units, see *Mixture-amounts designs* on page 21-11 and *Specifying the units for components* on page 21-35.

3 If you have process variables in your design, enter the columns in **Process variables**.

4 If you have an amount variable, under **Mixture Amount**, choose **In column**, and enter the column that contains the amount data.

5 Click **Lower/Upper**.



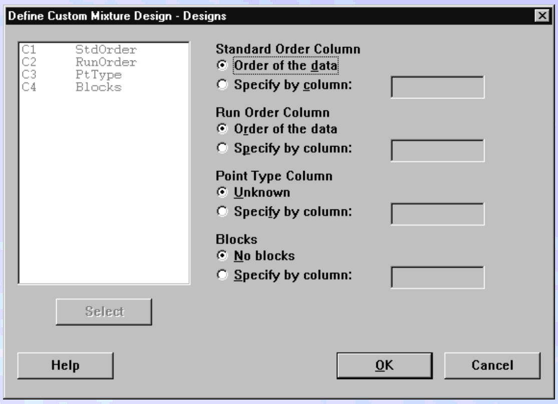
6 If you have an mixture-amounts experiment, MINITAB will enter the smallest value in your amount column in **Total value matching Lower/Upper bounds**. If this is not the value you want, change it to any other total in your amount column.

7 MINITAB will fill in the lower and upper bound table from the worksheet. Make any necessary corrections, then click **OK**.

8 Do one of the following:

- If you do not have any columns containing the standard order, run order, point type, or blocks, click **OK**.

- If you have columns that contain data for the standard order, run order, point type, or blocks, click **Designs**.



1. If you have a column that contains the standard order of the experiment, under **Standard Order Column**, choose **Specify by column** and enter the column containing the standard order.
2. If you have a column that contains the run order of the experiment, under **Run Order Column**, choose **Specify by column** and enter the column containing the run order.
3. If you have a column that contains the design point type, under **Point Type Column**, choose **Specify by column** and enter the column containing the point types.
4. If your design is blocked, under **Blocks**, choose **Specify by column** and enter the column containing the blocks.
5. Click **OK** in each dialog box.

Options

Lower/Upper subdialog box

- store the design parameters (amounts, upper and lower bounds of the components, and linear constraints) in separate columns in the worksheet—see *Storing the design* on page 21-19
- set one or more linear constraints for the set of components—see *Setting linear constraints for extreme vertices designs* on page 21-13

Modifying Designs

After creating a design and storing it in the worksheet, you can use Modify Design to make the following modifications:

- rename the components (below)

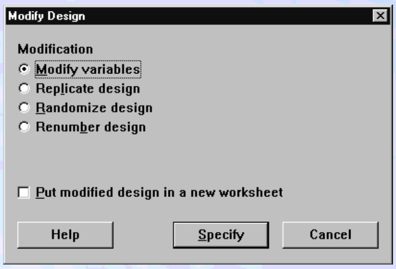
- rename process variables and change levels (page 21-32)
- replicate the design (page 21-33)
- randomize the design (page 21-33)
- renumber the design (page 21-34)

By default, MINITAB will replace the current design with the modified design in the worksheet. To store the modified design in a new worksheet, check **Put modified design in a new worksheet**.

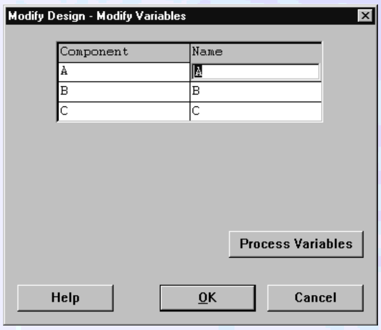
Renaming components

▶ To rename components

1 Choose **Stat > DOE > Modify Design**.



2 Choose **Modify variables** and click **Specify**.



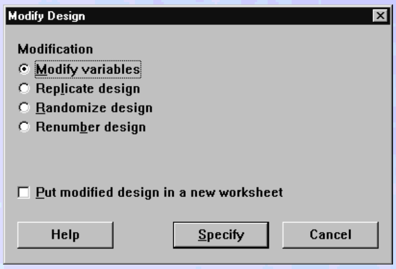
3 Under **Name**, click in the first row and type the name of the first component. Then, use the ↓ key to move down the column and enter the remaining names. Click **OK**.

Tip You can also type new component or process variable names directly into the Data window.

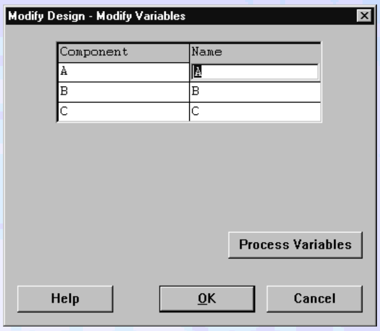
Renaming process variables or changing levels

▶ To rename process variables or change levels

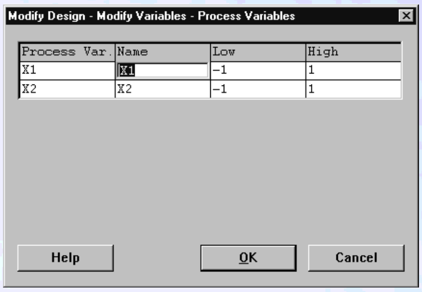
1 Choose **Stat ▯ DOE ▯ Modify Design**.



2 Choose **Modify variables** and click **Specify**.



3 Click **Process Variables**.



4 Do one or both of the following:

- Under **Name**, click in the first row and type the name of the first process variable. Then, use the [↓] key to move down the column and name the remaining process variables.
- Under **Low**, click in the process variable row you would like to assign values and enter any numeric or text value. Use the [→] key to move to **High** and enter a value. For numeric levels, the **High** value must be larger than **Low** value.

  Repeat to assign levels for other factors.

5 Click **OK**.

Tip You can also type new component or process variable names directly into the Data window.

Replicating the design

You can add up to ten replicates of your design. When you replicate a design, you duplicate the complete set of runs from the initial design. The runs that would be added to a three-component simplex lattice design are as follows:

Initial design	One replicate added (total of two replicates)	Two replicates added (total of three replicates)
A B C	A B C	A B C
1 0 0	1 0 0	1 0 0
0 1 0	0 1 0	0 1 0
0 0 1	0 0 1	0 0 1
	1 0 0	**1 0 0**
	0 1 0	**0 1 0**
	0 0 1	**0 0 1**
		1 0 0
		0 1 0
		0 0 1

True replication provides an estimate of the error or noise in your process and may allow for more precise estimates of effects.

▶ To replicate the design

1 Choose **Stat ▯ DOE ▯ Modify Design**.

2 Choose **Replicate design** and click **Specify**.

3 From **Number of replicates to add**, choose a number up to ten. Click **OK**.

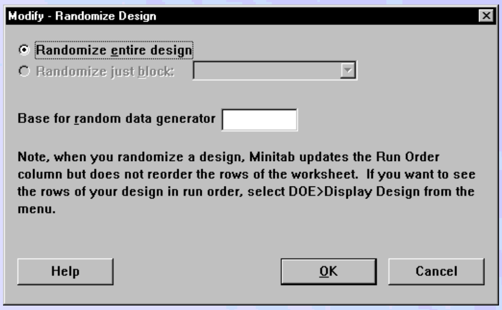
Randomizing the design

You can randomize the entire design or just randomize one of the blocks. For a general discussion of randomization, see page 21-19.

▶ To randomize the design

1 Choose **Stat ▯ DOE ▯ Modify Design**.

2 Choose **Randomize design** and click **Specify**.



3 Do one of the following:

- Choose **Randomize entire design**.
- Choose **Randomize just block**, and choose a block number from the list. (Mixture designs are not usually blocked.)

4 If you like, in **Base for random data generator**, enter a number. Click **OK**.

More You can use **Stat > DOE > Display Design** (page 21-35) to switch back and forth between a random and standard order display in the worksheet.

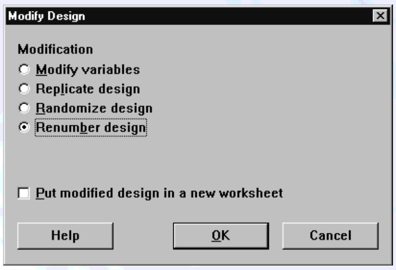
Renumbering the design

You can renumber the design. MINITAB will renumber the RunOrder column based on the order of design points in the worksheet. This is especially useful if you have selected an optimal design (see Chapter 22, *Optimal Designs*) and you would like to renumber the design to determine an order in which to perform the experiment.

▶ To renumber the design

1 Choose **Stat > DOE > Modify Design**.

2 Choose **Renumber design** and click **OK**.



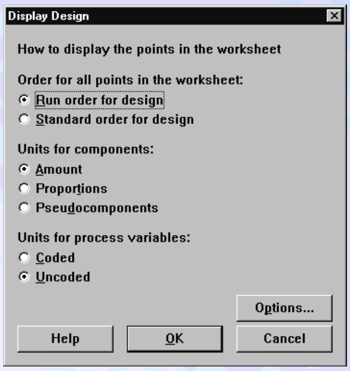
Displaying Designs

After you create a design, you can use Display Design to change the way the design points are stored in the worksheet. You can change the design points in two ways:

- display the points in either random and standard order. Run order is the order of the runs if the experiment was done in random order.
- express the components in amounts, proportions, or pseudocomponents.
- express process variables in coded or uncoded units.

▶ To change the display order of points in the worksheet

1 Choose **Stat > DOE > Display Design**.



2 Choose **Run order for the design** or **Standard order for the design**. If you do not randomize a design, the columns that contain the standard order and run order are the same.

3 Do one of the following:

- If you want to reorder all worksheet columns that are the same length as the design columns, click **OK**.
- If you have worksheet columns that you do not want to reorder:
  1 Click **Options**.
  2 In **Exclude the following columns when sorting**, enter the columns. These columns *cannot* be part of the design. Click **OK** in each dialog box.

Specifying the units for components

If you did not change the total for the mixture from the default value of one, MINITAB uses proportions to store your data. (This is equivalent to an amount total equal to one.) If you did change the total for the mixture, MINITAB uses amounts—what you actually measure—to express your data. Depending on the mixture total and the presence of constraints, you may want to represent the design in another scale.

You can choose one of three scales to represent the design: amounts, proportions, or pseudocomponents. With certain combinations of the mixture total and lower bound constraints, the various scalings are equivalent as shown in the following table:

Total mixture	Lower bounds	Equivalent scales
equal to 1	0	amounts proportions pseudocomponents
equal to 1	greater than 0	amounts proportions
not equal to 1	0	proportions pseudocomponents
not equal to 1	greater than 0	none

▶ To change the units for the components

1 Choose **Stat ▸ DOE ▸ Display Design**.

2 Choose **Amount**, **Proportions**, or **Pseudocomponents**. Click **OK**.

Pseudocomponents

Constrained designs (those in which you specify lower or upper bounds) produce coefficients which are highly correlated.

- Lower bounds are necessary when any of the components must be present in the mixture. For example, lemonade must contain lemon juice.
- Upper bounds are necessary when the mixture cannot contain more than a given proportion of an ingredient. For example, a cake mix cannot contain more than 5% baking powder.

Generally, you can reduce the correlations among the coefficients by transforming the components to pseudocomponents. For a complete discussion, see [1] and [3].

Pseudocomponents, in effect, rescale the constrained data area so the minimum allowable amount (the lower bound) of each component is zero. This makes a constrained design in pseudocomponents the same as an unconstrained design in proportions.

The table below shows two components expressed in amounts, proportions, and pseudocomponents. Suppose the total mixture is 50 ml. Let X1 and X2 be the amount scale.

Thus X1 + X2 = 50. Suppose X1 has a lower bound of 20 (this means that the upper bound of X2 is 50 minus 20, or 30). Here are some points on the three scales:

Amounts		Proportions		Pseudocomponents	
X1	X2	X1	X2	X1	X2
50	0	1.0	0.0	1.0	0.0
20	30	0.4	0.6	0.0	1.0
35	15	0.7	0.3	0.5	0.5

Collecting and Entering Data

After you create your design, you need to perform the experiment and collect the response (measurement) data. To print a data collection form, follow the instructions below. After you collect the response data, enter the data in any worksheet column not used for the design. For a discussion of worksheet structure, see *Storing the design* on page 21-19.

Printing a data collection form

You can generate a data collection form in two ways. You can simply print the Data window contents, or you can use a macro. A macro can generate a "nicer" data collection form—see Help for more information. Although printing the Data window will not produce the prettiest form, it is the easiest method. Just follow these steps:

1 When you create your experimental design, MINITAB stores the run order, components, process variables, and amount variable in the worksheet. These columns constitute the basis of your data collection form. If you did not name components or process variables when you created the design, and you want names on the form, use Modify Design (page 21-30).

2 In the worksheet, name the columns in which you will record the measurement data obtained when you perform your experiment.

3 Choose **File ▸ Print Worksheet**. Make sure **Print Grid Lines** is checked. Click **OK**.

More You can also copy the worksheet cells to the Clipboard by choosing **Edit ▸ Copy Cells**. Then paste the Clipboard contents into a word-processing application, such as Microsoft WordPad or Microsoft Word, where you can create your own form.

Analyzing Mixture Designs

To use Analyze Mixture Design, you must first create and store the design using Create Mixture Design, or create a design from data that you already have in the worksheet with Define Custom Mixture Design.

You can choose from six standard models (linear, quadratic, special cubic, full cubic, special quartic, or full quartic) or choose specific terms from a list of all estimable terms. See *Selecting model terms* on page 21-41 for details.

You can also select from four model fitting methods:

- mixture regression
- stepwise regression
- forward selection
- backward elimination

Data

Enter numeric response data column(s) that are equal in length to the design variables in the worksheet. Each row in the worksheet will contain the data for one run of your experiment. You may enter the response data in any columns not occupied by the design data. The number of columns reserved for the design data is dependent on the number of components in your design and whether or not you chose to store the design parameters (see *Storing the design* on page 21-19).

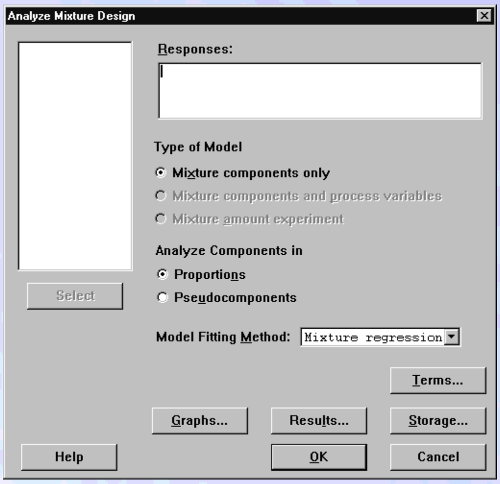
If there is more than one response variable, MINITAB fits separate models for each response.

MINITAB omits the rows containing missing data from all calculations.

Note When all the response variables do not have the same missing value pattern, MINITAB displays a message. When the responses do not have the same missing value pattern, you may want to perform the analysis separately for each response because you would get different results than if you included them all in a single analysis.

▶ To fit a mixture model

1 Choose **Stat > DOE > Mixture > Analyze Mixture Design**.



2 In **Responses**, enter up to 25 columns that contain the measurement data.

3 If you like, use any of the options listed below, then click **OK**.

Options

Analyze Mixture Design dialog box

- fit a model for mixture components only (default), or include process variables or amounts in the model. See *Mixture-amounts designs* on page 21-11 and *Mixture-process variable designs* on page 21-14 for more information.
- fit the model with the components expressed as proportions or pseudocomponents.
- choose from four model fitting methods: mixture regression (default), stepwise regression, forward selection, backward elimination.

Graphs subdialog box

- draw five different residual plots for regular, standardized, or deleted residuals—see *Choosing a residual type* on page 2-5. Available residual plots include a:
  – histogram.
  – normal probability plot.
  – plot of residuals versus the fitted values ($\hat{Y}$).
  – plot of residuals versus data order. The row number for each data point is shown on the x-axis (for example, 1 2 3 4… *n*).
  – separate plot for the residuals versus each specified column.

  For a discussion, see *Residual plots* on page 2-5.

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Terms subdialog box

- fit a model by specifying the maximum order of the terms, or choose which terms to include from a list of all estimable terms—see *Selecting model terms* on page 21-41.
- include inverse component terms, process variable terms, or an amount term in the model. You cannot include inverse terms if the lower bound for any component is zero or if you choose to analyze the design in pseudocomponents.

Options subdialog box

- If you choose the stepwise model fitting method, you can
  - designate a set of predictor variables that *cannot* be removed from the model, even when their p-values are less than α to enter.
  - specify a starting set of predictor variables. These variables *are* removed if their p-values are greater than α to enter.
  - set the α-value for entering a new variable in the model.
  - set the α-value for removing a variable from the model.
- If you choose the forward selection model fitting method, you can
  - designate a set of predictor variables that *cannot* be removed from the model, even when their p-values are less than α to enter.
  - set the α-value for entering a new variable in the model.
- If you choose the backward elimination model fitting method, you can
  - designate a set of predictor variables that *cannot* be removed from the model, even when their p-values are less than α to enter.
  - set the α-value for removing a variable from the model.
- display the next best alternate predictors up to the number requested. If a new predictor is entered into the model, MINITAB displays the predictor which was the second best choice, the third best choice, and so on, up to the requested number.

Results subdialog box

- display the following in the Session window:
  - no results
  - model selection information, a table of coefficients, and the analysis of variance table
  - the default results, which includes model selection information, a table of coefficients, the analysis of variance table, and the unusual values in the table of fits and residuals
  - the default results, plus a table of all fits and residuals

Storage subdialog box

- store the fits, and regular, standardized, and deleted residuals separately for each response—see *Choosing a residual type* on page 2-5.
- store the coefficients for the model, the design matrix, and model terms separately for each response. The design matrix multiplied by the coefficients will yield the fitted values. Since

Analyze Mixture Design does not allow a constant in the model, the design matrix does not contain a column of ones.

- store the leverages, Cook's distances, and DFITS, for identifying outliers—see *Identifying outliers* on page 2-9.

Selecting model terms

The model terms that are available depend on the type of mixture design. You can fit a model to a simple mixture design (components only), a mixture-process variable design (components and process variables), or a mixture-amounts design (components and amounts).

The order of the model you choose determines which terms are fit and whether or not you can model linear or curvilinear aspects of the response surface.

In the Terms subdialog box, you can choose a linear, quadratic, special cubic, full cubic model, special quartic, or full quartic model. Or, you can fit a model that is a subset of these terms. The following table summarizes these models. For a discussion of the various blending effects you can model, see [1].

This model type	fits these terms	and models this type of blending
linear (first-order)	linear	additive
quadratic (second-order)	linear and quadratic	additive nonlinear synergistic binary *or* additive nonlinear antagonistic binary
special cubic (third-order)	linear, quadratic, and special cubic	additive nonlinear synergistic ternary nonlinear antagonistic ternary
full cubic (third-order)	linear, quadratic, special cubic, and full cubic	additive nonlinear synergistic binary nonlinear antagonistic binary nonlinear synergistic ternary nonlinear antagonistic ternary
special quartic (fourth-order)	linear, quadratic, special cubic, full cubic, and special quartic	additive nonlinear synergistic binary nonlinear antagonistic binary nonlinear synergistic ternary nonlinear antagonistic ternary nonlinear synergistic quaternary nonlinear antagonistic quaternary

This model type	fits these terms	and models this type of blending
full quartic (fourth-order)	linear, quadratic, special cubic, full cubic, special quartic, and full quartic	additive nonlinear synergistic binary nonlinear antagonistic binary nonlinear synergistic ternary nonlinear antagonistic ternary nonlinear synergistic quaternary nonlinear antagonistic quaternary

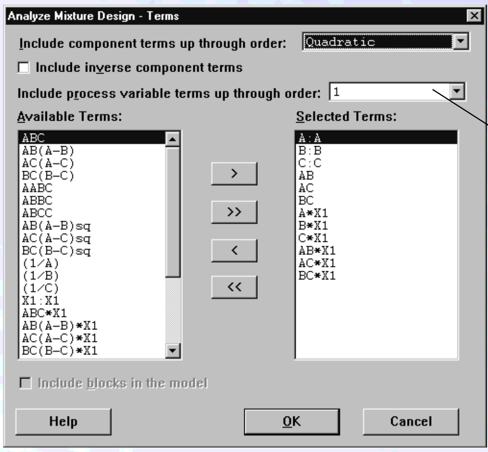
You can fit inverse terms with any of the above models as long as the lower bound for any component is not zero and you choose to analyze the design in proportions. Inverse terms allow you to model extreme changes in the response as the proportion of one or more components nears its boundary. Suppose you are formulating lemonade and you are interested in the acceptance rating for taste. An extreme change in the acceptance of lemonade occurs when the proportion of sweetener goes to zero. That is, the taste becomes unacceptably sour.

Analyze Mixture Design fits a model without a constant term. For example, a quadratic in three components is as follows:

$$Y = b_1A + b_2\square + b_3C + b_{12}AB + b_{13}AC + b_{23}BC$$

▶ To specify the model

1 In the Analyze Mixture Design dialog box, click **Terms**.



This option only displays when the mixture design contains process variables or amounts. The label changes depending on the variable type.

2 Do one of the following:

- from **Include the component terms up through order**, choose one of the following:

  linear, **quadratic**, **special cubic**, **full cubic**, **special quartic**, or **full quartic**

- move the terms you want to include in the model to **Selected Terms** using the arrow buttons
  – to move one or more terms, highlight the desired terms, then click [<] or [>]
  – to move all of the terms, click [<<] or [>>]

  You can also move a term by double-clicking it.

Note MINITAB represents components with the letters A, B, C, …, skipping the letter T, process variables with X1…Xn, and amounts with the letter T.

3 If you want to include inverse component terms, do one of the following:

- to include all the inverse component terms, check **Include inverse component terms**

- to include a subset of the inverse component terms, highlight the desired terms, then click [>]

4 If you want to include process variable or amount terms, do one of the following:

- from **Include process variables/mixture amount terms up through order**, and choose an order

- move terms you want to include in the model to **Selected Terms** using the arrow buttons
  – to move one or more terms, highlight the desired terms, then click [<] or [>]
  – to move all of the terms, click [<<] or [>>]

  You can also move a term by double-clicking it.

▶ Example of analyzing a simplex centroid design

This example fits a model for the design created in *Example of a simplex centroid design* on page 21-20. Recall that you are trying determine how the proportions of the components in an herbal blend household deodorizer affect the acceptance of the product based on scent. The three components are neroli oil, rose oil, and tangerine oil. Based on the design points, you mixed ten blends. The response measure (Acceptance) is the mean of five acceptance scores for each of the blends.

1 Open the worksheet DEODORIZ.MTW.

2 Choose **Stat** ▸ **DOE** ▸ **Mixture** ▸ **Analyze Mixture Design**.

3 In **Responses**, enter *Acceptance*. Click **OK**.

Session window output

Regression for Mixtures: Acceptance versus Neroli, Rose, Tangerine

```
Estimated Regression Coefficients for Acceptance (component proportions)

Term                   Coef    SE Coef      T      P       VIF
Neroli                5.856     0.4728      *      *     1.964
Rose                  7.141     0.4728      *      *     1.964
Tangerin              7.448     0.4728      *      *     1.964
Neroli*Rose           1.795     2.1791   0.82  0.456     1.982
Neroli*Tangerin       5.090     2.1791   2.34  0.080     1.982
Rose*Tangerin        -1.941     2.1791  -0.89  0.423     1.982

S = 0.49023            PRESS = 11.440
R-Sq = 73.84%          R-Sq(pred) = 0.00%      R-Sq(adj) = 41.14%

Analysis of Variance for Acceptance (component proportions)

Source              DF     Seq SS     Adj SS     Adj MS      F      P
Regression           5    2.71329    2.71329   0.542659   2.26  0.225
   Linear            2    1.04563    1.56873   0.784366   3.26  0.144
   Quadratic         3    1.66766    1.66766   0.555887   2.31  0.218
Residual Error       4    0.96132    0.96132   0.240329
Total                9    3.67461
```

Interpreting the results

The magnitude of the coefficients for the three pure mixtures indicate that tangerine oil (7.448) and rose oil (7.141) produce deodorizers with higher acceptance levels than neroli oil (5.856).

Positive coefficients for two-blend mixtures indicate that the two components act synergistically or are complementary. That is, the mean acceptance score for the blend is greater than you would obtain by calculating the simple mean of the two acceptance scores for each pure mixture.

Negative coefficients indicate that the two components are antagonistic towards one another. That is, the mean acceptance score is lower than you would obtain by calculating the simple mean of the two acceptance scores.

The neroli oil by tangerine mixture is the only two-blend mixture that might be judged as significant (t = 2.34; p = 0.08).

For a general discussion of analysis results, see [1].

Displaying Factorial Plots

Factorial plots are available for process variables in a mixture design. You can produce three types of factorial plots to help you visualize process variable effects: main effects plots, interaction plots, and cube plots. These plots can be used to show how a response variable relates to one or more process variable.

These plots are described in Chapter 19, *Factorial Designs*. See *Displaying Factorial Plots* on page 19-52 for details.

Displaying Mixture Plots

You can produce three types of mixture plots to help you visualize effects:

- response trace plot—see *Response trace plots* on page 21-45
- contour plot—see *Contour and surface (wireframe) plots* on page 21-49
- surface (wireframe) plot—see *Contour and surface (wireframe) plots* on page 21-49

These plots show how a response variable relates to the design variables based on a model equation.

More You can use a simplex design plot to visualize the mixture design space (or a slice of the design space if you have more than three components). MINITAB plots the design points on triangular axes. See *Displaying Simplex Design Plots* on page 21-24.

Data

Trace plots, contour plots, and surface plots are model dependent. Thus, you *must* fit a model using Analyze Mixture Design before you can display these plots. MINITAB looks in the worksheet for the necessary model information to generate these plots.

Response trace plots

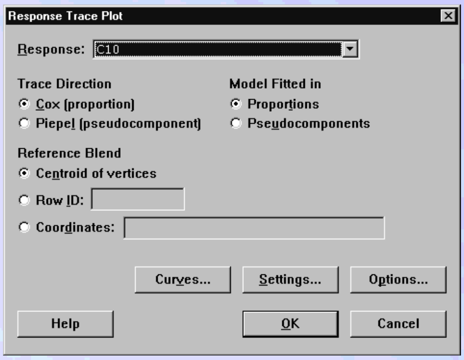
A response trace plot (also called a component effects plot) shows the effect of each component on the response. Several response traces, which are a series of predictions from the fitted model, are plotted along a component direction. The trace curves show the effect of changing the corresponding component along an imaginary line (direction) connecting the reference blend to the vertex.

Each component in the mixture has a corresponding trace direction. The points along a trace direction of a component are connected thereby producing as many curves as there are components in the mixture.

Response trace plots are especially useful when there are more than three components in the mixture and the complete response surface cannot be visualized on a contour or surface plot. You can use the response trace plot to identify the most influential components and then use them for a contour or surface plot.

▶ To display a response trace plot.

1 Choose **Stat > DOE > Mixture > Response Trace Plot**.



2 From **Response**, choose a response to plot. If an expected response is not in the list, fit a model to it with Analyze Mixture Design.

3 Click **OK**.

Options

Response Trace Plot dialog box

- specify the trace direction: Cox (proportion) or Piepel (pseudocomponent)—see *Component direction* on page 21-47
- specify the model units: proportions or pseudocomponents
- define the reference blend (the default is the centroid of the experimental region)

Curves subdialog box

- specify the line style and line color for the trace curves

Settings subdialog box

- specify hold values for process variables (the default is the low setting) and the amount variable (the default is the average amount)

Options subdialog box

- define minimum and maximum values for the x-axis and y-axis
- replace the default title with your own title

Component direction

When changing the proportion of a component in a mixture to determine its effect on a response, you must make offsetting changes in the other mixture components because the sum of the proportions must always be one. The changes in the component whose effect you are evaluating along with the offsetting changes in the other components can be thought of as a *direction* through the experimental region.

There are two commonly used trace directions along which the estimated responses are calculated: Cox's direction and Piepel's direction.

- When the design is not constrained and the reference point lies at the centroid of the unconstrained experimental region, both Cox's directions and Piepel's directions are the axes of the simplex.
- When the design is constrained, the default reference mixture point lies at the centroid of the constrained experimental region that is different than the centroid of the unconstrained experimental region. In this case, Cox's direction is defined in the original design space, whereas, Piepel's direction is defined in the L-pseudocomponent space.

▶ Example of a response trace plot

In the *Example of a simplex centroid design* on page 21-20, you created a design to study how the proportions of three ingredients (neroli oil, rose oil, and tangerine oil) in an herbal blend household deodorizer affect the acceptance of the product based on scent. Next, you analyzed the response (Acceptance) in the *Example of analyzing a simplex centroid design* on page 21-43. Now, to help you visualize the component effects, you display a response trace plot.

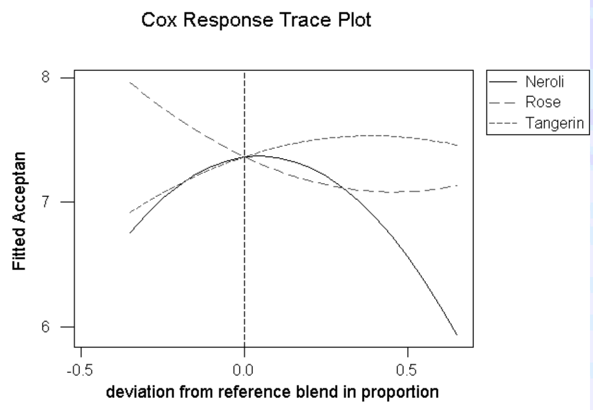
1 Open the worksheet DEODORIZ2.MTW.

2 Choose **Stat** ➤ **DOE** ➤ **Mixture** ➤ **Response Trace Plot**.

3 Click **Curves**.

4 Under **Line Styles**, choose **Use different types**. Click **OK** in each dialog box.

Graph window output



Interpreting the results

The trace plot shows how each component effects the response relative to the reference blend. In this example, the reference blend is the centroid of the design vertices. This trace plot provides the following information about the component effects. Starting at the location corresponding to the reference blend:

- As the proportion of neroli oil (solid curve) in the mixture
  - increases (and the other mixture components decrease), the acceptance rating of the deodorizer decreases
  - decreases (and the other mixture components increase), the acceptance rating of the deodorizer decreases

  The proportion of neroli oil in the reference blend is near optimal.

- As the proportion of rose oil (long-dashed curve) in the mixture
  - increases (and the other mixture components decrease), the acceptance rating of the deodorizer decreases slightly
  - decreases (and the other mixture components increase), the acceptance rating of the deodorizer increases

  A decrease in the proportion of rose oil relative to the reference blend may improve the acceptance rating.

- As the proportion of tangerine oil (short-dashed curve) in the mixture
  - increases (and the other mixture components decrease), the acceptance rating of the deodorizer increases slightly
  - decreases (and the other mixture components decrease), the acceptance rating of the deodorizer decreases

  An increase in the proportion of tangerine oil relative to the reference blend may improve the acceptance rating.

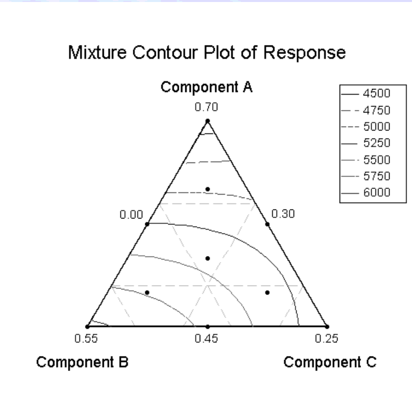
Keep the following in mind when you are interpreting a response trace plot:

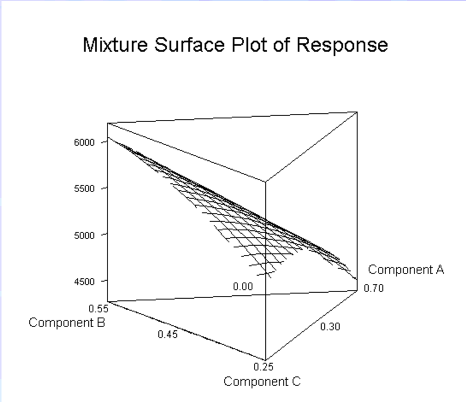
- All components are interpreted relative to the reference blend.
- Components with the greatest effect on the response will have the steepest response traces.
- Components with larger ranges (upper bound − lower bound) will have longer response traces; components with smaller ranges will have shorter response traces.
- The total effect of a component depends on both the range of the component and the steepness of its response trace. The total effect is defined as the difference in the response between the effect direction point at which the component is at its upper bound and the effect direction point at which the component is at its lower bound.
- Components with approximately horizontal response traces, with respect to the reference blend, have virtually no effect on the response.
- Components with similar response traces will have similar effects on the response.

Contour and surface (wireframe) plots

In a contour plot, the response surface is viewed as a two-dimensional plane where all points that have the same response are connected to produce contour lines of constant responses. Contour plots are useful for establishing desirable response values and mixture blends.

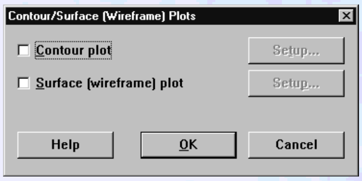
A surface plot displays a three-dimensional view of the surface. Like contour plots, they are useful for establishing desirable response values and mixture blends. Surface plots may provide a clearer picture of the response surface. The illustrations below compare these two types of response surface plots.





▶ To plot the response surface

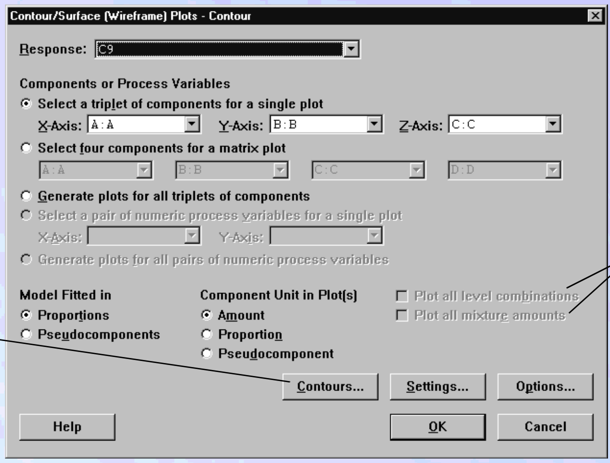
1 Choose **Stat** ▯ **DOE** ▯ **Mixture** ▯ **Contour/Surface (Wireframe) Plots**.



2 Do one or both of the following:

▯ to generate a contour plot, check **Contour plot** and click **Setup**

- to generate a surface (wireframe) plot, check **Surface (wireframe) plot** and click **Setup**



3 From **Response**, choose a response to plot. If an expected response is not in the list, fit a model to it with Analyze Mixture Design.

4 If you like, use any of the options listed below, then click **OK**.

Options

Setup subdialog box

- select a triplet of components for a single plot
- display four contour plots in a single page layout
- generate plots for all triplets of components
- display plots for numeric process variables
- display the plot in amounts, proportions, or pseudocomponents
- for a single contour plot, include all the levels of the process variables in a single layout
- include an amount variable (by default, MINITAB will hold the amount variable at its first defined value)

Contours subdialog box

- for contour plots, specify the number or location of the contour levels, and the contour line color and style—see *Controlling the number, type, and color of the contour lines* on page 21-52

Wireframe subdialog box

- for surface (wireframe) plots, specify the color of the wireframe (mesh) and the surface

Settings subdialog box

- specify values for design variables that are not included in the plot—see *Settings for extra components, process variables, and an amount variable* below

Options subdialog box

- define minimum and maximum values for the x-axis, y-axis, and z-axis
- for contour plots, define the background grid or suppress grid lines
- for contour plots, suppress or display design points on the plot
- replace the default title with your own title

Settings for extra components, process variables, and an amount variable

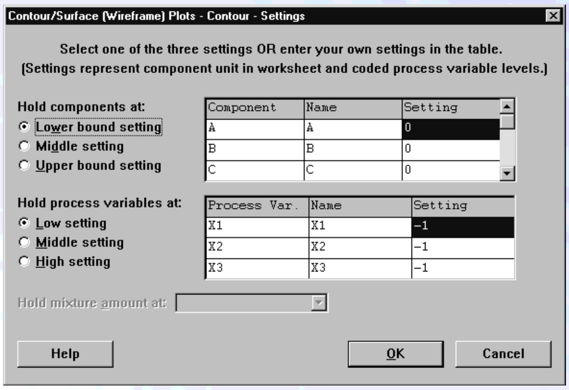
You can set the holding level for components, and process variables that are not in the plot at their highest or lowest settings, or you can set specific levels to hold each. The hold values must be expressed in the following units:

- components in the *units displayed in the worksheet*
- process variables in *coded units*

Note If you have text process variables in your design, you can only set their holding values at one of the text levels.

▶ To set the holding level for design variables not in the plot

1 In the Setup subdialog box, click **Settings**.



2 Do one or more of the following to set the holding values:

- For components (only available for design with more than three components):

  - To use the preset values for components, choose **Lower bound setting**, **Middle setting**, or **Upper bound setting** under **Hold components at**. When you use a preset value, *all* components not in the plot will be held at their lower bound, middle, or upper bound.
  - To specify the value at which to hold the components, enter a number in **Setting** for each component that you want to control. This option allows you to set a different holding value for each component.

- For process variables:
  - To use the preset values for process variables, choose **High setting** or **Low setting** under **Hold process variables at**. When you use a preset value, *all* variables not in the plot will be held at their high or low settings.
  - To specify the value at which to hold the process variables, enter a number in **Setting** for each of the process variables you want to control. This option allows you to set a different holding value for each process variable.

- For an amount variable:
  - In **Hold mixture amount at**, choose one of the mixture totals. MINITAB displays the multiple totals that you entered in the Components subdialog box when you were creating the design. The default hold value is the average of the multiple totals.

3 Click **OK**.

Controlling the number, type, and color of the contour lines

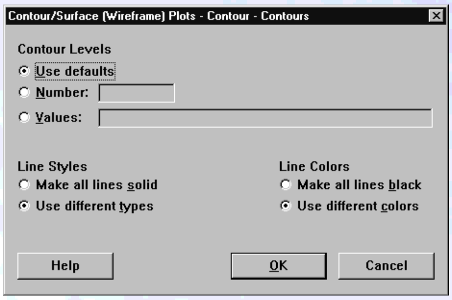
MINITAB displays from four to seven contour levels—depending on the data—by default. However, you can specify from 2 to 15 contour lines.

You can also change the line type and color of the lines.

▶ To control plotting of contour lines

1 In the **Contour/Surface (Wireframe) Plots** dialog box, check **Contour plot** and click **Setup**.

2 Click **Contours**.



3 To change the number of contour lines, do one of the following:

- Choose **Number** and enter a number from 2 to 15.

- Choose **Values** and enter from 2 to 15 contour level values in the units of your data. You must enter the values in increasing order.

4 To define the line style, choose **Make all lines solid** or **Use different types** under **Line Styles**.

5 To define the line color, choose **Make all lines black** or **Use different colors** under **Line Colors**.

6 Click **OK**.

▶ Example of a contour plot and a surface plot

In the deodorizer example on page 21-43, you fit a model to try and determine how the proportions of the components in an herbal blend household deodorizer affect the acceptance of the product based on scent. The three components are neroli oil, rose oil, and tangerine oil. Based on the design points, you mixed ten blends. The response measure (Acceptance) is the mean of five acceptance scores for each of the blends.

Now you generate a contour and a surface plot to help identify the component proportions that yield the highest acceptance score for the herbal blend.

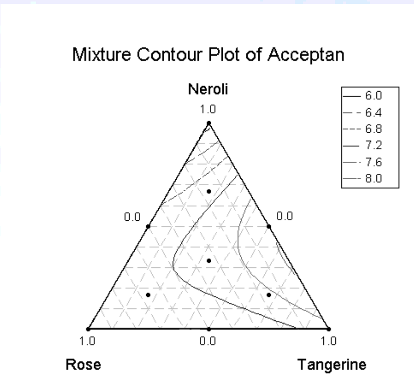
1 Open the worksheet DEODORIZ2.MTW.

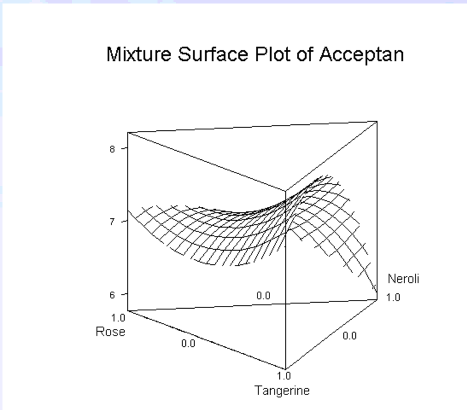
2 Choose **Stat** > **DOE** > **Mixture** > **Contour/Surface (Wireframe) Plots**.

3 Choose **Contour plot** and click **Setup**. Click **OK**.

4 Choose **Surface (wireframe) plot** and click **Setup**. Click **OK** in each dialog box.

Graph window output





Interpreting the results

The area of the highest acceptance is located on the right edge of the plots. Both the contour and the surface plot show that the acceptance of the herbal deodorizer is highest when the mixture contains little or no rose oil and slightly more tangerine oil than neroli oil.

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References

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[2] D.C. Montgomery and S.R. Voth (1994). “Multicollinearity and Leverage in Mixture Experiments,” Journal of Quality Technology 26, pp. 96–108.

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Appendix for Mixture Designs

Triangular coordinate systems

Triangular coordinate systems allow you to visualize the relationships between the components in a three-component mixture. In a mixture, the components are restricted by one another in that the components must add up to the total amount or whole. Triangular coordinate systems in this section show the minimum of the x_1, x_2, and x_3 components as 0, with the maximums at 1.

The following illustration shows the general layout of a triangular coordinate system. The components in mixture models are referred to in terms of their proportion to the whole, with the whole as 1. The vertices of the triangle represent *pure* mixtures (also called single-component blends). In pure mixtures, the proportion of one component is 1 and the rest are 0.