Getting Started with the SAS® 9.2 ADX Interface for Design of Experiments

SAS® Documentation

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Getting Started with the SAS® 9.2 ADX Interface for Design of Experiments

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Contents

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The final responsibility for the SAS System lies with SAS Institute alone. We hope that you will always let us know your opinions about the SAS System and its documentation. It is through your participation that SAS software is continuously improved.

Chapter 1

What's New in SAS 9 ADX Interface for Design of Experiments

Chapter Contents

Chapter 1

What's New in SAS 9 ADX Interface for Design of Experiments

Overview

The SAS ADX Interface for Design of Experiments includes enhancements related to response surface designs, mixture designs, general factorial designs, and split-plot designs. Furthermore, ADX can now import data from SAS data sets or external file formats, and it can export design information to SAS data sets or external file formats.

The SAS 9 ADX Interface now enables you to do the following:

- create general factorial designs with factors having up to nine levels
- construct and analzye two-level full factorial and fractional factorial split-plot designs
- choose a mixed level design from a new expanded design selection
- analyze unstructured experimental data imported from external sources
- analyze fitted models using the new graphical ANOVA
- construct a lambda plot to evalulate the need for a response transformation
- add center points to a design before or after replication
- add replicated points in a new block
- apply a user-specified alpha value for the graphical techniques in fit and optimize
- delete inactive factors and project a fractional-factorial design to a higher-resolution design
- join the means in a box plot
- show clear and aliased effects in the alias structure
- display confidence intervals in the response calculator and experiment report
- honor block structure in a blocked design during design randomization

Details

Response Surface Designs

ADX can now create designs based on Hartley's (1959) small response surface designs.

Variance dispersion graphs are generated in the design details so you can compare designs and choose the best number of center points. This option requires SAS/IML software.

Mixed Level Designs

The number of mixed-level designs offered in ADX has been extensively expanded from the original 213 designs to 25,115 designs. You can now construct designs with up to 9 levels (originally 2 and 3 levels only) and up to 513 runs (originally 108 runs).

Mixture Designs

Process variables can now be included in the creation and analysis of mixture designs. Mixture designs with process variables are created using the optimal design interface. The analysis will determine whether process variables are significant, but all such variables will be included in the optimization process. In the optimization tools, process variables are treated as fixed-level factors.

General Factorial Designs

General factorial designs are designs that run all combinations of factor levels. In ADX, you can create general factorials with factors having any number of levels.

Split-Plot Designs

ADX can now create full factorial and two-level minimum aberration fractional factorial generalized split-plot designs as described in Huang, Chen, and Voelkel (1998).

Observational Data Analysis

Prior to the 9.2 release, ADX could analyze only experimental data from designs that are formally constructed. But ADX customers have reported that there are many situations where they carry out an experiment that is informally designed and want to analyze the data in ADX. ADX can now be used to first import this type of data and then analyze using appropriate statistical and graphical techniques including basic statistical methods such as one-way ANOVA, *t* test, and histogram. This new functionality labeled "Analyze Observational Data" is available from the File menu of the ADX Desktop.

Data Import and Export

ADX can import factor and response values from SAS data sets or external files. You can create the design in ADX and import only the response information, or you can import both the factor levels and the response.

ADX can export design information to SAS data sets and external files for inclusion in a data warehouse. You can export variable information, experiment details, and values for the factors and response.

Access to external file formats requires SAS/ACCESS software.

References

Hartley, H. O. (1959), "Smallest Composite Designs for Quadratic Response Surfaces," *Biometrics*, 15, 611–624.

Huang, P., Chen, D., and Voelkel, J. O. (1998), "Minimum-Aberration Two-Level Split-Plot Designs," *Technometrics*, 40, 314–326.

Chapter 2

Overview of ADX

Chapter Contents

Chapter 2

Overview of ADX

The ADX Interface

Welcome to the SAS ADX Interface for Design of Experiments. The ADX Interface features powerful, intuitive tools for designing and analyzing experiments.

Using This Book

Getting Started with the SAS ADX Interface for Design of Experiments is intended to help you quickly learn the primary features of the ADX Interface. This tutorial takes you through the steps of creating and analyzing the various types of experimental designs offered by ADX.

This book is not intended as comprehensive documentation, nor should it be considered as an experimental design text. However, the Appendices provide a glossary of terms and a list of references you might find useful.

To use this book, you should have some understanding of design of experiments and be familiar with such terms as factorial screening design and normal plots. Of course, ADX provides some new and exciting ways to analyze your experimental designs.

Chapter Topics

In this chapter, you get acquainted with the ADX environment by working through a simple example.

Covered in This Chapter

- Creating a new two-level design
- Selecting a design
- Editing responses
- Exploring data
- Using a main-effects plot
- Using a cube plot
- Using ADX Help

Task List

- Get acquainted with the ADX desktop.
- Learn how ADX organizes designs.
- Learn how designs achieve particular experimental objectives.
- Create a simple two-level factorial design.

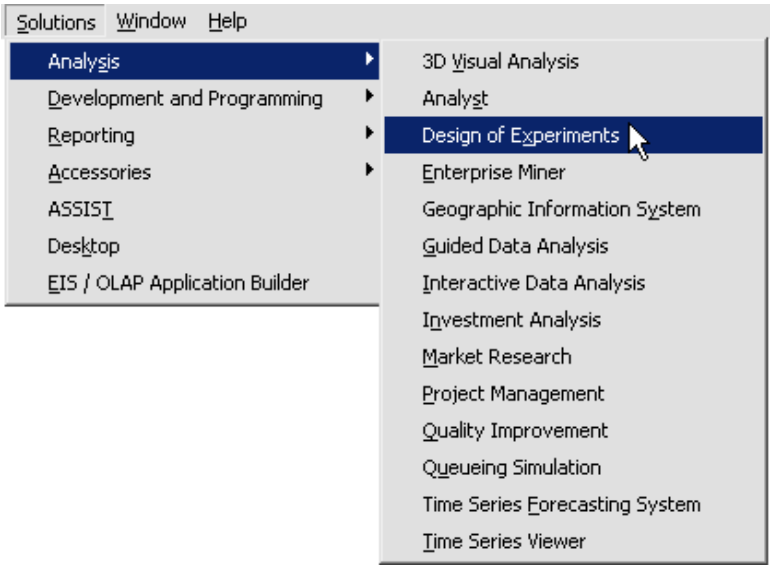
Your First ADX Session

You do not need to know SAS programming to get started with ADX. The organization of the ADX Interface guides you step by step through the process of constructing a design, analyzing the data, and creating a report.

ADX provides menus and tool buttons for performing each task in this process. The menus change to correspond with the ADX window that is open on the desktop.

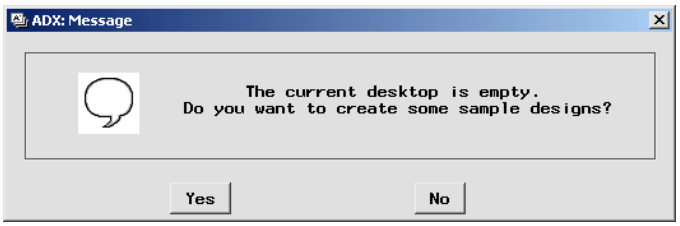
Starting ADX

To access ADX, first access the SAS System from your desktop. Then select **Solutions** → **Analysis** → **Design of Experiments** from the main menu in the SAS windowing environment.



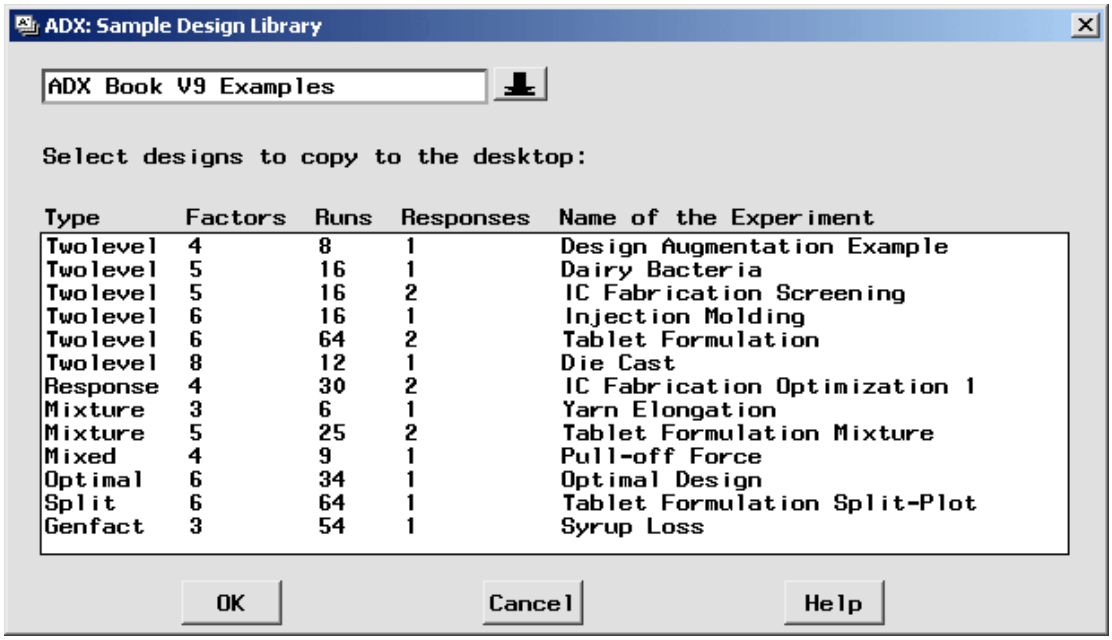
Initial ADX Call

If this is the first time ADX is called, you will see the following Message dialog box.



Follow these steps:

1. Click **Yes**. In the next window you select the sample designs to put on the ADX desktop.
2. To create the designs used in this book, click **ADX Book V9 Examples**. Hold down the SHIFT key and select all the designs.



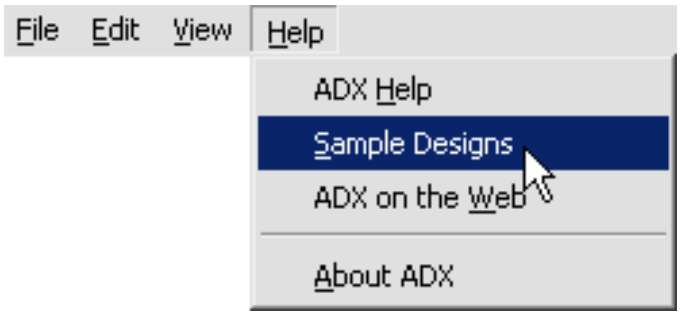
3. Click **OK**. Once ADX creates the sample designs, it puts them into the ADXPARM folder.

Adding Sample Designs to the Desktop Folder

If you are accessing ADX subsequent to an initial call, you want to add the sample designs to the current folder. (Your folder of sample designs might have different designs, depending on which sample designs were selected during the initial ADX call.)

To add sample designs to the current folder, follow these steps:

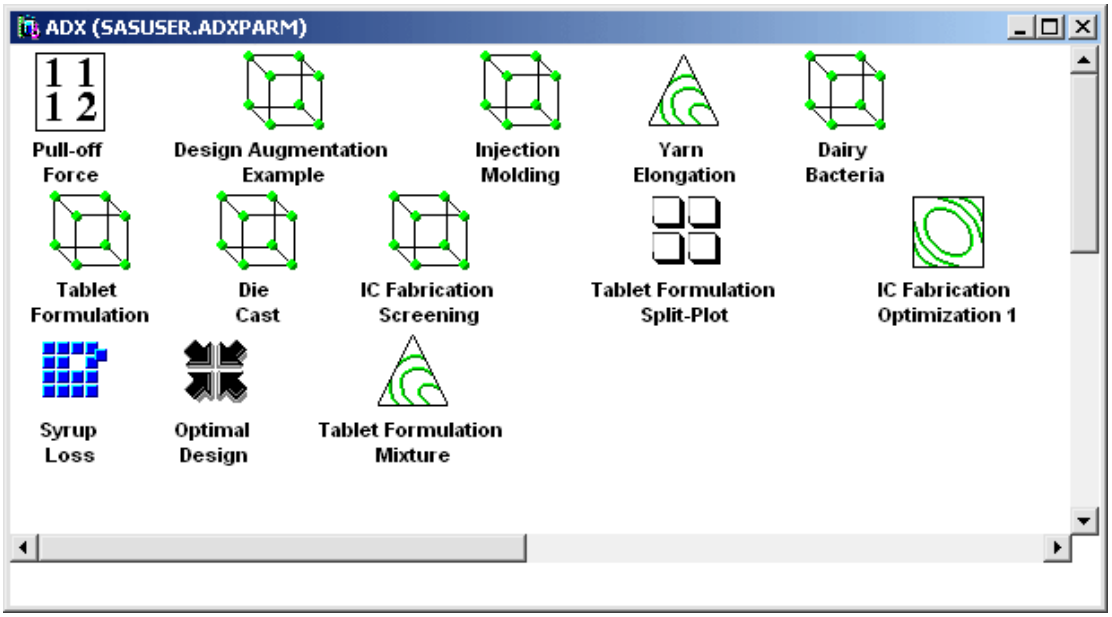
1. Select **Help** → **Sample Designs** from the ADX desktop.



2. ADX instructs you to select the designs you want to copy.
3. Click **ADX Book V9 Examples**.
4. Select all the designs (hold down the SHIFT or CTRL key and click to select multiple designs).

Managing Your Designs with the ADX Desktop

The ADX desktop is the starting point for working with designs. From the desktop, you can access folders of designs, each of which appears in a separate window. Within each folder, designs are organized by type. Each design type has its own icon.



The name of the default folder is ADXPARM. Use the commands on the **File** menu or the folder icons on the toolbar to create new folders or to change the current folder. If you create a new design, it will be added to the current folder.

See Chapter 14 for more information about organizing your designs.

Design of Experiments Process

Design of experiments is a process in which designing the experiment is only one step. For any experiment, follow these steps:

1. Determine the experimental objective.
2. Determine the factors and responses.
3. Design the experiment to meet the objective.
4. Collect the data.
5. Analyze the data with graphs, plots, and statistics.
6. Report the experimental results.
7. Design a new experiment.

Design Objectives

Designs offered by ADX can be used to achieve specific experimental objectives, as shown in Table 2.1.

Table 2.1. Design Types and Their Objectives

Design Type	Model Objective
Two-level screening	Identify factors of greatest impact on response
Response surface	Model curvature effects
Mixture	Model effects that are components of a blend
Mixed level	Model with two- and three-level, mixed quantitative and qualitative factors
Optimal	Model with D- and A-optimal designs for irregular design regions
Split-plot	Model effects where some levels are hard to change
General factorial	Model with full factorial designs and factors with several levels

Getting Started with a Simple Example

The best way to learn the ADX Interface is to work through a simple example. This example creates a fractional factorial design and illustrates a few of the plots you can use to explore the data.

Experimental Objective

Suppose you are doing a pilot study to examine five strains of bacteria (X1–X5) and determine which, if any, might be worth further study for use in dairy products. Since the eventual goal is to minimize the pH of milk in which these bacteria are placed, a screening experiment will be used to identify the strains that influence the pH.

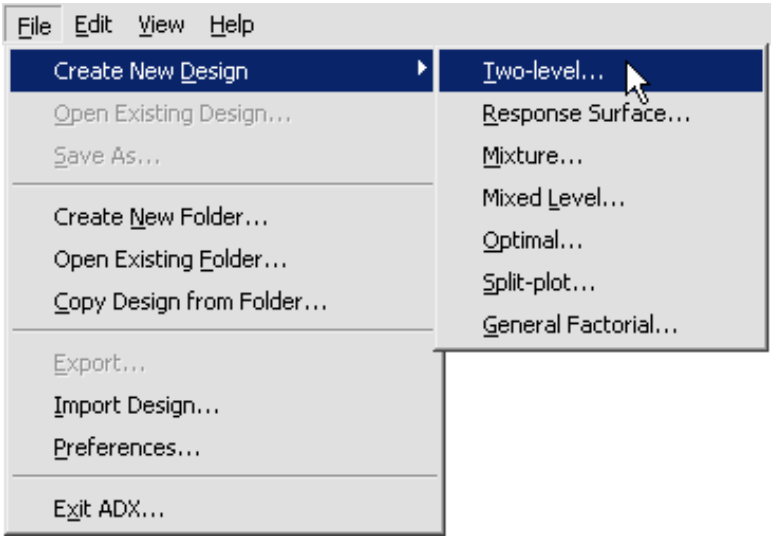
The factors in this experiment are the five strains (X1–X5). In each run of the experiment, a factor can have a coded value of -1 (strain absent) or $+1$ (strain present). The response variable is pH.

Task List

- Create a two-level factorial design.
- Type the response values into the design.
- Examine main-effects plots and cube plots to see which bacterial strains are worth further investigation.

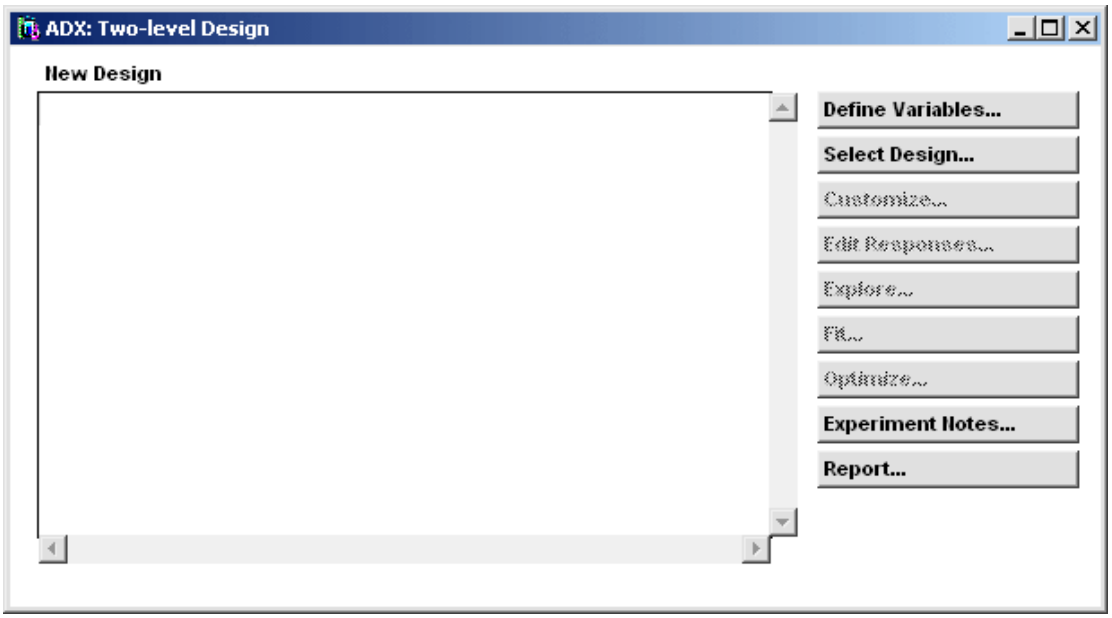
Creating the Design

Select **File** → **Create New Design** → **Two-level**from the ADX desktop.



Alternatively, you can click the **Two-level design** icon on the toolbar.

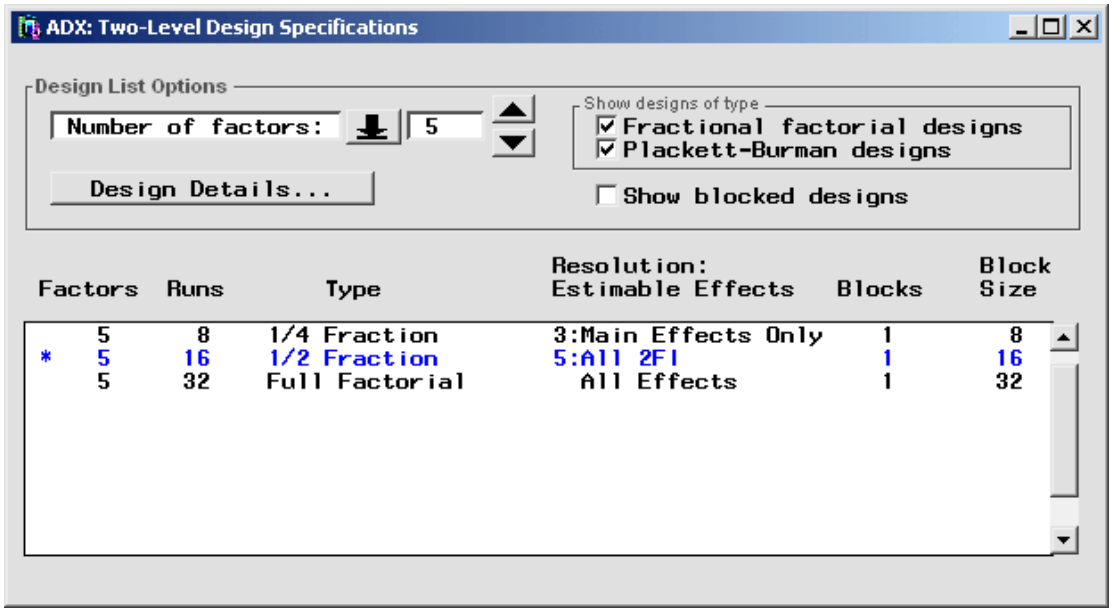
ADX brings up the main design window, which is titled Two-level Design.



The main design window is conveniently arranged to facilitate designing and analyzing an experiment. The task buttons are listed to the right of the design display area. The area on the left is blank until you select a design. (Some of the task buttons are unavailable until preliminary steps are completed.)

To create the design for the strains, follow these steps:

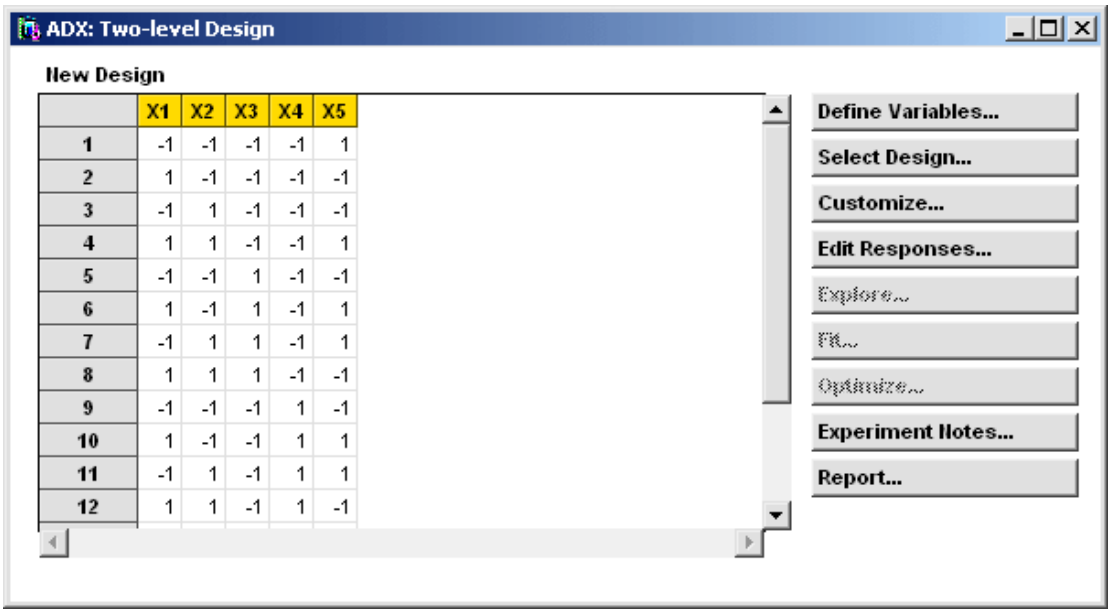
1. Click **Select Design** to open the Two-Level Design Specifications window.
2. Type **5**, the number of strains, for **Number of factors**:
3. Select the **1/2 Fraction** design, a 16-run Resolution 5 design.



4. Close the window (select **File** → **Close** or click ☒) to use the design.

The Message dialog box gives you a chance to change your mind.

Click **Yes** to use the selected design. ADX returns to the main design window and displays a table of the runs in the design.

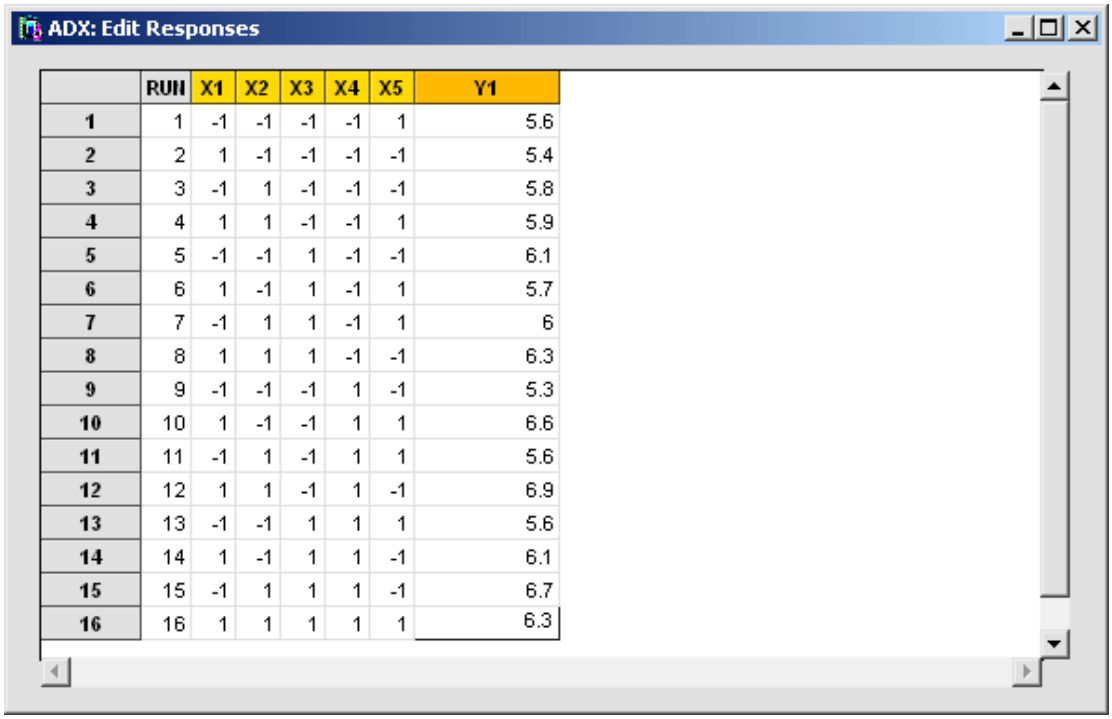


	X1	X2	X3	X4	X5
1	-1	-1	-1	-1	1
2	1	-1	-1	-1	-1
3	-1	1	-1	-1	-1
4	1	1	-1	-1	1
5	-1	-1	1	-1	-1
6	1	-1	1	-1	1
7	-1	1	1	-1	1
8	1	1	1	-1	-1
9	-1	-1	-1	1	-1
10	1	-1	-1	1	1
11	-1	1	-1	1	1
12	1	1	-1	1	-1

Default factor names are given at the tops of the columns, and the levels of each factor are the rows. For the purposes of this experiment, X1 corresponds to the presence or absence of bacterial strain 1, X2 corresponds to strain 2, and so on.

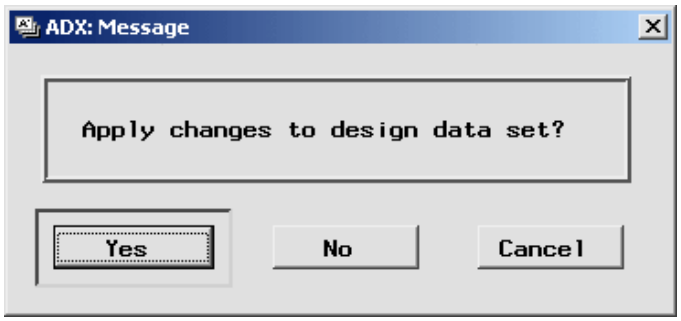
To enter the response data into the design, follow these steps:

1. Click **Edit Responses**. ADX takes you to the Edit Responses window and provides a column, called **Y1**, for you to enter the pH response values.
2. Type the following pH values in the default response column **Y1** (in order from row 1 to 16): 5.6, 5.4, 5.8, 5.9, 6.1, 5.7, 6, 6.3, 5.3, 6.6, 5.6, 6.9, 5.6, 6.1, 6.7, 6.3.



	RUN	X1	X2	X3	X4	X5	Y1
1	1	-1	-1	-1	-1	1	5.6
2	2	1	-1	-1	-1	-1	5.4
3	3	-1	1	-1	-1	-1	5.8
4	4	1	1	-1	-1	1	5.9
5	5	-1	-1	1	-1	-1	6.1
6	6	1	-1	1	-1	1	5.7
7	7	-1	1	1	-1	1	6
8	8	1	1	1	-1	-1	6.3
9	9	-1	-1	-1	1	-1	5.3
10	10	1	-1	-1	1	1	6.6
11	11	-1	1	-1	1	1	5.6
12	12	1	1	-1	1	-1	6.9
13	13	-1	-1	1	1	1	5.6
14	14	1	-1	1	1	-1	6.1
15	15	-1	1	1	1	-1	6.7
16	16	1	1	1	1	1	6.3

3. Close the window.
4. Click **Yes** in the Message dialog box to apply the changes. ADX will return you to the main design window and show the new response values.

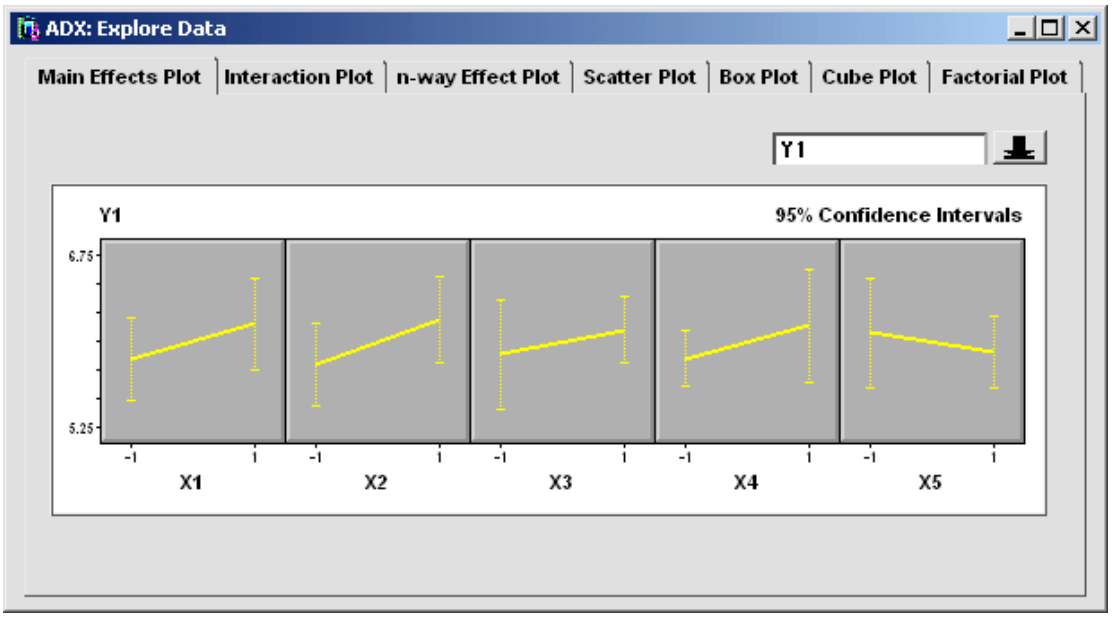


Once a design has response values, you can use the **Explore**, **Fit**, and **Optimize** features for exploring and analyzing the data. However, you cannot select a different design.

Exploring Results

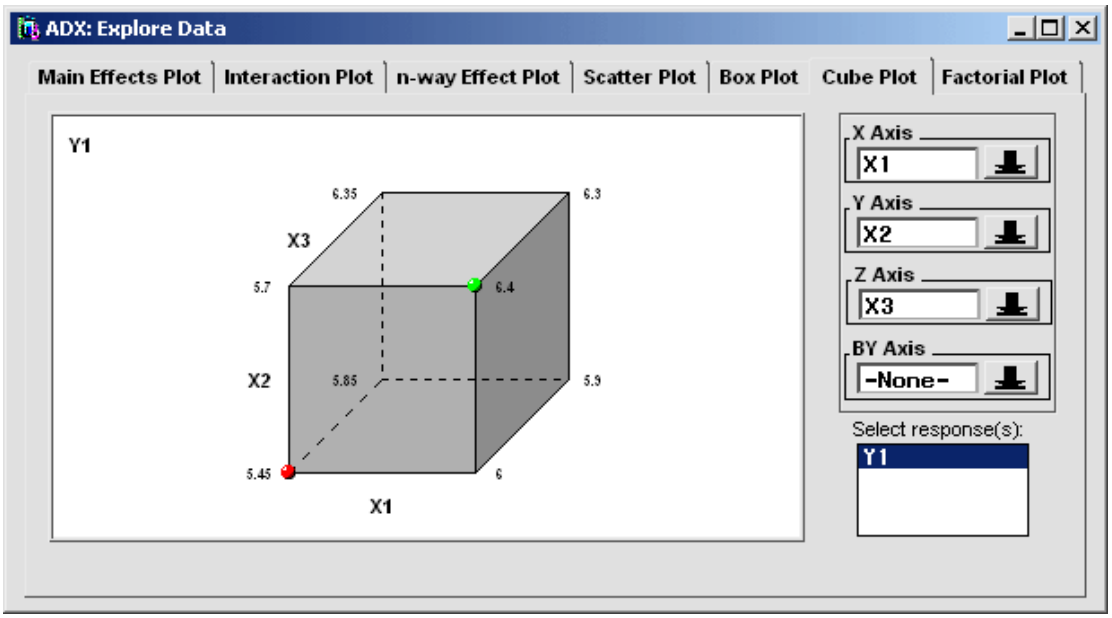
To view the main-effects and interaction plots, click **Explore**. The Explore Data window will open.

In a main-effects plot, the slope of the line connecting the low level to the high level indicates the strength of the effect or, in this case, the ability of the strain to change the response, pH.



Switch to the cube plot by clicking the **Cube Plot** tab.

The cube plot, like all the graphics displays in ADX, is interactive. For example, place the mouse pointer over the X1 label. The arrow changes to a hand to indicate that you can click and drag the label to another edge of the cube. You will learn about other interactive features in later chapters.



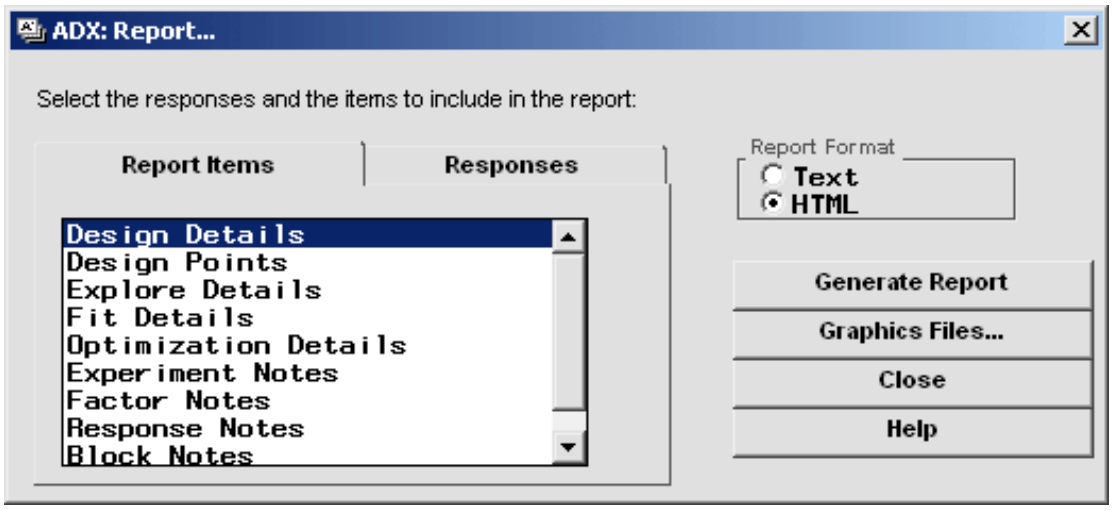
The values at the corners are averages of the response over all runs where the labeled factors in the plot are at the given value. For example, in this plot the average value

of Y1 over all runs where strains X1, X2, and X3 are absent is 6.3. The symbols at certain corners indicate which combinations of levels give the highest and the lowest pH (Y1) values. The lowest average pH of 5.45 occurs when strains X1, X2, and X3 are present.

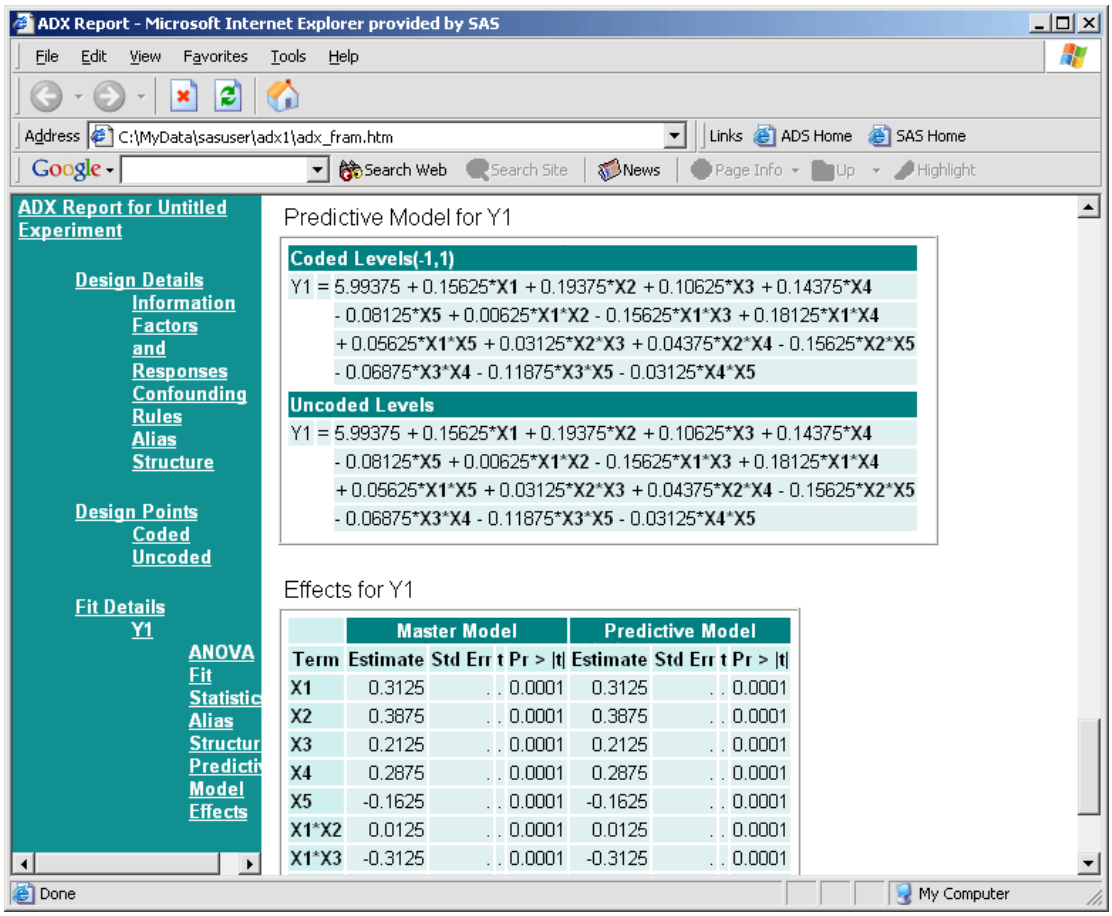
Close the Explore Data window to return to the main design window.

HTML Reports

To create a report on the results of the experiment, click **Report** in the main design window. ADX will open a window that enables you to customize your report.



Select the items and responses you want to include in the report and click **Generate Report**. The following HTML report is displayed with Microsoft Internet Explorer.



	Master Model				Predictive Model			
Term	Estimate	Std Err	t	Pr > |t|	Estimate	Std Err	t	Pr > |t|
X1	0.3125	.	.	0.0001	0.3125	.	.	0.0001
X2	0.3875	.	.	0.0001	0.3875	.	.	0.0001
X3	0.2125	.	.	0.0001	0.2125	.	.	0.0001
X4	0.2875	.	.	0.0001	0.2875	.	.	0.0001
X5	-0.1625	.	.	0.0001	-0.1625	.	.	0.0001
X1*X2	0.0125	.	.	0.0001	0.0125	.	.	0.0001
X1*X3	-0.3125	.	.	0.0001	-0.3125	.	.	0.0001

Text Reports

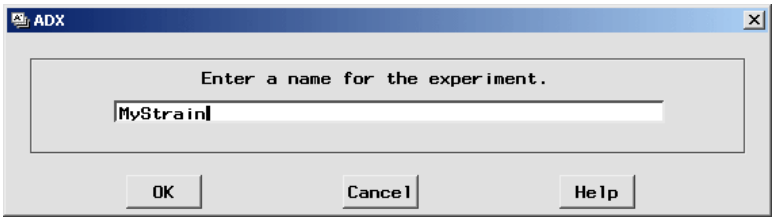
Selecting the **Text** option in the Report window generates a text-only report that you can edit. To save the text file, select **File** → **Save as** and select **Write to file** or **Write to object**.

Exiting ADX

When you are finished working with a design, close the main design window. A Message dialog box appears to ask if you want to save the changes to the design permanently.

To save your design with the response values entered, follow these steps:

1. Click **Yes**.



2. Type **MyStrain** as the name for this design.
3. Click **OK**.

ADX adds the new MyStrain design to the open desktop folder so you can use it later.

To exit ADX, follow these steps:

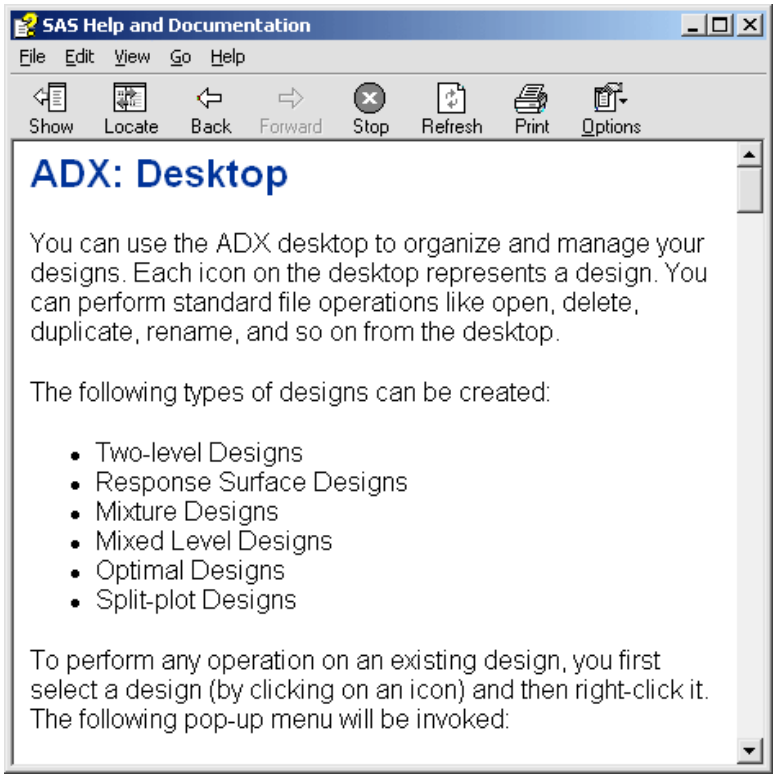
1. Return to the ADX desktop.
2. Select **File** → **Exit ADX** or close the desktop window.
3. A confirmation dialog box appears. Click **OK**.

4. To exit the SAS System, select **File** → **Exit**.

Congratulations! You have just analyzed your first experiment with the ADX Interface.

Using ADX Help

ADX Help provides information about how to use ADX and how to design experiments. Select **Help** → **ADX Help** from the ADX desktop to open the Help window.



Select **File** → **Close** or click ☒ to close the Help window.

Points to Remember

- ADX has features for creating and analyzing experimental designs through a simple point-and-click interface.
- ADX is organized by type of experimental design.
- Different designs accomplish different types of experimental objectives.
- ADX uses folders to group designs so that you can organize designs according to projects.
- ADXPARM is the name for the default desktop folder that contains designs. By default, sample designs that accompany this book are placed in the ADXBK9 folder.
- The main design window contains all the commands you need in order to refine, edit, explore, and analyze your experiment. They are arranged from top to bottom in the order that you should follow.
- Click **Explore** in the main design window to show plots such as the main-effects and cube plots.
- The online ADX Help system provides useful information about experimental design and analysis methods, and it explains how to implement them in the ADX interface.

Chapter 3

Full Factorial Designs

Chapter Contents

Chapter 3

Full Factorial Designs

Chapter Topics

In a two-level full factorial design, all combinations of the factor levels are run at least once. Consequently, these designs have full resolution, and all effects, including main effects, two-way interaction effects, and higher-order interactions, can be estimated.

Covered in This Chapter

- Defining variables
- Reviewing design details
- Exploring data
  - Using a main-effects plot
  - Using an interaction plot
  - Using a factorial plot
  - Using a box plot
- Fitting models for responses
  - Using automatic selection methods
  - Using a normal plot
  - Using a Pareto plot
  - Using the effect selector
- Optimizing multiple responses
  - Using the prediction profiler
  - Incorporating a desirability function

Experimental Objective

The following example is based on a case study described by Fossceco (1999). A pharmaceutical manufacturer formulates tablets by mixing excipients with active ingredients and processing this mixture. The mixture is passed through an extruder to make spaghetti-like strands, which are spheronized to create small pellets and then compressed into tablet form. An experiment is performed to maximize the yield (YIELD) and assure that the mean particle size (MPS) is about 1000 microns.

The factors represent different steps in the manufacturing process as shown in Table 3.1.

Table 3.1. Factors of the Tablet Formulation Example

Type	Name	Low	High	Description
Factor	FLUID	90	115	Moisture content (%)
	MIX	15	45	Mixing time (min)
	EXTRUDER	36	132	Extruder speed (rpm)
	SCREEN	0.6	1.0	Spheronizing screen size (mm)
	RESID	2	5	Residence time (min)
	DISK	450	900	Disk speed (rpm)
Response	YIELD			Drug yield (%)
	MPS			Mean particle size (microns)

Task List

- Create a two-level screening design.
- Define variables and review design details.
- Explore the data from the two-level screening design with plots.
- Fit a model to each response (YIELD and MPS).
- Optimize both responses by using a desirability function.

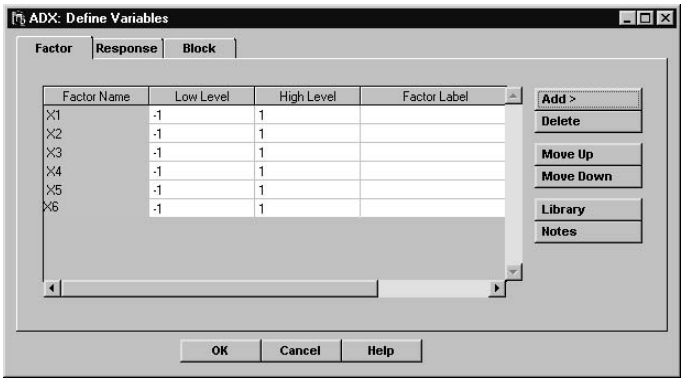
Creating a Full Factorial Design

In the section "Getting Started with a Simple Example" on page 13, you created a two-level design with default variable names. In this example, you will use the Define Variables window to specify information about factor names and factor levels. You will then select the full factorial design from several standard factorial designs recommended by ADX.

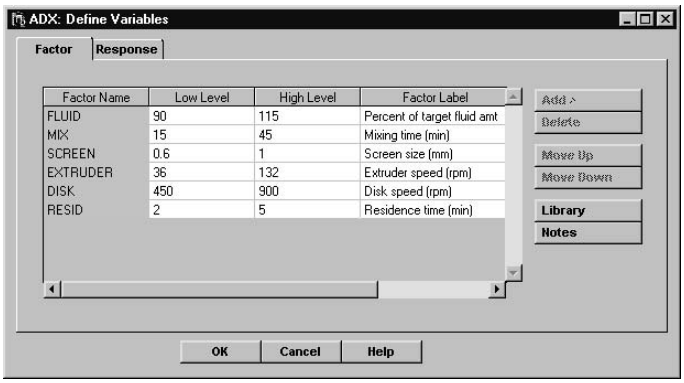
Defining Factors and Responses

The Tablet Formulation design includes responses. Here, however, you re-create this design so that you can learn how to define the variables for a design by following these steps:

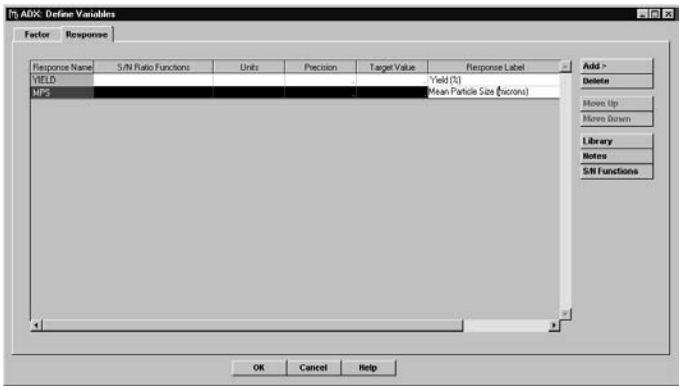
1. Select **File** → **Create New Design** → **Two-level** from the ADX desktop to open the main design window.
2. Click **Define Variables**.
3. Click **Add** and select **6** as the number of rows to add. ADX adds one row for each factor and automatically fills in coded levels for each of the factors.



4. Type a **Factor Name**, **Low Level**, **High Level**, and **Factor Label** for each factor as in Table 3.1. The factor name must be eight characters or less. The factor label is optional and will be used in graphs and reports if ADX has enough room to display it.



5. Click the **Response** tab to enter response variables.
6. Click **Add** and then select **1** from the number of rows. Note that one row is always provided for the first response variable.
7. Type the response names and labels for YIELD and MPS.

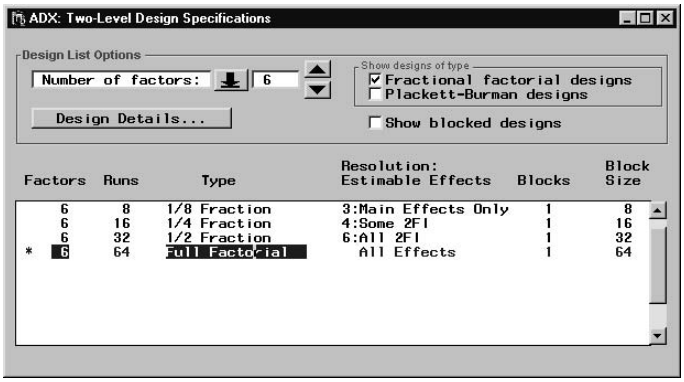


8. Click **OK** when finished. ADX asks if you want to save the changes.
9. Click **Yes**.

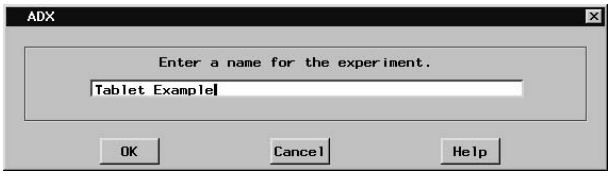
Selecting the Design

To complete the design, follow these steps:

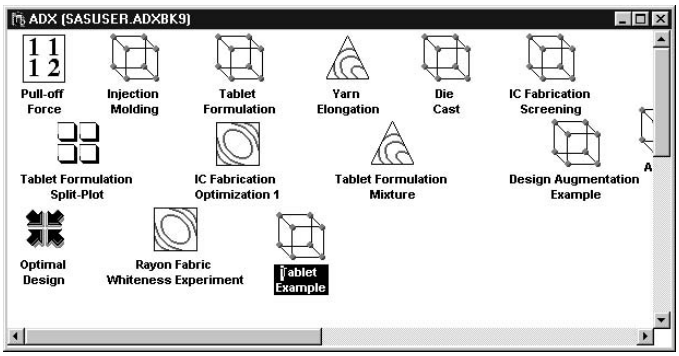
1. Click **Select Design** in the Two-level Design window.
2. Choose the full factorial design with **64** runs. This design enables estimation of all effects.



3. Close the Two-Level Design Specifications and Two-level Design windows, and click **Yes** to save the changes to the design.
4. Type **Tablet Example** in the resulting ADX dialog box.
5. Click **OK**.



The design is now saved.



Editing the Response Values

In practice, once your experiment is run and the response values are available, you click **Edit Responses** to enter the responses as explained in the section "Getting Started with a Simple Example" on page 13. Once the responses are entered, the design factors and their levels cannot be changed.

For this example, you can continue by opening the design named Tablet Formulation. This design is the same as the one you just created, but it includes the response values.

Reviewing the Design Details

Once the responses are entered into a design, you can review the design details.

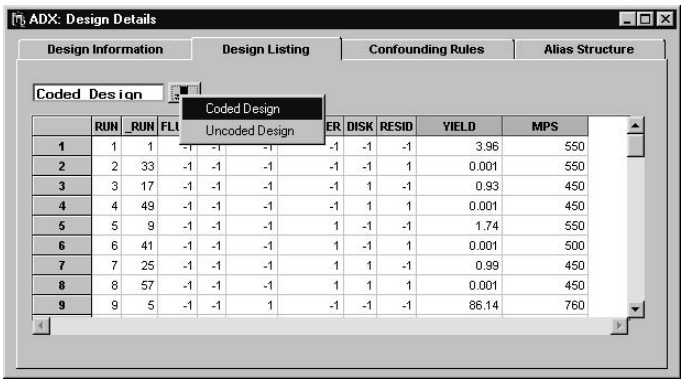
To access and review Tablet Formulation, follow these steps:

1. Select Tablet Formulation by double-clicking the **Tablet Formulation** design icon.
2. Click **Design Details**. Review the information on the **Design Information** and **Design Listing** tabs.

The design listing shows the uncoded design. Analyses are done on the coded design, which has a low level of -1 and a high level of 1. However, parameter estimates can be shown in uncoded form.

To view the coded design, follow these steps:

1. Click the **Coding Options Menu** icon at the top left to change to the coded design.
2. Close the window.



	RUN	_RUN	FLU			ER	DISK	RESID	YIELD	MPS
1	1	1	-1	-1	-1	-1	-1	-1	3.96	550
2	2	33	-1	-1	-1	-1	-1	1	0.001	550
3	3	17	-1	-1	-1	-1	1	-1	0.93	450
4	4	49	-1	-1	-1	-1	1	1	0.001	450
5	5	9	-1	-1	-1	1	-1	-1	1.74	550
6	6	41	-1	-1	-1	1	-1	1	0.001	500
7	7	25	-1	-1	-1	1	1	-1	0.99	450
8	8	57	-1	-1	-1	1	1	1	0.001	450
9	9	5	-1	-1	1	-1	-1	-1	86.14	760

Analyzing a Full Factorial Design

The ADX Interface provides a large repertoire of graphical tools and statistical methods for analyzing designed experiments. However, only a small subset of these techniques is needed for any given experiment.

The analysis strategy followed here for the Tablet Formulation design is as follows:

- Explore each response by using a main-effects plot, an interaction plot, an n-way effect plot, and a factorial plot with the Explore Data window.
- Select and investigate a model with the Choose a Response window.
- Determine which combination of factor levels will simultaneously provide the desired responses by using the prediction profiler in the Response Optimization window.

Note that for a design with sufficient observations to estimate the variance of the experimental error (underlying noise), ADX computes t-statistics with corresponding p-values for a formal assessment of statistical significance. This will always be the case for factorial designs, unless you set the master model to include every possible effect up to the highest-order interaction.

Exploring the Response Data

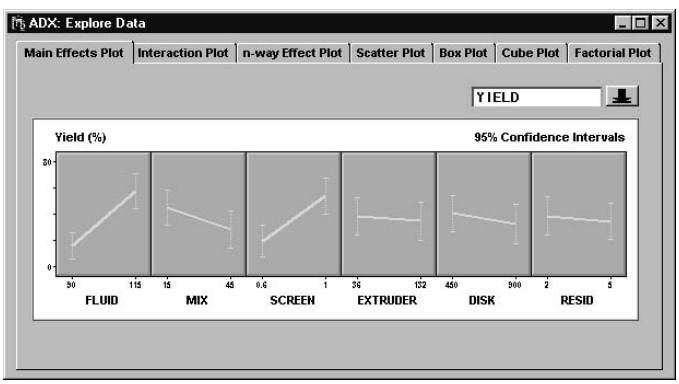
You can use the graphical tools listed in Table 3.2 in the Explore Data window to understand your data before fitting a model.

Table 3.2. Plots in the Explore Data Window and Their Uses

Plot	Use
Main effects	Examine main effect of factors
Interaction	Check for presence of 2-way interactions
n-way effect	Check for presence of up to 4-way interactions
Scatter	Examine run-order effects
Box	Compare response distributions across combinations of factor levels
Cube	Compare means for levels of factors
Factorial	Visualize factorial structure of responses with tree

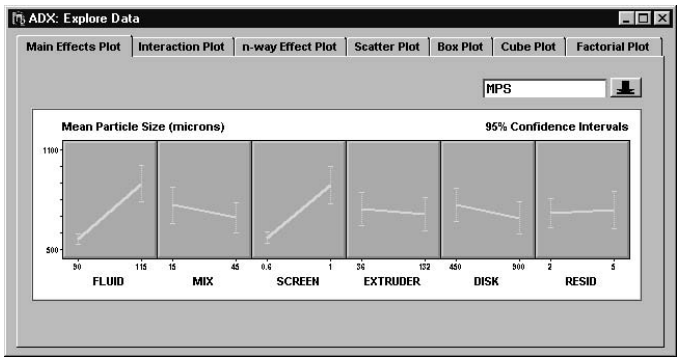
Main-Effects Plot

To view a main-effects plot, click **Explore**.



From this plot, it is clear that both FLUID and SCREEN individually have an impact on YIELD. The other factors seem to have less of an impact, and it is not clear whether their main effects will be flagged as significant in a formal test.

You can view the main-effects plot for MPS by clicking the down arrow beside **YIELD** and selecting **MPS**.



Before moving on to the interaction plot, select **View** → **Include in report** to save the main-effects plot for later reporting. You might want to increase the window size to make room for the whole plot.

Interaction Plot

Since a full factorial design provides information for all possible two-factor interactions, you should examine interaction plots.

Click the **Interaction Plot** tab.

The off-diagonal cells in the matrix are interaction plots, which show how the effect of one factor on the response changes based on the level of another factor. The diagonal cells are main-effects plots.

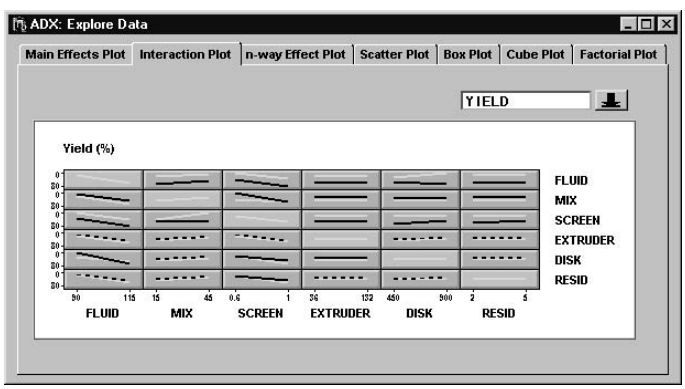


Table 3.3 explains how to interpret an interaction plot.

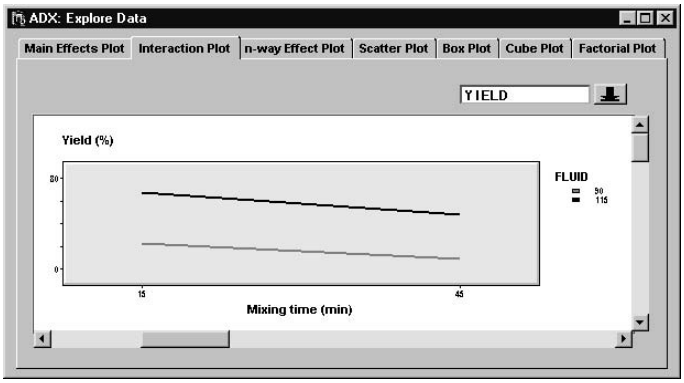
Table 3.3. Interpreting an Interaction Plot

Pattern	Interpretation
Parallel lines	No interaction effect
Intersecting lines	Interaction effect
Single striped line	Effects of factor pair coincide
Nonparallel nonintersecting lines	Possible interaction effect

The matrix of interaction plots shows several potentially significant interaction effects on YIELD, including FLUID*DISK, MIX*SCREEN, MIX*RESID, SCREEN*DISK, SCREEN*RESID, and EXTRUDER*DISK.

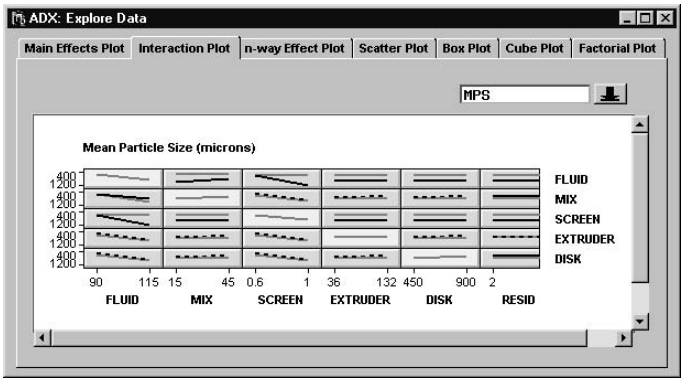
Individual plots in the matrix might be too small to see when there are a large number of factors. To increase the size of a cell, do one of the following:

- Right-click and select **Zoom**. The arrow changes to a magnifying glass. Click on the cell that you want to examine. This cell now takes up the whole screen. Right-click and clear **Zoom** to restore the matrix.
- Click and drag the lower-right corner of any cell to simultaneously resize all the cells. If you resize the window containing the interaction plot, the cells are resized automatically so that the plot continues to fill the window.



When the lines are not parallel but do not cross in the range of observed values, then it helps to look at confidence intervals. Right-click and select **Confidence intervals** to display 95% confidence intervals as error bars at the endpoints of the lines.

Click the down arrow and select **MPS** to view the interaction plot for the MPS response.



After exploring the interaction plot in detail, you should identify the following interaction effects as potentially significant as shown in Table 3.4.

Table 3.4. Potentially Significant Interactions

Response	Two-Factor Interactions
YIELD	FLUID*DISK, MIX*SCREEN, MIX*RESID, SCREEN*DISK, SCREEN*RESID, and FLUID*RESID
MPS	RESID*FLUID, RESID*MIX, RESID*SCREEN, RESID*DISK, FLUID*MIX

Of course, you should use a formal test, such as an analysis of variance, before drawing any firm conclusions. This is done in the section "Fitting a Model" on page 38.

The right mouse button offers other options. For example, you can label the plot lines directly by toggling off **Effects legend**. You can change fonts, colors, and line styles by selecting **Properties**.

Select **View** → **Include in report** to save the interaction plot in a report, which will be generated at the end of your session.

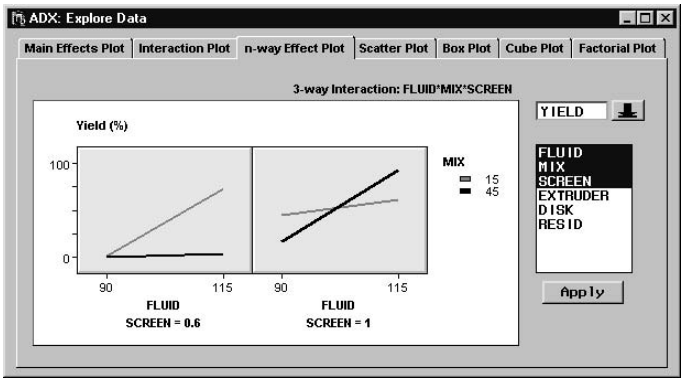
n-way Effect Plot

You can use the n-way effect plot to examine possible three- and four-way interactions. Since higher-order interactions are more subtle than two-way interactions, these plots are more complex.

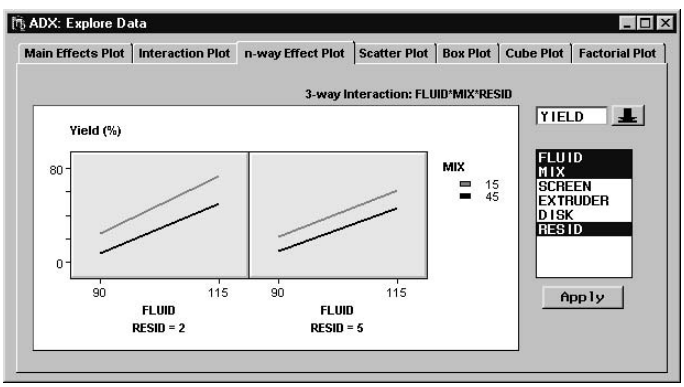
Click the **n-way Effect Plot** tab. ADX starts by presenting the two-way interaction plot for FLUID and MIX (this might change if you have used this window with this design before). In this case, 20 different three-way interaction plots can be generated, since there are 20 ways to select three factors from six factors.

To explore the three-way interactions, do the following:

1. Select **SCREEN** from the Select Effects list to highlight it. Click **Apply** to generate a three-way interaction plot for FLUID, MIX, and SCREEN.
2. The difference between the slopes of the two lines in each plot changes considerably between the two plots. This suggests the presence of a FLUID*MIX*SCREEN effect. A formal test of this effect is recommended; see the section "Fitting a Model" on page 38. In fact, a formal test will confirm the significance of this effect.



3. Select **View** → **Include in report** to save this graphic for later reporting. Keep the name in the resulting dialog box, and click **OK**.
4. Select **SCREEN** to clear it, and then select **RESID** to highlight that effect. Click **Apply** to generate a three-way interaction plot for FLUID, MIX, and RESID.



5. The two resulting plots look similar. This suggests that there is no three-way interaction between FLUID, MIX, and RESID.
6. Follow a similar process to examine some of the other possible 18 three-way interactions.

Note: In a three-way interaction plot, you look for a difference in the relationship between the slopes of the two lines between plots.

Alternatively, you can create an n-way effect plot from the **Interaction Plot** tab by moving the mouse pointer over the cell with the first two effects, right-clicking, and selecting **3FI plot->** . You can repeat this sequence from the resulting three-way interaction plot to generate a four-way interaction plot, or you can select four effects in the n-way plot.

Scatter Plot

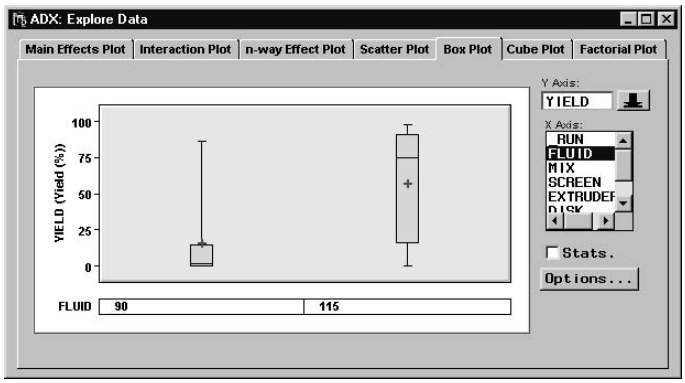
You can use scatter plots to look for run-order effects, also called serial, time-dependent, or learning effects. The scatter plot in ADX is interactive and is flexible enough to display any variable on the X or Y axis or as BY variables.

Scatter plots are discussed in detail in the section "Scatter Plot" on page 67.

Box Plot

You can use box plots to display the response distribution at different combinations of factor levels. Box plots can reveal differences in the response mean at different levels, suggesting main effects. Box plots can also reveal whether the response variation is homogeneous across factor levels, an assumption made in analysis of variance.

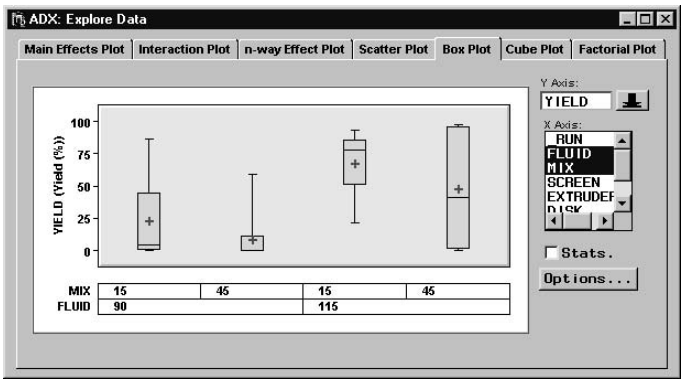
In the Explore Data window, click the **Box Plot** tab. A box plot with default settings will appear. A symbol, by default a plus sign (+), is drawn at the mean response for each factor level. The bottom and top of the box represent the first and third quartiles of the response, and a line is drawn at the median response. The whiskers represent the low and high values of the response.



The Y axis variable is YIELD, and the X axis variable is FLUID. To look at information about the response within a level of FLUID, double-click the box. The arrow changes to a magnifying glass, indicating the presence of detailed information.

Select **Stats.** to display some of these statistics under each box in the box plot. By default, ADX displays the number of responses, the mean, and the standard deviation. You can choose which statistics to display by clicking **Options** in the Box Plot window.

You can display more than one stratification variable at a time by selecting multiple variable names in the X Axis box. You do not have to hold down the CTRL key and click to select multiple stratification variables. Clicking on a variable already highlighted will deselect it.



Once you have selected the stratification variables, you can rearrange them by vertically dragging their names at the left of their level label boxes. Note that the arrow changes to a hand when you can drag variables.

Further options are available from the Box Plot window, which you can open by clicking the **Options** button. Options for changing fonts and colors are available when you right-click and select **Properties**.

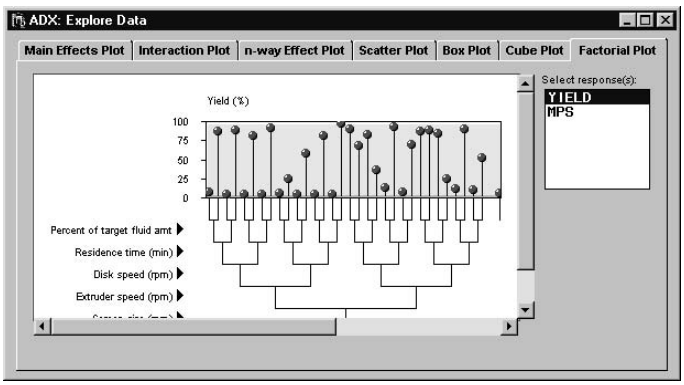
Cube Plot

The cube plot shows the average response at the high and low levels of three factors at a time, arranged on a cube. Further information can be found in the section "Cube Plot" on page 66.

Factorial Plot

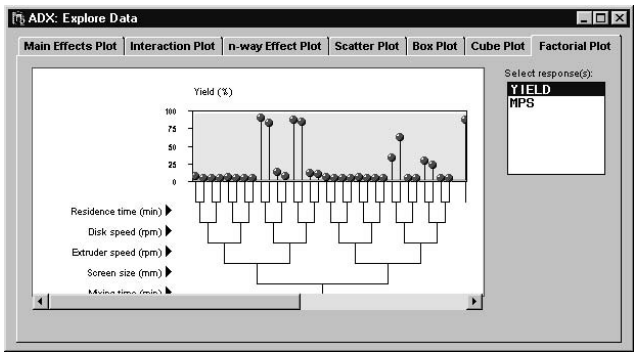
The factorial plot displays the mean response for the combination of factor levels displayed. The display changes if you change the order of the factors of the tree. Refer to Beckman (1996) for an in-depth discussion of factorial plots.

Click the **Factorial Plot** tab to display the factorial plot.



Interacting with the factorial plot helps you visualize which factors cause the largest change in response going from low to high. (You might want to maximize your window to view more of the plot.)

Place the mouse pointer over FLUID; it will change to a vertical double arrow. Click and drag to move FLUID so that it is the lowest branch, and observe the change in the factorial plot. Since moving FLUID to the bottom seems to separate most of the high responses from the low responses, it appears that FLUID is a significant main effect.



You can hide the factor level labels by clicking on the arrow to the right of the factor name. This helps you view more of the plot.

Fitting a Model

After exploring the data, you need to decide on a model you will use to predict or optimize the response. This model, referred to as the predictive model, will typically contain only effects that are considered to be significant.

When you first choose a design, ADX automatically defines a default master model to go with that design. Usually, the model includes an intercept, all main effects, and all two-factor interactions. Of course, you can choose a different master model. When you click **Fit**, ADX automatically fits the master model and highlights significant (active) effects in the Effect Selection for Yield (%) window. You can accept this list or refine it interactively by applying other automatic effect selection methods or by overriding the default effect selection. When you finish the effect selection process, ADX will retain the significant effects in a final model, which is called the predictive model.

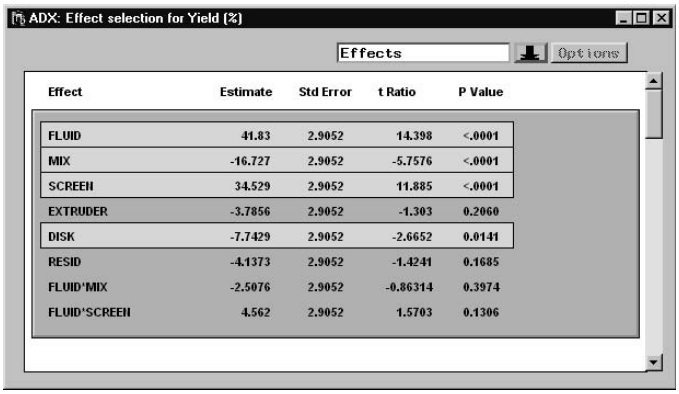
You should create a predictive model before using **Optimize**, but if you do not, ADX will use the master model for optimization.

To fit the master model, follow these steps:

1. Click **Fit** in the main design window. Since this design has more than one response, a dialog box will appear to let you to choose a response.

2. Select the **YIELD** response and click **Run**.
3. ADX will display a Check Fit Assumptions window. Since you want to analyze untransformed data for now, close this window.

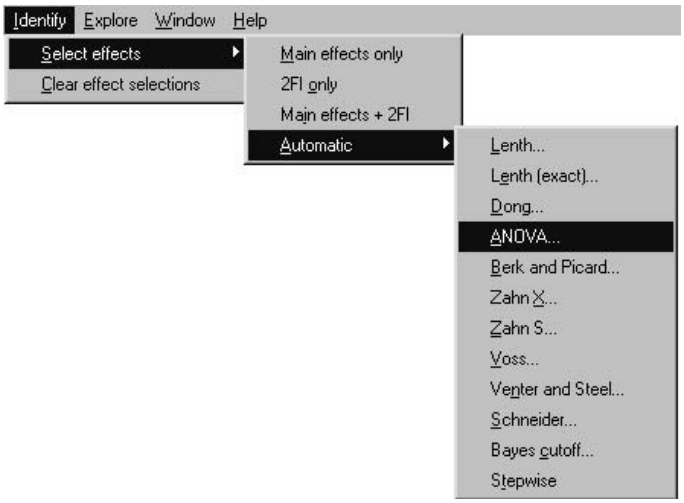
The Effect Selection for Yield (%) window displays the fitted master model and highlights the significant effects, which are determined by an automatic effect selection method. In this example, the master model includes all main effects and all two-factor interactions. Four of the main effects (highlighted) and a number of two-factor interactions (not shown) were found to be significant based on analysis of variance, which is the automatic effect selection method used by default.



Effect	Estimate	Std Error	t Ratio	P Value
FLUID	41.83	2.9052	14.398	<.0001
MIX	-16.727	2.9052	-5.7576	<.0001
SCREEN	34.529	2.9052	11.885	<.0001
EXTRUDER	-3.7856	2.9052	-1.303	0.2060
DISK	-7.7429	2.9052	-2.6652	0.0141
RESID	-4.1373	2.9052	-1.4241	0.1685
FLUID*MIX	-2.5076	2.9052	-0.86314	0.3974
FLUID*SCREEN	4.562	2.9052	1.5703	0.1306

ADX provides a variety of automatic selection methods to determine significant effects. Each of these methods is explained in the ADX Help.

You can see the methods available for effect selection by selecting **Identify** → **Select effects** → **Automatic**.



When there are enough runs to form an independent estimate of the error variance, analysis of variance (ANOVA) is the default method used for determining the selected effects. When the design is saturated (insufficient runs to estimate an error variance), Lenth's (1989) method for selecting effects is used. See the section "Analyzing Saturated Designs" on page 72 for more details on which effect selection methods are available for two-level designs.

Selecting **ANOVA** brings up the Parameters window, which enables you to change the alpha level used for effect selection. Note that other selection methods might have different parameters; the Parameters window will vary depending on the selection method you choose.

ADX highlights effects in the fitted model that are significant. By default, ADX selects the following significant effects:

- Main effects: FLUID, MIX, SCREEN, DISK
- Two-factor interactions: FLUID*DISK, MIX*SCREEN, SCREEN*DISK, SCREEN*RESID

ADX provides the ability to override selected effects. If you click on a highlighted effect to exclude it from the predictive model, ADX will consider it not to be significant, and the highlighting will disappear. If you click on an effect that is not highlighted, ADX will treat it as a significant effect, and it will be highlighted.

By default, ADX tests only two-way interactions. This is because the master model includes only intercept, main effects, and two-factor interactions. However, you might want to test for the presence of three-way interactions in this design. If so, you must change the master model. Follow these steps:

1. In the Effect Selection for Yield (%) window, select **Model → Change master model**.

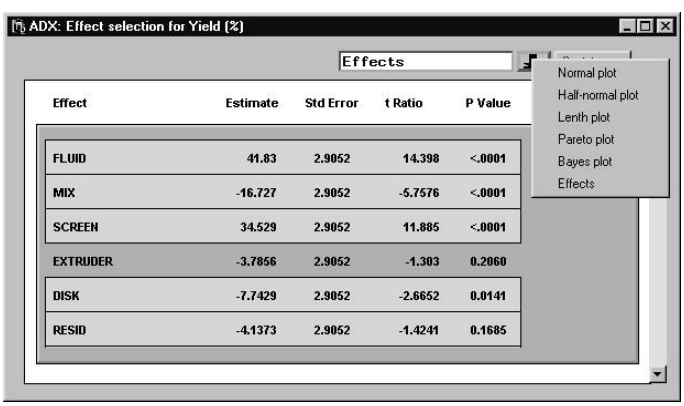
2. Select all the factors. This can be done by clicking FLUID and dragging down the list or by holding down the CTRL key and clicking on each factor.
3. In the edit box under the **Interaction** button, change the number to **3**. You can click the right arrow button.
4. Click **Interaction**. All combinations of three-way interactions will be added to the **Effects in Master Model** list. ADX will now test for these effects.
5. Click **OK**. ADX might open the Check Fit Assumptions window and indicate that a response transform is necessary. For now, close this window without making any changes.
6. Scroll through the Effect Selection for Yield (%) window and notice the presence of three-way interactions. The FLUID*MIX*SCREEN effect is automatically selected, indicating that this effect is statistically significant at the $\alpha = 0.05$ level. This agrees with the assessment made previously with the n-way interaction plot. ADX also selects FLUID*MIX*DISK, FLUID*SCREEN*DISK,
FLUID*SCREEN*RESID, MIX*SCREEN*DISK, and
MIX*SCREEN*RESID.

The effect selector is one of several displays you can use to display effects. Click the icon at the top to see a list of the different types of displays available for effect selection. Note that the selection of significant (active) effects is maintained from one display to another.

Normal Plot Display

The normal plot is a common method for displaying significant effects in factorial designs.

To display the normal plot, click the down arrow and select **Normal plot** from the pop-up menu. ADX highlights significant effects (according to the ANOVA method of selection) by using large, round symbol markers.



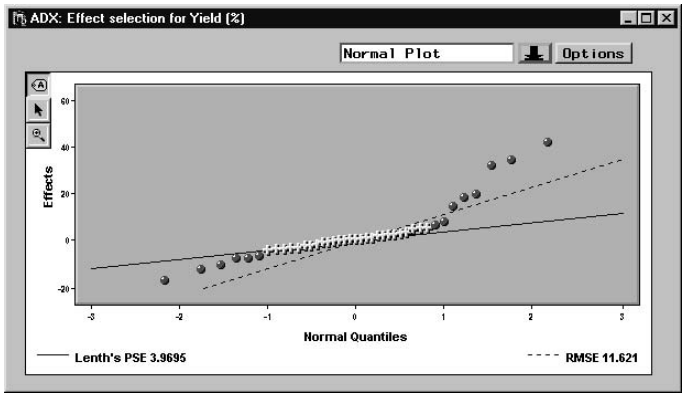
Effect	Estimate	Std Error	t Ratio	P Value
FLUID	41.83	2.9052	14.398	<.0001
MIX	-16.727	2.9052	-5.7576	<.0001
SCREEN	34.529	2.9052	11.885	<.0001
EXTRUDER	-3.7856	2.9052	-1.303	0.2060
DISK	-7.7429	2.9052	-2.6652	0.0141
RESID	-4.1373	2.9052	-1.4241	0.1685

Three different modes are available for interacting with this plot. Click on the corresponding icon to enter each mode:

Use the labeling mode to display the label for an effect by clicking on the point you want to label or remove the label from.

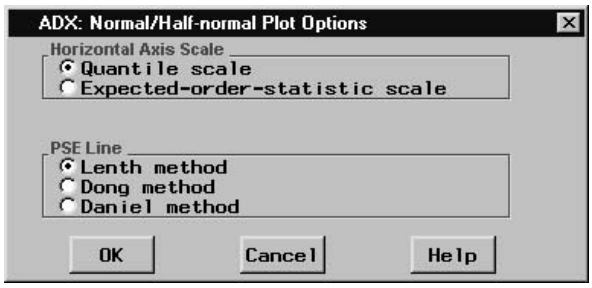
Use the selection mode to overwrite the selection of significant (active) effects by clicking on points you want to select or deselect. Significant (active) effects are highlighted.

Use the magnification mode to drag a rectangular area in the normal plot for magnification.



Note that two reference lines are displayed in the normal plot. These lines can be used for visual assessment of effects. Points that depart from the lines are considered to correspond with active effects.

Both lines pass through the origin. The slope of the dashed line is the root mean squared error (RMSE) calculated from ANOVA. This line is displayed only when an ANOVA can be performed. The slope of the solid line is Lenth's pseudostandard error (PSE). You can display alternative PSE reference lines by clicking the **Options** button from the **Normal Plot**. ADX provides options for the horizontal axis scale and for computing the pseudostandard error.



Select which options you want, and click **OK** to make the change.

Half-Normal Plot

Some experimenters prefer the half-normal plot over the normal plot. In a half-normal plot the magnitudes of the effects are displayed rather than the effects themselves.

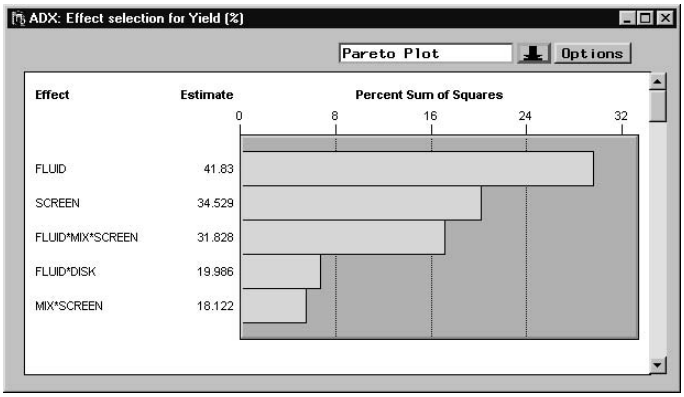
To display the half-normal plot, click the down arrow and select **Half-normal Plot** from the pop-up menu.

You can use exactly the same methods for changing the options and selected effects that you use in the normal plot.

Pareto Plot

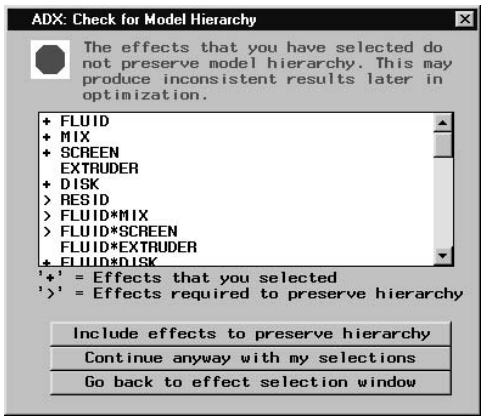
The Pareto plot displays effect estimates in decreasing order from largest to smallest. This makes it easy to determine the most important effects in the model. Pareto plot options can be used to change the type of estimate displayed from percent sum of squares to absolute effect.

To view the estimates with the Pareto plot display, click the down arrow and select **Pareto Plot** from the pop-up menu.



Determining the Predictive Model

Close the Effect Selection for YIELD (%) window. ADX will display a Check for Model Hierarchy window. ADX displays this window only when an interaction effect has been selected but not the corresponding lower-order interactions or main effects that come below it in the model hierarchy. For example, ANOVA identified the SCREEN*RESID effect as significant, but did not identify RESID.



In this window, ADX identifies selected effects with a (+) and effects that should be included in the predictive model according to the model hierarchy assumption with a (>). When this window appears, you should usually click **Include effects to preserve hierarchy** or **Go back to effect selection window** to change the selection in the Effect Selection for Yield (%) window. Click **Include effects to preserve hierarchy** now to return to the main design window.

Next, construct a predictive model for the MPS response by following these steps:

1. Click **Fit**.
2. Choose MPS as the response to fit. Click **Run**.
3. Close the Check Fit Assumptions window.
4. Change the master model to include three-factor interaction effects by selecting **Model** → **Change master model**. Select all effects, click the right arrow under **Interaction**, and then click **Interaction**. Click **OK**.
5. Close the Check Fit Assumptions window again.
6. Open the Effects Selection for MPS window with the Pareto plot.
7. Close the Effect Selection window for MPS, and click **Yes** to apply effect selections.
8. The Check for Model Hierarchy window appears. Click **Include effects to preserve hierarchy**.
9. In addition to the effects selected through ANOVA, ADX will include RESID, FLUID*DISK, MIX*SCREEN, MIX*DISK, and SCREEN*DISK in the predictive model for MPS.

Optimizing Multiple Responses

ADX provides a variety of methods for determining which factor settings yield optimal values for one or more responses. One of these methods uses an interactive response profile plot, referred to as the prediction profiler, which you can augment with

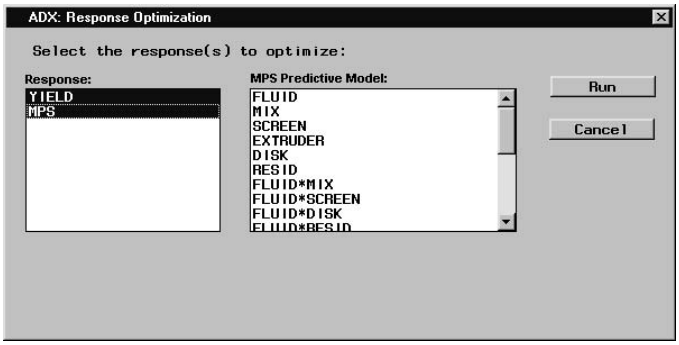
a desirability function for each response. For theoretical details, refer to Derringer and Suich (1980) and Montgomery (1997).

To find the optimal factor settings, do the following:

1. For each response you should have a predictive model. If not, ADX will use the master model for any response that does not have a predictive model.
2. Click **Optimize** in the main design window to open the Response Optimization window. Click **Run** to open the **Prediction Profiler**.
3. Review the **Prediction Profiler** settings.
4. Review the interactive features by right-clicking in the **Prediction Profiler**.
5. View the desirability function.
6. Set the desirability function for each response so that high values of YIELD are desirable, and set a target of 1000 for MPS where values even moderately far away have very low desirability.
7. Review the factor settings that maximize the overall desirability, where the overall desirability function is the geometric mean of all the individual desirability functions.
8. Use the prediction calculator to determine the predicted responses along with their standard errors.

Optimizing Factor Settings

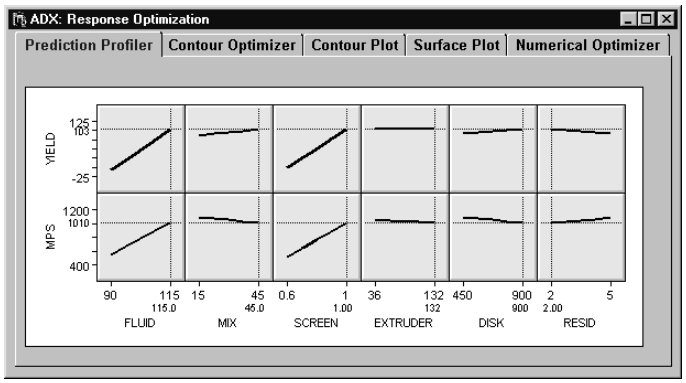
To get started, click **Optimize**. When you have multiple responses, ADX opens a window for you to select which responses to include in the optimization. Select both responses, YIELD and MPS. For each response ADX will remind you of the effects in the predictive model, as in the following illustration:



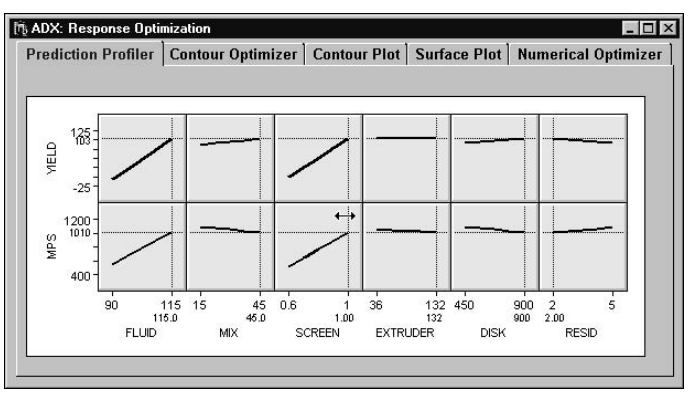
Click **Run**. ADX then displays the **Prediction Profiler** tab, which contains an interactive optimization tool that describes the change in responses as each factor is changed.

Interactive Prediction Profiler

The various components of the **Prediction Profiler** tab are as follows:



- The horizontal axis displays the factor names or labels with current settings indicated by vertical lines.
- The current setting for a factor can be changed by dragging the vertical line to the left or right.
- The vertical axis displays the predicted response for each response variable.
- The horizontal line is the predicted response for the current factor settings and will change as you change the factor settings.
- The plotted line in each plot is the prediction line for that response and that factor, assuming that all the other factors are held constant at the settings indicated by vertical lines.
- Prediction intervals can be toggled on or off by right-clicking and selecting **Prediction intervals** from the menu.

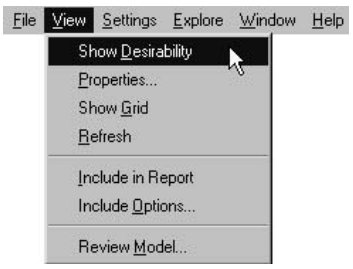


Simultaneous Optimization with Desirability Functions

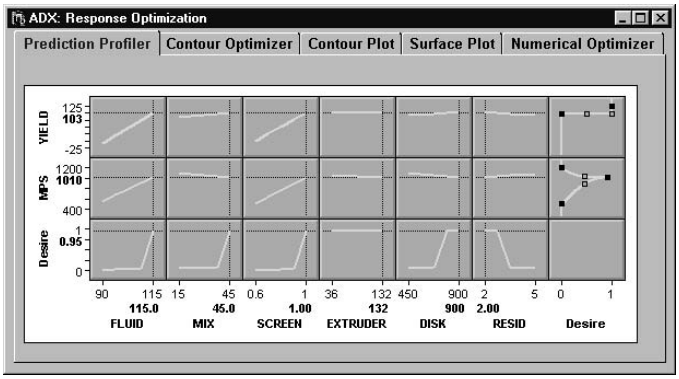
The performance of a product or process frequently depends on whether the responses meet certain criteria. Here you want to maximize YIELD while holding MPS to a target value.

Alternatively, you specify a desirability function for each response that expresses its criterion. ADX computes an overall desirability as the geometric mean (the nth root of the product of the individual desirability function, where n is the number of responses). You can then change the factor settings to find values that maximize the overall desirability. Refer to Derringer and Suich (1980) and Montgomery (1997) for more details.

Select **View** → **Show Desirability**.



ADX adds a desirability function for each response and an overall desirability trace for each factor.



The last column of cells is an interactive graph showing the desirability function for each response. The bottom row of cells displays the desirability trace corresponding to the settings of each factor.

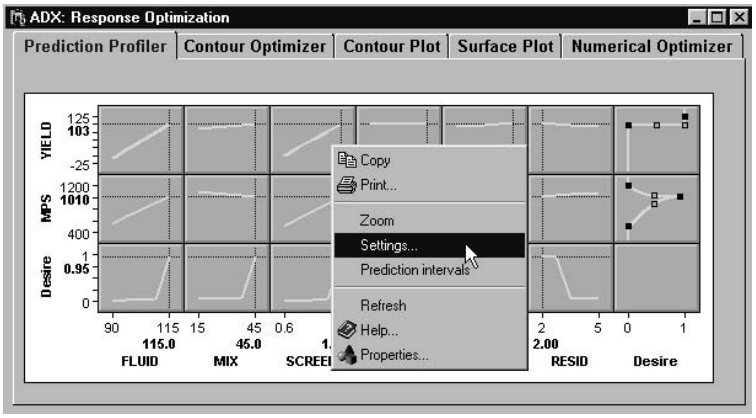
The desirability function has three points that can be set: high, low, and center. These points take on values from 0 to 1, where 0 is least desirable and 1 is most desirable. By default, this function is linear and maximizes the response.

Since only very high values of YIELD are desirable, you need to reset the function. You can set the desirability function in two ways:

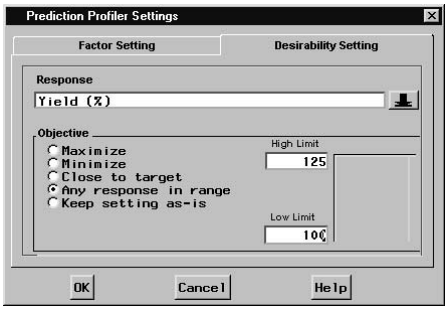
- indirectly, by changing the desirability settings in the Prediction Profiler Settings window
- directly, by clicking and dragging on the function line

To change the settings by using the Prediction Profiler Settings window, follow these steps:

1. Right-click and select **Settings** from the menu.



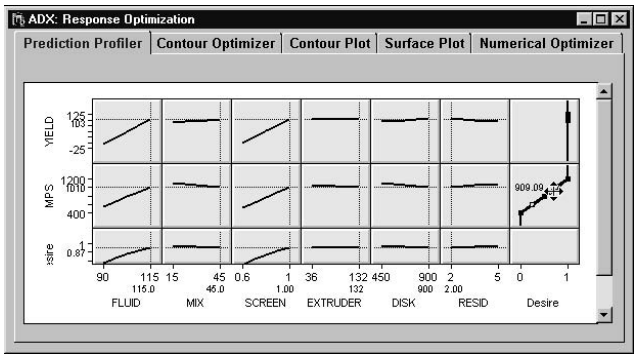
2. Click **Desirability Setting**.
3. The YIELD response should already be chosen; if not, click the down arrow and select it.
4. Select **Any response in range**.
5. Type **100** for the low limit. Keep the high limit setting.



6. Click **OK**.

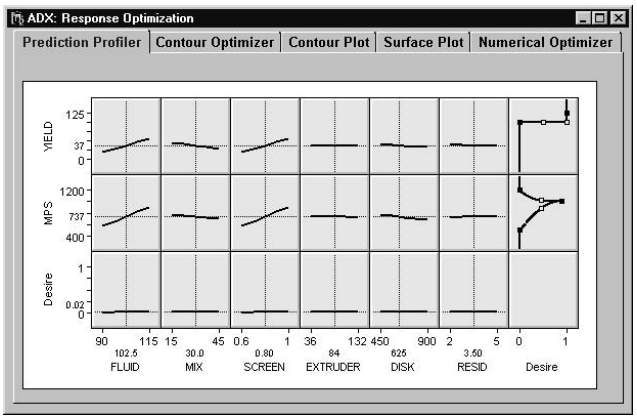
To change the settings by clicking and dragging, follow these steps:

1. Click and drag on the middle of the function line to the right so that the response has a desirability of 1 near 1000.



2. Click and drag the high and low ends of the function line to the left so that values not near 1000 have low desirability.
3. Since you want the desirability to decrease rapidly as the value moves away from 1000, drag the hollow lines to change the curvature of the desirability line.

The result should look like the following figure:

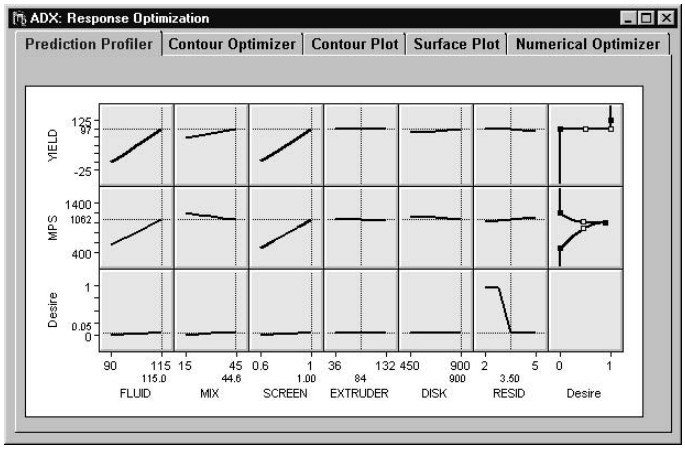


The new desirability traces for each factor are given in the row at the bottom of the **Prediction Profiler**. The goal is to find factor settings that provide an overall desirability value close to 1. The individual factor desirability traces indicate how a factor will affect desirability. For example, shifting MPS away from 1000 decreases the desirability rapidly, and shifting YIELD to less than 100 results in a zero desirability.

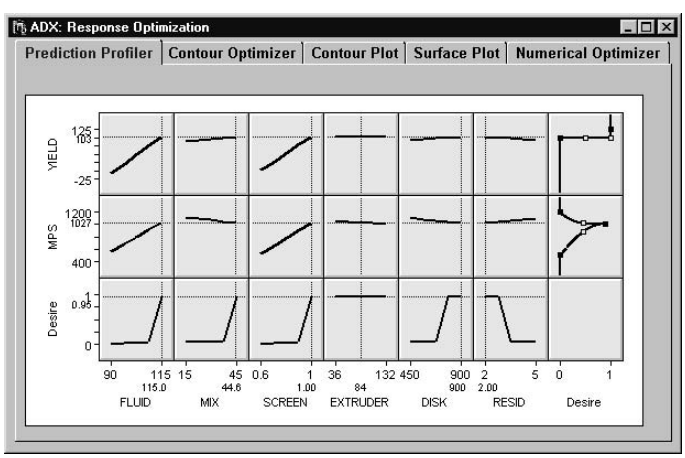
At the factor setting where all factors are at their midpoint, the lack of slope for each factor indicates that desirability will be little affected by shifting any one factor.

This is because the desirability is zero over a large interval of YIELD. However, the desirability traces are likely to change once factor settings are changed, especially since several significant interactions are identified. (Note that you might see slight differences between what is on your screen and what is shown here. The appearance of the traces depends on how the desirability functions are set.)

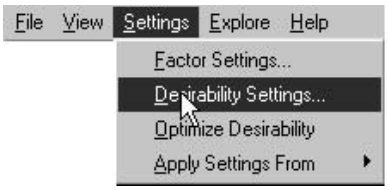
Shift FLUID, MIX, SCREEN, and DISK to their highest settings. The desirability trace for RESID changes dramatically.



Shift RESID to its lowest settings. The desirability for this new setting is greater than 0.9. Note that the trace for EXTRUDER is flat; this indicates that you can set EXTRUDER according to other conditions without severely affecting your optimization.



You can also find the settings that maximize the desirability by selecting **Optimize Desirability** from the **Settings** menu. In this case, doing so with the preceding settings will only move EXTRUDER to its highest setting (this raises the desirability by a very small amount).

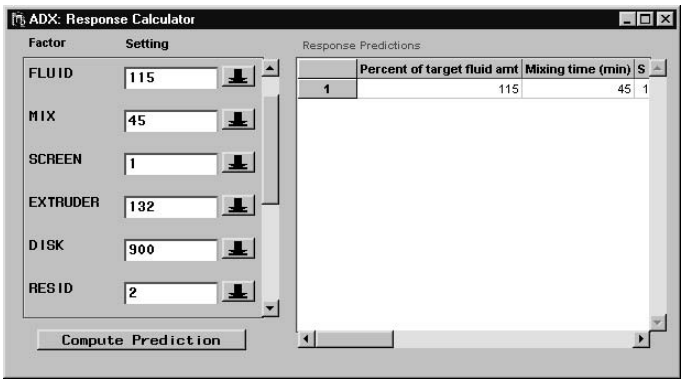


Once you have maximized desirability, you can review the individual factor traces to see how changing each factor changes the desirability, and in what direction.

Using the Optimization Results

There are several facilities you can use once you have identified the optimal factor settings:

1. Select **View** → **Include in Report** and click **OK** to save the **Prediction Profiler** display in a report.
2. Select **Explore** → **Response calculator**. The Response Calculator window will appear. Note that the factor settings are the same as those in the **Prediction Profiler**.
3. Click **Compute Prediction**. A row will be added to the spreadsheet. This row contains the factor settings, the predicted values for all responses, and the standard errors for all predictions within parentheses.



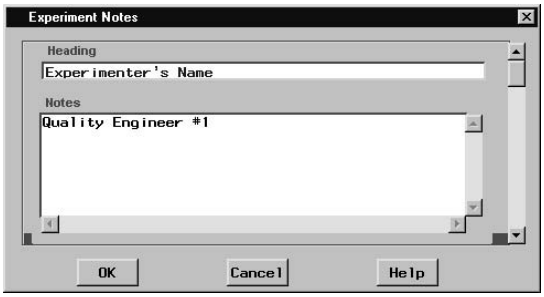
4. Close the window and click **OK** to return to the Response Optimization window.
5. Close the Response Optimization window and click **Yes** to return to the main design window.

You are now ready to report your results.

Tying It All Together

The reporting mechanism in ADX enables you to share your results on a corporate local area network or the World Wide Web. Before generating a report, do the following:

1. Click **Experiment Notes**.

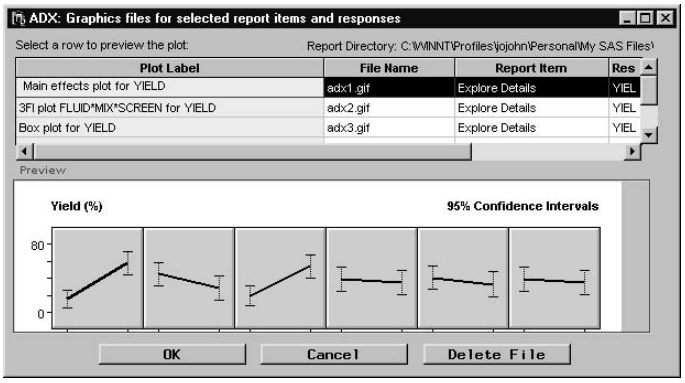


2. A dialog box will appear with two fields: **Heading** and **Notes**. The heading in this case is Experimenter's Name. Type your name in the second field.
3. Scroll down and enter other pertinent information about your experiment.
4. Click **OK** to return to the main design window.

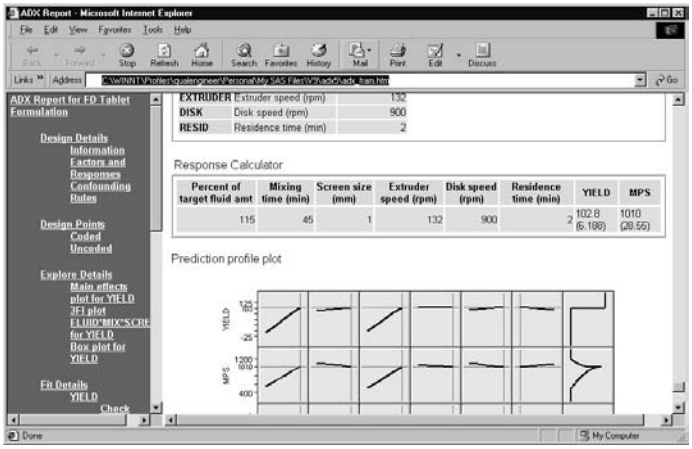
It is always a good idea to enter this information, especially if the results of this experiment will be stored in an experimental database or data warehouse.

To generate a report, do the following:

1. Click **Report** in the main design window.
2. The ADX Report window will appear. Ensure that all report items are selected (holding down the SHIFT key and clicking if necessary).
3. Click the **Responses** tab, and hold down the SHIFT key and click to ensure that all responses are selected.
4. Select **HTML**.
5. Click **Graphics Files**. A window with a list at the top and an image viewer at the bottom will appear. Every plot for which you selected **View** → **Include in Report** will appear here. Click the appropriate row to view the graphic.



6. If you decide not to include a particular graphic, select the appropriate row and click **Delete File**.
7. Click **OK** to close the window and return to the ADX Report window.
8. Click **Generate Report** to generate an HTML report and view it in your default browser.



Points to Remember

- You can create different folders for organizing your designs in ADX.
- Once responses are entered into a design, the design is frozen and can no longer be changed.
- ADX uses coded values (-1 for low and 1 for high) for factors when fitting.
- The Explore Data window provides a variety of graphical displays for examining the structure of your data prior to model fitting.
- Main-effects plots provide a way to look at the effects of individual factors on the response.

- Interaction plots indicate the presence and strength of two-factor interactions.
- The Zoom feature provides more detail for individual cells within the interaction matrix.
- Factorial plots help you to visualize the factorial structure in tree form.
- The Effect Selection window provides a wealth of methods for automatically selecting significant effects in a fitted master model.
- ADX uses ANOVA as the automatic effect selection method for a full factorial model with degrees of freedom for estimating error. ADX uses Lenth's method for saturated factorial designs.
- The Effect Selection window offers a variety of graphical methods for displaying significant effects, including normal and Pareto plots.
- ADX follows the principle of model hierarchy for building the predictive model. You can override this principle.
- The **Prediction Profiler** is an interactive tool for exploring the effect of changing factor settings on predicted values.
- You can augment the **Prediction Profiler** with desirability functions that you can use to find those factor settings that maximize the overall desirability.

Chapter 4

Fractional Factorial Designs

Chapter Contents

Chapter 4

Fractional Factorial Designs

Chapter Topics

Fractional factorial designs are commonly used for finding important effects, especially when runs are expensive. ADX helps you choose an appropriate two-level fractional factorial design and analyze the responses to determine significant effects.

Covered in This Chapter

- Defining variables
  - Using the factor library
- Selecting a design
  - Design information
  - Confounding rules
  - Alias structure
  - Custom designs using the ADX Interface to the FACTEX procedure
- Exploring data
  - Interaction plots
  - Factorial plots
- Fitting a model
  - Checking assumptions
  - Using half-normal plots
- Optimizing a response
  - Prediction profiler
  - Desirability function
- Running an experiment-saturated design with a saturated design

Experimental Objective

A quality engineer observes that too many units manufactured by an injection molding process exhibit excessive shrinkage. He designs a fractional factorial screening design to determine the causes of shrinkage with variables as shown in Table 4.1.

Table 4.1. Variables in the Injection Molding Experiment

Type	Variable	Factor Name	Low	High
Factors	MTEMP	Mold temperature	-1	$+1$
	SSPD	Screw speed	-1	$+1$
	HTIME	Holding time	-1	$+1$
	CTIME	Cycle time	-1	$+1$
	GSIZE	Gate size	-1	$+1$
	HPRESS	Holding pressure	-1	$+1$
Response	SHRINK	Observed shrinkage ($\times$ 10)		

The goal is to minimize shrinkage.

Task List

- Select and create a fractional factorial design.
- Review the confounding rules for the design.
- Review the aliasing structure of the design.
- Explore the response data with interaction and factorial plots.
- Fit a model for the response.
- Find factor settings for optimum response.

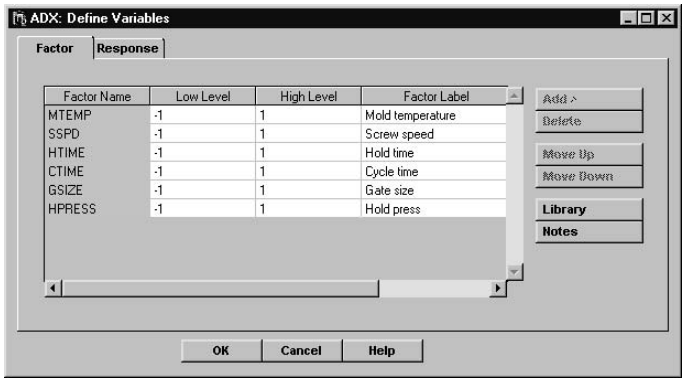
Selecting a Fractional Factorial Design

ADX shows the properties of a design under consideration. Using the tools in ADX, you can select the fractional factorial design that best fits your experimental situation.

Defining Variables

Defining the variables for a fractional factorial design is the same as those for a full factorial design, which are described in the section "Creating a Full Factorial Design" on page 26. Follow these steps:

1. Select **File**→ **Create New Design**→ **Two-level** from the ADX desktop to open the main design window.
2. Click **Define Variables**.
3. The Define Variables window will appear. Click **Add** and select **6** as the number of rows to add. Recall that the low level is set to -1 and the high level is set to 1. Enter the factor names as shown in the illustration.



4. Click the **Response** tab to enter response variables.
5. Change the response name to **SHRINK** and the label to **Observed Shrinkage**.
6. Click **OK**.
7. ADX asks if you want to save the changes. Click **Yes**.

Selecting Standard Designs

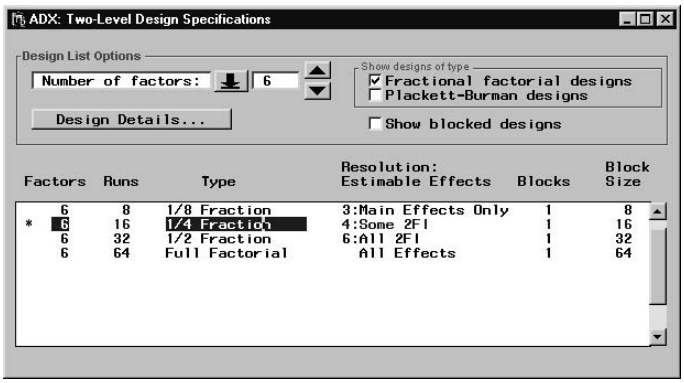
Selecting a fractional factorial design is more complicated than selecting a full factorial design, since there are additional properties to consider. ADX shows the properties of each design before creating it so that you can make the best decision. These properties are as follows:

- Design fraction
- Number of runs
- Design resolution
- Design listing, both coded and uncoded
- Confounding rules
- Alias structure
- Variance dispersion

To select a standard fractional factorial design, do the following:

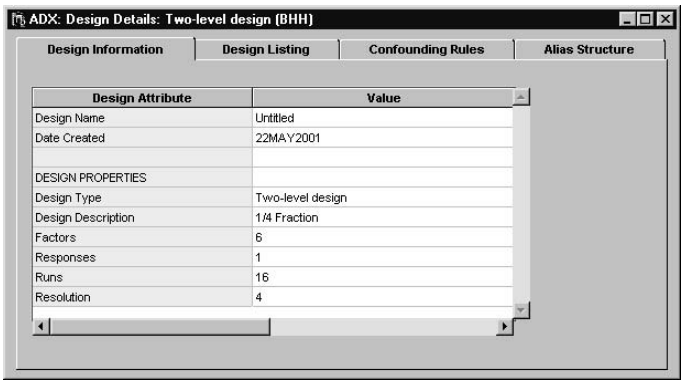
1. In the main design window, click **Select Design**.
2. The Two-Level Design Specifications window will appear. The default number of factors selected will be the same number as you created in the Define Variables window.
3. By clicking the down arrow beside **Number of factors**, you can choose other properties you want the design to have: number of runs, resolution, number of blocks, and block size. Usually, it is easiest to leave **Number of factors** selected.

4. You can choose a list of fractional factorial designs, Plackett-Burman designs, or both by selecting the appropriate boxes. For this example, select **Fractional factorial designs** and clear **Plackett-Burman designs**.
5. If your design has more than one block, check **Show blocked designs**. In this case, you are not using a blocked design, so leave **Show blocked designs** cleared.
6. Select the **1/4 Fraction** design.



Viewing Design Properties

Click **Design Details** (in the design selection window) to determine the resolution of the design.



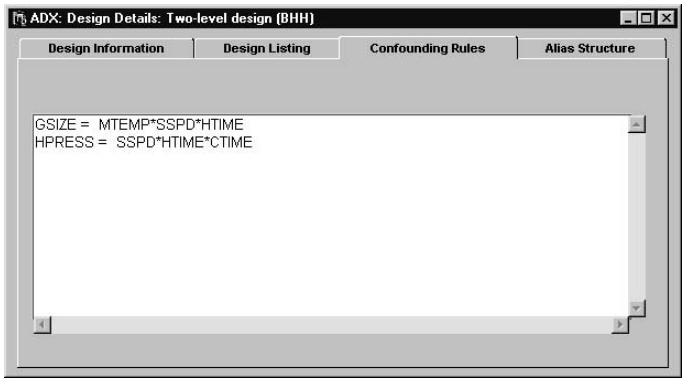
This design has Resolution 4, which means that main effects are free of two-factor interactions, but some two-factor interactions are aliased with each other.

Confounding

The **Confounding Rules** tab tells you how the design was generated. This design was generated according to two rules:

- GSIZE = MTEMP*SSPD*HTIME
- HPRESS = SSPD*HTIME*CTIME

Thus, in each run, the coded level of GSIZE is the product of the coded levels of MTEMP, SSPD, and HTIME, and the coded level of HPRESS is the product of the coded levels of SSPD, HTIME, and CTIME.

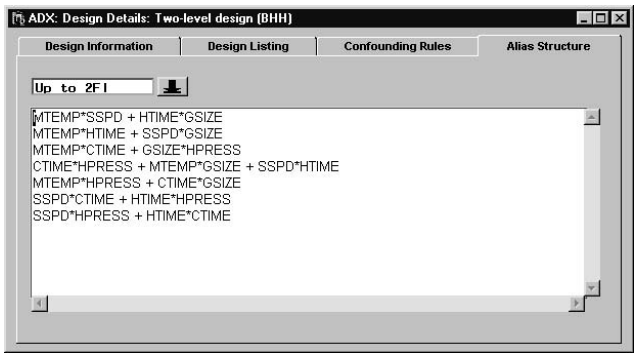


Alias Structure

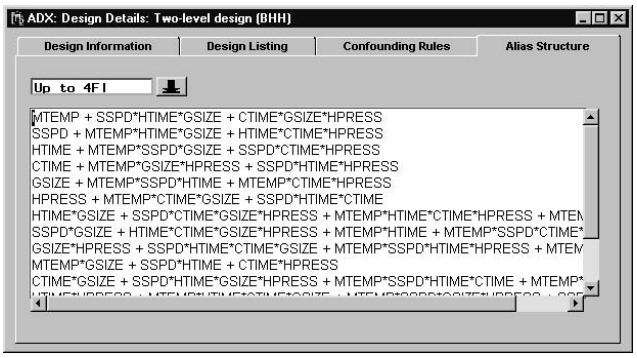
In fractional factorial designs, some effects are aliased with others. The **Alias Structure** tab describes the aliasing for main effects and for two-factor, three-factor, and four-factor interactions. It is important to review the aliasing structure of a design to make sure that potentially important interactions will be estimable in your design.

To view the alias structure, follow these steps:

1. Click the **Alias Structure** tab.



2. By default, ADX shows any aliasing that occurs between main effects and two-factor interactions. Since this is a Resolution 4 design, main effects do not appear in alias strings with two-factor interactions, but some two-factor interactions are aliased with each other. For example, the string MTEMP*SSPD+HTIME*GSIZE means that the interaction between MTEMP and SSPD will be indistinguishable from the interaction between HTIME and GSIZE. If no more than one of these interactions is potentially important, then this aliasing is acceptable.
3. Use the arrow in the upper-left to view the alias structure for higher-order interactions. The window shows the aliasing between main effects and three-factor interactions and among two-factor interactions, other two-factor interactions, and four-factor interactions.



4. Close the window to create the design.

For more information about these standard designs, refer to Box, Hunter, and Hunter (1978).

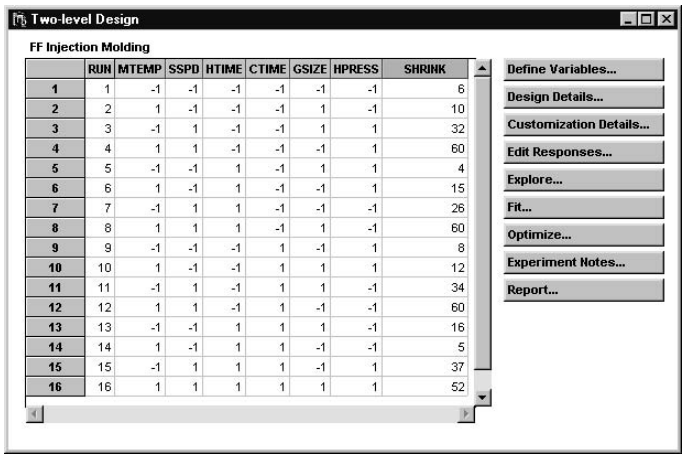
Randomizing the Run Order

After you have selected the design and before you run the experiment, you should randomize the order of the runs. In the main design window, click **Edit Responses**. Randomize the run order by selecting **Design** → **Randomize Design**.

In practice, you would be ready to run the experiment at this point. You can print a copy of the design by selecting **File** → **Print** or export an electronic copy by selecting **File** → **Export Design**.

Entering Response Values

Assuming you had completed the experiment, you could enter the responses in the spreadsheet in the Edit Responses window or import them as in Chapter 14, "Useful Techniques." Here, you can complete the design by entering the responses shown in the following window. However, it will be faster to close this design and open the Injection Molding design, which already contains the responses.



	RUN	MTEMP	SSPD	HTIME	CTIME	GSIZE	HPRESS	SHRINK
1	1	-1	-1	-1	-1	-1	-1	6
2	2	1	-1	-1	-1	1	-1	10
3	3	-1	1	-1	-1	1	1	32
4	4	1	1	-1	-1	-1	1	60
5	5	-1	-1	1	-1	1	1	4
6	6	1	-1	1	-1	-1	1	15
7	7	-1	1	1	-1	-1	-1	26
8	8	1	1	1	-1	1	-1	60
9	9	-1	-1	-1	1	-1	1	8
10	10	1	-1	-1	1	1	1	12
11	11	-1	1	-1	1	1	-1	34
12	12	1	1	-1	1	-1	-1	60
13	13	-1	-1	1	1	1	-1	16
14	14	1	-1	1	1	-1	-1	5
15	15	-1	1	1	1	-1	1	37
16	16	1	1	1	1	1	1	52

Note: Once you have edited the responses for a design, you cannot modify the factors of the design.

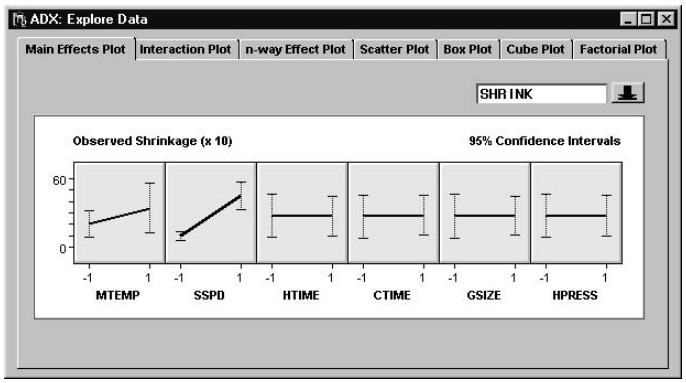
Exploring Responses

The data exploration tools for a full factorial design, discussed in Chapter 3, are available for a fractional factorial design. However, due to aliasing, they should be used with care.

To open the Explore Data window, click **Explore** in the main design window.

Main-Effects Plot

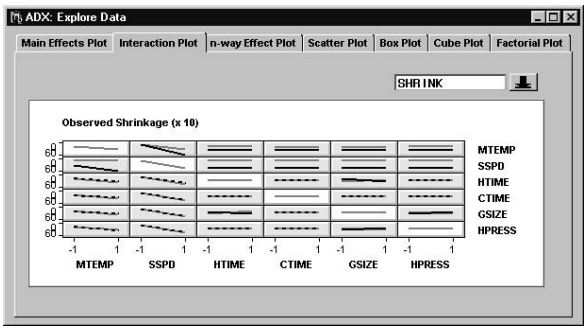
In any regular fractional factorial design, uncorrelated estimates of the main effects are available. However, you should keep in mind that main effects are aliased with certain interaction effects. If any of the interactions aliased with a main effect are active, the main-effect estimate will be biased. Usually, if a main effect is part of a significant contrast, the main effect is assumed to be significant. The effects in the alias string can be further explored in subsequent experiments, which are designed to “break the alias chain” by ensuring that effects of interest are estimable and free of other effects.



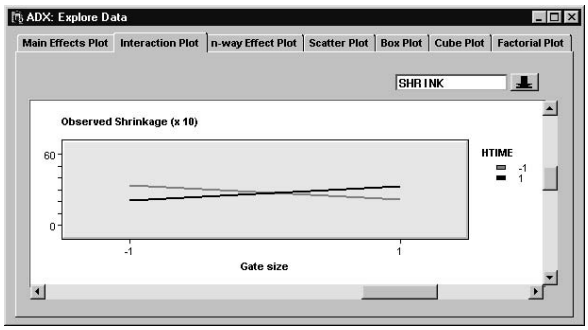
Interaction Plot

The interaction plot is also available for regular fractional factorial experiments. This plot is not recommended for use with Resolution 3 designs, because two-factor interactions are aliased with main effects. For Resolution 4 designs, it is possible to estimate some two-factor interactions, but you should refer to the alias structure when using the interaction plot. In Resolution 5 designs, all two-factor interactions are free of each other (though they might be aliased with even higher-order interactions). For this reason, it is safest to use the interaction plot in the Resolution 5 case.

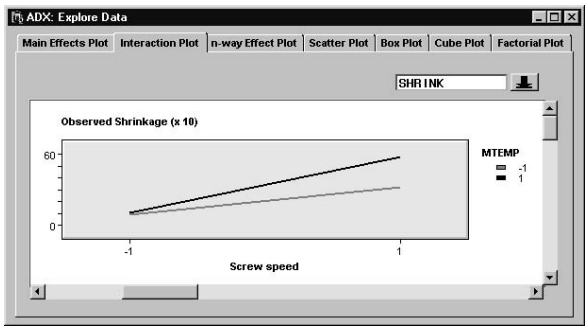
To view the interaction plot, click the **Interaction Plot** tab.



There is an apparent interaction between HTIME and GSIZE. Right-click, select **Zoom**, and click on the HTIME*GSIZE cell to magnify it.



Now, zoom in on the MTEMP*SSPD cell. If you were to calculate the difference in slopes between these two lines, it would be the same as the difference in slopes between the two lines in the HTIME*GSIZE cell.

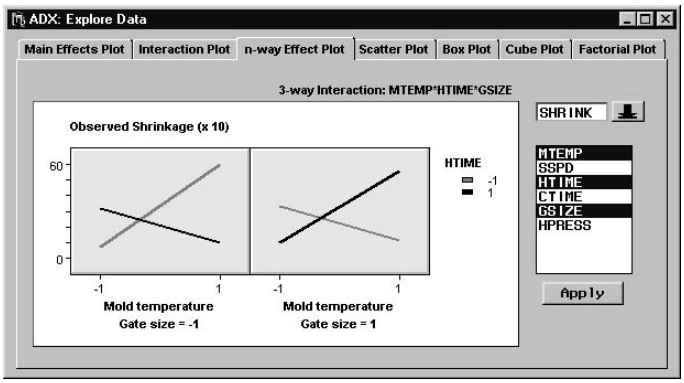


Recall that MTEMP*SSPD and HTIME*GSIZE are aliased. Therefore, it is impossible to determine whether one or both of these effects are significant, even though their interaction plot strongly suggests a significant effect. These effects could be separated through a follow-up. See Chapter 13 on design augmentation to break an alias chain.

n-way Effect Plot

Because of aliasing, the n-way effect plot is seldom used for fractional factorial designs, and when it is used it should be interpreted with care. Three- and four-factor interactions tend to be aliased with main effects or two-factor interactions, rendering the n-way effect plot for these effects meaningless.

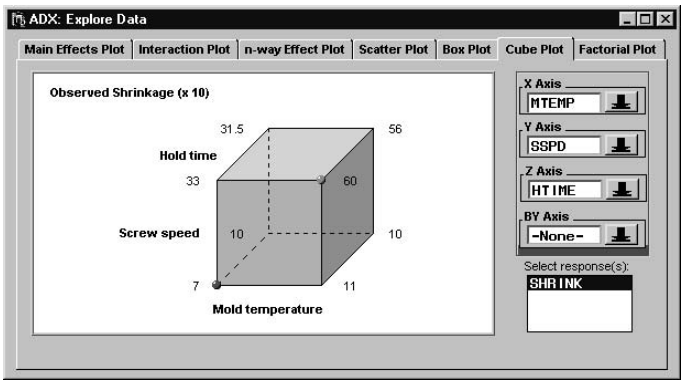
For example, the following plot suggests a significant effect (because the lines are crossed), but the three-factor interaction is aliased with SSPD, which the main-effects plot suggests is significant. Formal tests cannot unravel the two effects. If there is good reason to suspect that MTEMP*HTIME*GSIZE is active, separating it from SSPD will require more experimentation.



Cube Plot

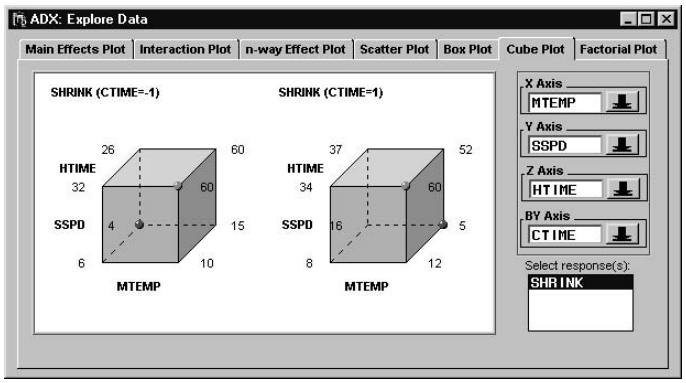
Click **Explore** and then the **Cube Plot** tab to display a cube plot. (See the section "Getting Started with a Simple Example" on page 13 for another example of using cube plots.)

The response means of the factor levels are displayed on the corners of the cube. Low levels of the factors are to the left, front, or bottom, and high levels are to the right, back, or front of the cube dimension. Different colored symbols mark the high and low responses on the cube.



The extreme values occur when HTIME and MTEMP are both at their lowest values and when HTIME and MTEMP are both at their highest values. Since the shrinkage averages at the front of the cube are close to those in the corresponding positions at the back, you might conclude that SSPD is not active. On the other hand, the shrinkage averages in the other dimensions indicate that the HTIME and MTEMP main effects, and their interaction, are active.

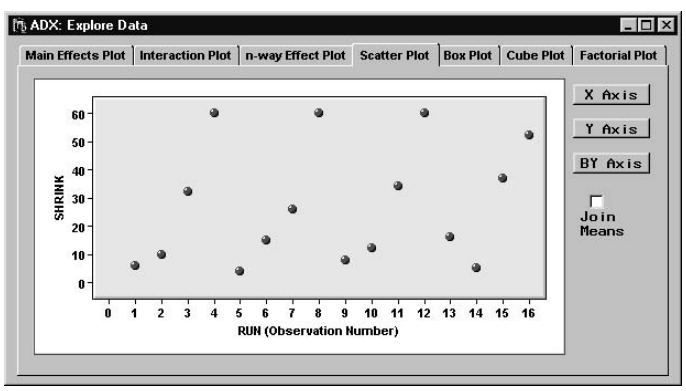
The ADX system also provides side-by-side cube plots at different levels of a fourth factor. To view cube plots side by side, select a factor not already displayed from the **BY Axis** list.



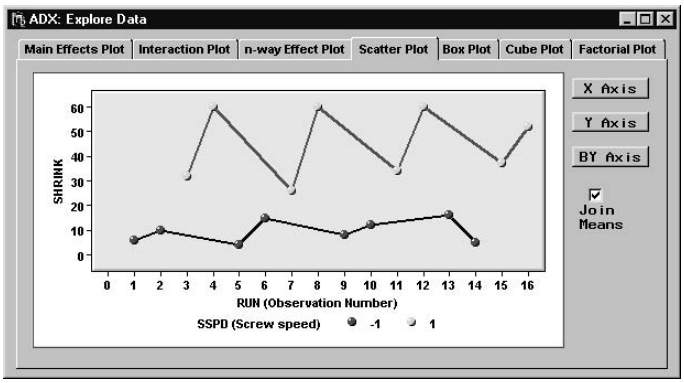
The difference in average shrinkage at the rear left bottom corners of the cubes is -12, while the difference at the rear right bottom corners is 10. This suggests a possible interaction between CTIME and MTEMP. However, this needs to be confirmed with a formal test.

Scatter Plot

A scatter plot is often used to determine run-order effects. Click the **Scatter Plot** tab. The default plot displays an unusual pattern, which might be the result of a time dependence.

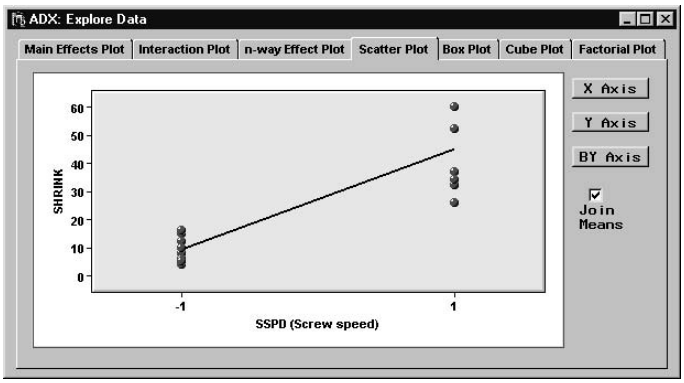


However, it is revealing to select **SSPD** as the **BY Axis** variable and select **Join Means**.

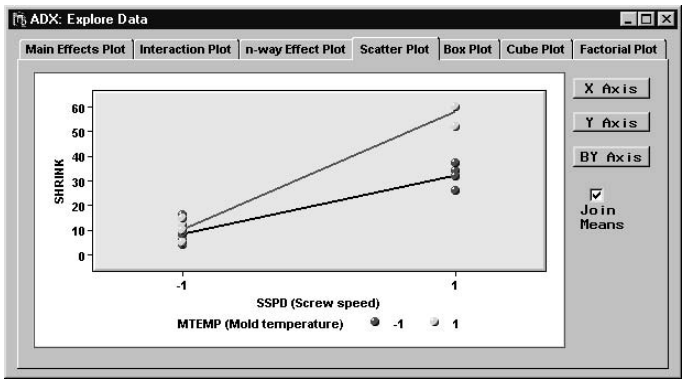


This plot suggests that SSPD is significant and that run order is not randomized.

You can also use the scatter plot to create a main-effects plot in which the individual response values are displayed in addition to their averages. For example, the following plot shows the main effect of SSPD.



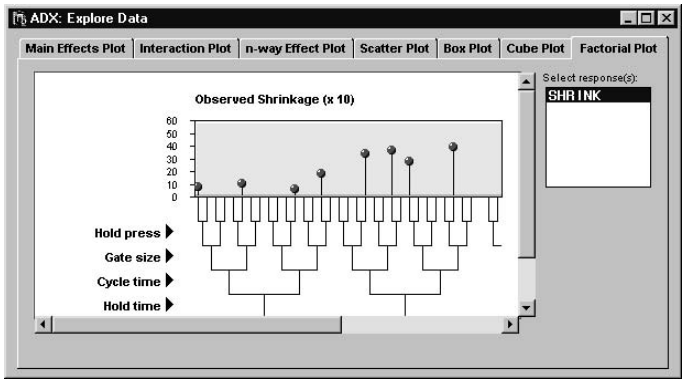
Likewise, you can use the scatter plot facility to create an interaction plot in which the individual response values are displayed. For example, the following is an interaction plot for MTEMP*SSPD, which you can create by selecting MTEMP as a BY variable by clicking the **BY Axis** button.



You can use the scatter plot to plot any variable in the design against any other variable by selecting a third BY variable (from the menu that appears when you click the **BY Axis** button) to classify the points on the plot. This is useful for creating custom plots for situations in which the standard plots might not apply.

Factorial Plot

The factorial plot was discussed in detail in the section "Factorial Plot" on page 37. When you use the factorial plot for a fractional factorial design, not all of the tree leaves are present because not all combinations of factor levels are present.



Analyzing a Fractional Factorial Design

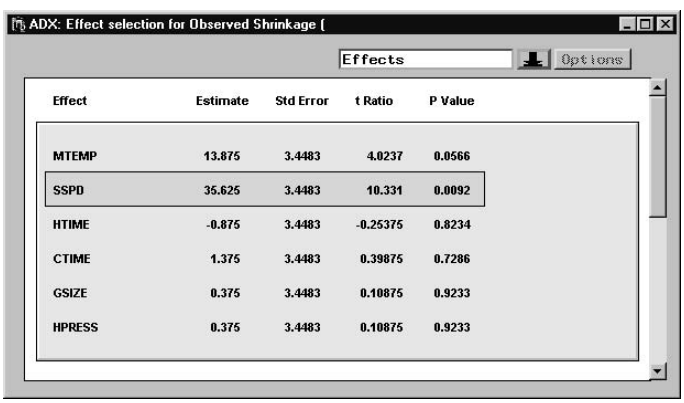
The analysis of a fractional factorial design differs from that of a full factorial design. One important difference is the care needed in the estimation of aliased effects. A second difference is the need for alternatives to the analysis of variance, which arises when the design is saturated (see the section "Analyzing Saturated Designs" beginning on page 72). To begin the analysis of a design, click **Fit** in the main design window.

Checking Assumptions

ADX automatically checks for outliers and the need for a response transform when you begin to fit the master model. (For a complete discussion of this process, see the section "Fitting a Model" on page 70.) If outliers are present, or if a Box-Cox analysis suggests a response transformation, the Check Assumptions window will open automatically. In this case, you should explore the assumptions that are colored blue. Otherwise, ADX proceeds directly to fitting the model.

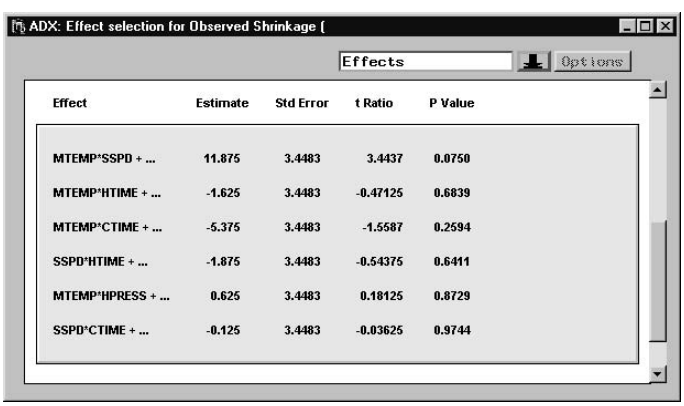
Fitting a Model

When you fit a master model, ADX brings up the effect selector, which shows the effect name, the effect estimate in the coded design, and its associated t statistic (when an analysis of variance is possible). If ADX detects a significant effect (at the $\alpha = 0.05$ level), it will highlight that effect. As discussed in Chapter 3, you can accept the selection of significant effects or refine it before you proceed to response optimization.



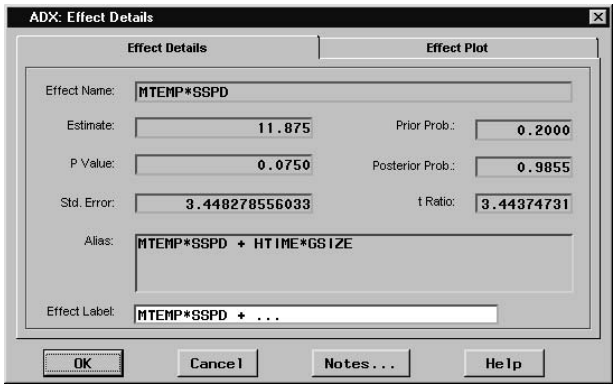
Effect	Estimate	Std Error	t Ratio	P Value
MTEMP	13.875	3.4483	4.0237	0.0566
SSPD	35.625	3.4483	10.331	0.0092
HTIME	-0.875	3.4483	-0.25375	0.8234
CTIME	1.375	3.4483	0.39875	0.7286
GSIZE	0.375	3.4483	0.10875	0.9233
HPRESS	0.375	3.4483	0.10875	0.9233

If you scroll down farther, you will notice that certain effects have a "+ . . ." appended to their labels. This indicates aliasing between effects in the master model. Since main effects are aliased with effects that are not in the master model, their labels do not indicate aliasing.



Effect	Estimate	Std Error	t Ratio	P Value
MTEMP*SSPD + ...	11.875	3.4483	3.4437	0.0750
MTEMP*HTIME + ...	-1.625	3.4483	-0.47125	0.6839
MTEMP*CTIME + ...	-5.375	3.4483	-1.5587	0.2594
SSPD*HTIME + ...	-1.875	3.4483	-0.54375	0.6411
MTEMP*HPRESS + ...	0.625	3.4483	0.18125	0.8729
SSPD*CTIME + ...	-0.125	3.4483	-0.03625	0.9744

If you double-click on the effect, you get a window with detailed information about the effect. For example, double-click MTEMP*SSPD.



This window provides the full alias string as shown on the **Alias** tab of the Design Information window. You can also click the **Effect Plot** tab to display the same effect plot shown in the Explore Data window in the section "Exploring Responses" on page 63.

You can choose alternate methods for automatically identifying active effects, such as stepwise regression and Lenth's (1989) method. Follow these steps:

1. Select **Identify** → **Select effects** → **Automatic**. You will be presented with a menu of effect selection methods. By default, **ANOVA** is selected because it is currently used to select effects.
2. Select **Lenth** as the effect selection method.

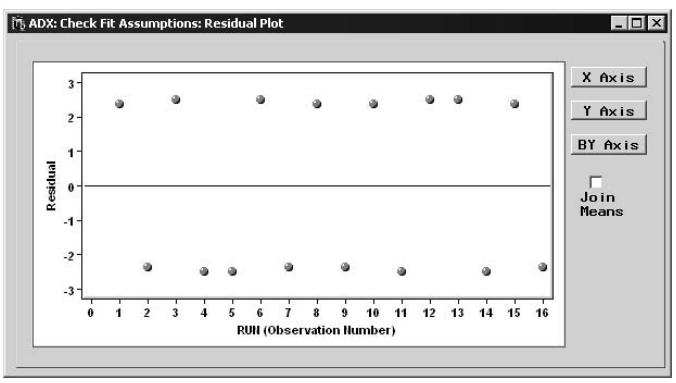
3. A Parameters window will appear, depending on the method. In this case, it asks for a value for α and assumes a value of 0.05. Click **OK**.
4. ADX will reevaluate the significance of the effects according to Lenth's method and highlight those found to be significant.

Note: The automatic effect selection method available will vary according to the design properties. See "Analyzing Saturated Designs" for more details.

Analyzing Residuals

You can view residual plots in ADX by selecting **Model** → **Check Assumptions** and clicking the **Perform Residual Analysis** button. The interactive display features are the same as those of the scatter plot, and you can display the following diagnostics by clicking the **BY Axis** button:

- Residuals
- Standardized residuals
- Normal score for residuals
- Cook's D influence statistic
- PRESS statistic (deleted residuals)
- Studentized deleted residuals



Analyzing Saturated Designs

If a design is saturated, there are only enough degrees of freedom to estimate the parameters specified in the master model, including the overall mean. It is impossible to estimate the error variance without making additional assumptions, such as the effect sparsity assumption used in Lenth's (1989) method.

Furthermore, it is impossible to detect outliers or the need for a response transform. Therefore, the Check Fit Assumptions window is not available. When you analyze responses in a saturated design, you have to assume that there are no outliers and that your data will require no transformation.

The analysis of a saturated design differs from that of an unsaturated design as follows:

1. By default, ADX displays a normal plot instead of the effect selector, and it highlights the effects determined to be active with Lenth's (1989) method. The error estimate, called a pseudostandard error (PSE), arises from the assumption that approximately 20% of the effects in any given situation will be active, and the rest of the effect estimates are zero-mean jointly normal random variables.

2. The effect selector will not show any values for a t test, since these tests are unavailable.
3. You can select active effects through any of the automatic selection methods except ANOVA.
4. You cannot open the Check Assumptions window.

Optimizing Responses

You can optimize the responses for a regular fractional factorial design by following the process described in the section "Optimizing Multiple Responses" on page 44. To open the optimization window, click **Optimize** in the main design window. The prediction profiler will appear, and it can be used in the same way as described in Chapter 3. In this case, setting SSPD at the lowest level will minimize the shrinkage. The other factors can be set according to other criteria without significantly affecting shrinkage.

Tying It All Together

The significant factors for response SHRINK are MTEMP and SSPD. MTEMP is involved in significant interactions with SSPD.

Points to Remember

- Regular fractional factorial designs have fewer runs than full factorial designs.
- ADX provides a large repertoire of standard fractional factorial designs.
- You should always refer to the alias structure of a fractional factorial design when exploring or estimating effects, especially interactions.
- Analysis of a saturated fractional factorial design requires additional assumptions and special methods to determine which effects are active.

Chapter 5

Fractional Factorial Designs with Blocks and Center Points

Chapter Contents

Chapter 5

Fractional Factorial Designs with Blocks and Center Points

Chapter Topics

Fractional factorial designs are commonly used to screen for important effects, especially when runs are expensive. Adding center points is useful for detecting nonlinearity in the response. Replicated center points also provide an estimate of variance. Blocks are helpful for removing nuisance effects, such as those caused by running an experiment over several days, from the response data.

Covered in This Chapter

- Defining variables
  - Using the factor library
- Selecting a design
- Customizing a design
  - Adding center points
  - Blocking
- Interaction plots
- Fitting a model
  - Checking assumptions
  - Using Pareto plots

Experimental Objective

At a plant where integrated circuit chips are fabricated, engineers want to screen for important effects in the etch process. For this experiment, they investigated the five factors and two responses listed in Table 5.1.

Table 5.1. Variables of the IC Fabrication Screening Experiment

Type	Name	Low	High	Description
Factors	TEMP	1210	1220	Deposition temp (C)
	FLOW	55	60	Arsenic flow rate
	TIME	10	16	Deposition time
	ETCH	1180	1220	Etch rate
	ACID	6	14	Acid flow rate
Responses	THCKNESS			Thickness of film
	RESTIVTY			Resistivity

Since this experiment is run over two days, the design will have two blocks.

The goal of this experiment is to identify important factors for further study. These important factors are ones that significantly influence film thickness or resistivity.

Task List

- Create a customized screening design with center points and replicates.
- Review the confounding rules for the design.
- Review the aliasing structure of the design.
- View customization details for the IC Fabrication Screening design.
- Explore the response data with interaction and cube plots.
- Fit a model for each response.
- Optimize the responses to find factor settings for a follow-up response surface experiment.

Creating a Customized Fractional Factorial Design

This section covers the following steps used to create a fractional factorial design with two blocks and center points:

- Defining variables
- Creating a two-level 1/2 fractional factorial with two blocks
- Using the Customization Details window to add center points

Defining Factor, Response, and Block Variables

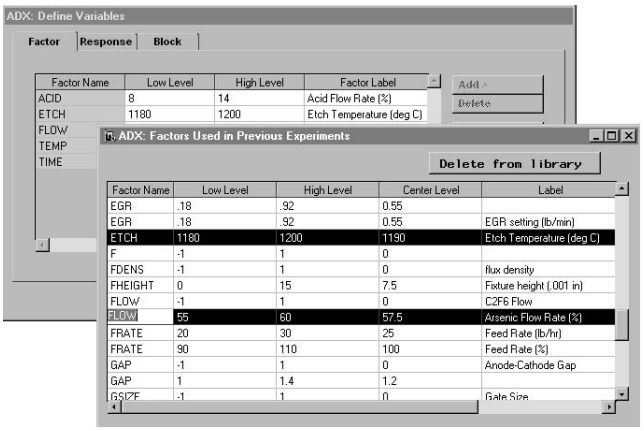
To build the design, return to the ADX desktop and follow these steps:

1. Select **File** → **Create New Design** → **Two-level** from the ADX desktop.
2. Click **Define Variables**.

Normally, you would type in the factor names, high and low values, and descriptions. However, you can use the factor library as a shortcut. The factor library stores the names, levels, and descriptions of all previously used factors. Follow these steps:

1. Click **Library**.

2. Hold down the CTRL key and click to select the factors ACID, ETCH, FLOW, TEMP, and TIME. Factors in the library are organized alphabetically.



3. Close the Factor Used in Previous Experiments window.

Follow the same steps to define the response:

1. Click the **Response** tab.
2. Click **Library**.
3. Select **THCKNESS** and **RESTIVTY** from the Responses Used in Previous Experiments window.
4. Close the Responses Used in Previous Experiments window.
5. Delete the **Y1** response.

Because the experiment takes two days to run, define the two blocks. Follow these steps:

1. Click the **Block** tab.
2. Click **Add** and select **1** to add another row to the block levels.

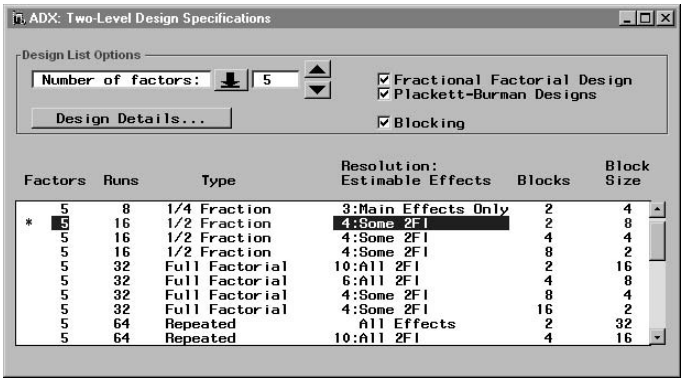
Click **OK** to return to the main design window.

Creating a Fractional Factorial Design with Blocks

Now that you have defined factors, responses, and blocks, follow these steps to specify the design:

1. Click **Select Design** to open the Two-Level Design Specifications window. ADX displays all standard designs with 5 factors.

2. Select the **16** run **1/2 Fraction** design with **2** blocks.

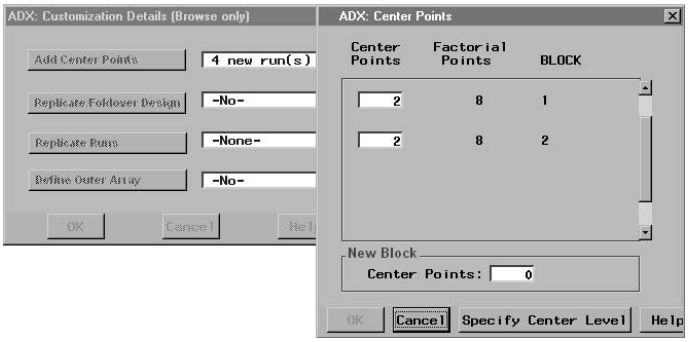


3. Close the window and click **Yes** to use the design.

Using the Customize Window to Add Center Points

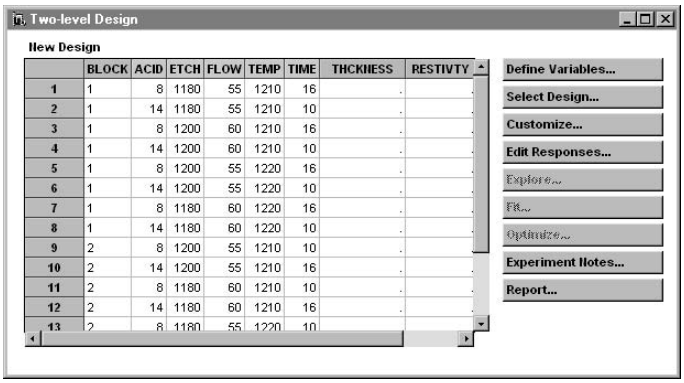
Since the budget allows four more runs, four center points will be added, two to each block. This provides for the detection of a nonlinear response and an independent estimate of variance. To add center points, follow these steps:

1. Click **Customize**.
2. Click **Add Center Points**.
3. Type **2** for the number of center points for each block.



4. Click **OK**.

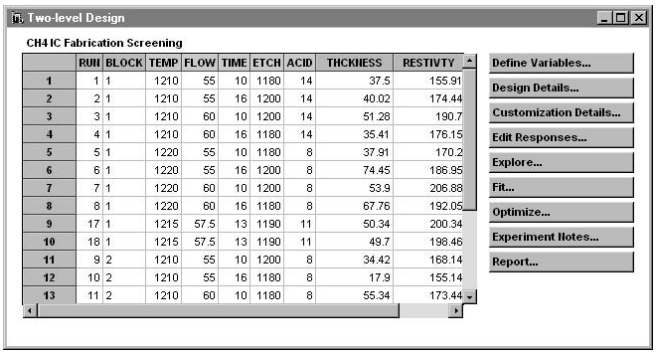
ADX reports that **4** new runs have been added that are center points. The design now has **20** runs.



	BLOCK	ACID	ETCH	FLOW	TEMP	TIME	THCKNESS	RESTIVTY
1	1	8	1180	55	1210	16	.	.
2	1	14	1180	55	1210	10	.	.
3	1	8	1200	60	1210	16	.	.
4	1	14	1200	60	1210	10	.	.
5	1	8	1200	55	1220	16	.	.
6	1	14	1200	55	1220	10	.	.
7	1	8	1180	60	1220	16	.	.
8	1	14	1180	60	1220	10	.	.
9	2	8	1200	55	1210	10	.	.
10	2	14	1200	55	1210	16	.	.
11	2	8	1180	60	1210	10	.	.
12	2	14	1180	60	1210	16	.	.
13	2	8	1180	55	1220	10		

Reviewing a Customized Fractional Factorial Design

You can close the design you just created. Since there is a sample design in ADX that contains response values for this experiment, double-click the IC Fabrication Screening design to view the design factors and responses.



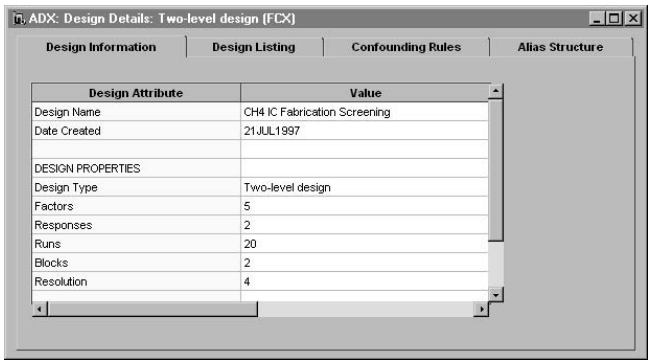
	RUN	BLOCK	TEMP	FLOW	TIME	ETCH	ACID	THCKNESS	RESTIVTY
1	1	1	1210	55	10	1180	14	37.5	155.91
2	2	1	1210	55	16	1200	14	40.02	174.44
3	3	1	1210	60	10	1200	14	51.28	190.7
4	4	1	1210	60	16	1180	14	35.41	176.15
5	5	1	1220	55	10	1180	8	37.91	170.2
6	6	1	1220	55	16	1200	8	74.45	186.95
7	7	1	1220	60	10	1200	8	53.9	206.88
8	8	1	1220	60	16	1180	8	67.76	192.05
9	17	1	1215	57.5	13	1190	11	50.34	200.34
10	18	1	1215	57.5	13	1190	11	49.7	198.46
11	9	2	1210	55	10	1200	8	34.42	168.14
12	10	2	1210	55	16	1180	8	17.9	155.14
13	11	2	1210	60	10	1180	8	55.34	173.44

Customization Details

A design can be customized only while it is being created. Although you can view the Customization Details window for any design, ADX prevents you from modifying a design after you have added the response values.

Design Details

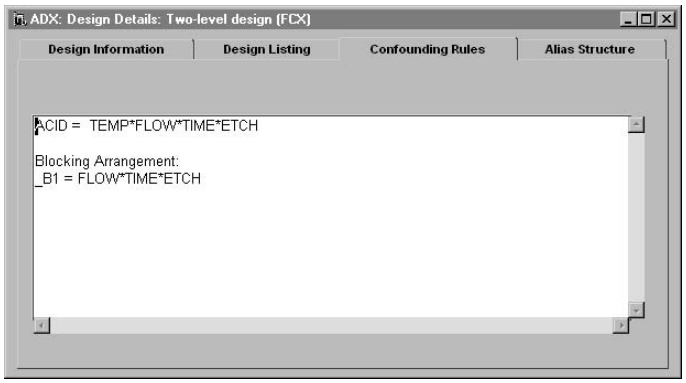
View the Design Details (from the main design window) to determine the resolution of the IC Fabrication Screening design. The design has Resolution 4, which means that you can estimate all main effects and some two-factor interactions.



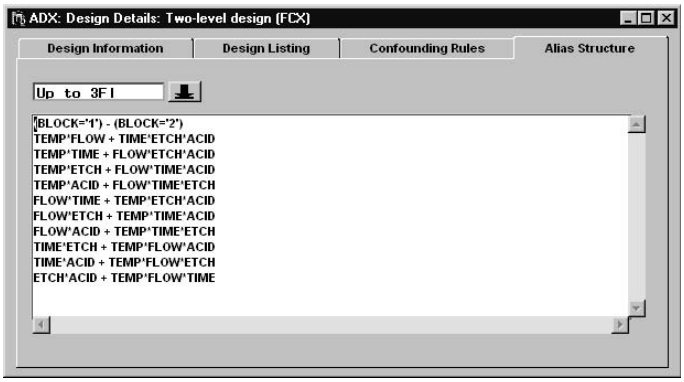
Design Attribute	Value
Design Name	CH4 IC Fabrication Screening
Date Created	21JUL1997
DESIGN PROPERTIES	
Design Type	Two-level design
Factors	5
Responses	2
Runs	20
Blocks	2
Resolution	4

Confounding and Aliasing

This example, like all fractional factorial designs, was generated according to certain confounding rules, which are shown on the **Confounding Rules** tab of the Design Details window. Note that blocks are confounded with the three-factor interaction FLOW*TIME*ETCH. Therefore, you cannot estimate this interaction.



Click the **Alias Structure** tab of the Design Details window to view the alias sets of the design.



See the section "Confounding" on page 61 for more information about confounding and the section "Alias Structure" on page 61 for more information about aliasing.

Analyzing the Response Data

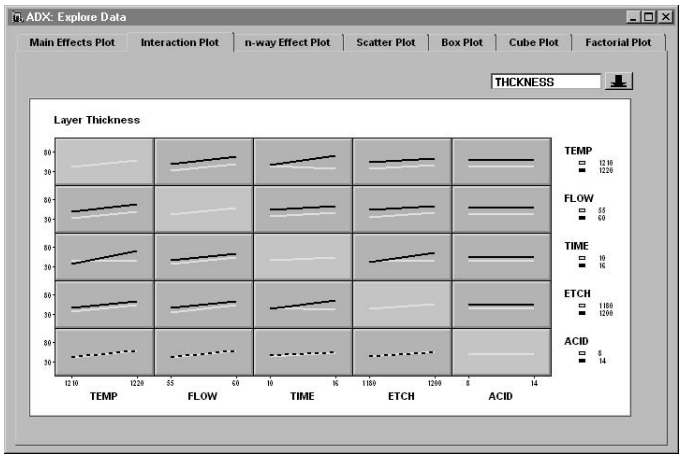
The steps for fitting a model to the responses are as follows:

1. Check for interaction with interaction plots.
2. Find significant effects with the ANOVA and Bayes automatic selection methods.
3. View significant effects with Pareto and Bayes plots.

Interaction Plot

The interaction plot is described in detail in the section "Interaction Plot" on page 32, and the use of the interaction plot with fractional factorial designs is described in the section "Interaction Plot" on page 64.

Click **Explore** and then the **Interaction Plot** tab. It is best to examine the alias structure of the design before using this plot.



The plots for TEMP*TIME and TIME*ETCH indicate interaction effects that might be significant. Since the three-factor interaction FLOW*ETCH*ACID is aliased with the two-factor interaction TEMP*TIME, you would need to assume that FLOW*ETCH*ACID is not active if you test TEMP*TIME for significance. Otherwise, these two effects should be explored further; see Chapter 13, "Special Topics," for further details.

Fitting a Model

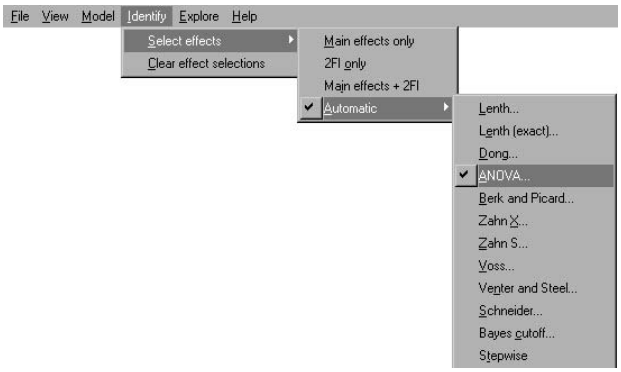
ADX provides numerous ways to analyze the design and find significant effects for two-level factorial designs. See the section "Fitting a Model" on page 70 and the section "Analyzing Saturated Designs" on page 72 for more details.

To fit each response model, follow these steps:

1. Click **Fit**.

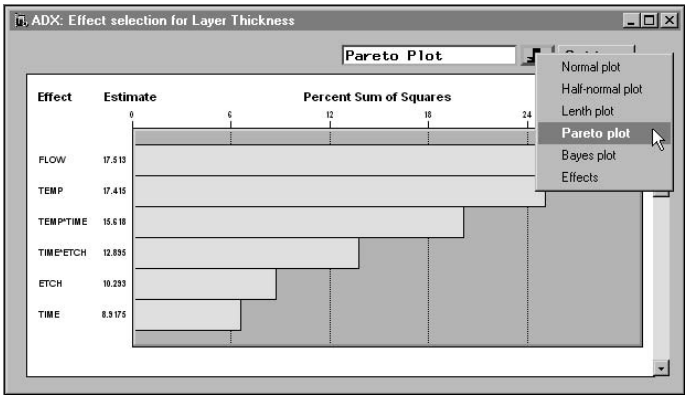
2. Select **THCKNESS**.
3. Click **Run**.

Select **Identify** → **Select effects** → **Automatic** → **ANOVA** to see how ADX selected significant effects.



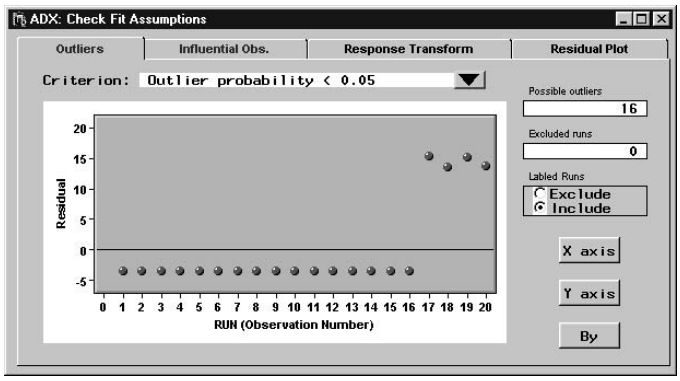
Since this design has center points that can be used for estimating error, ADX uses the default ANOVA method to determine which effects in the master model are significant.

To view the effect selections with a Pareto plot of the estimates, click the down arrow in the Effect selection for Layer Thickness window and select **Pareto Plot** from the pop-up menu.



Close the Effect Selection for Layer Thickness window. From the main design window, click **Fit** and select **RESTIVTY** as the response to fit.

When you fit the resistivity response, the Check Fit Assumptions window opens and displays the outlier probability plot. For the purpose of this example, keep all of the runs and close the Check Fit Assumptions window.



No effects are significant for resistivity at $\alpha = 0.05$.

Close the Fit window.

Tying It All Together

The significant factors for thickness are TEMP, FLOW, ETCH, and TIME. TEMP is involved in significant interactions with ETCH and TIME. There are no significant effects for resistivity. The next step is to perform a response surface experiment with just these four factors, to determine the optimum setting by including curvature effects in the model. This will be done in Chapter 7.

Points to Remember

- ADX has a factor library that stores factor names, levels, and labels for saved designs. You can use the factor library to define variables for a design.
- Blocking can help remove nuisance effects from variability.
- Blocks are typically aliased with other effects in a design.
- Adding center points enables detection of response nonlinearity and an estimate of variance.
- Once responses have been entered into a design, you can view customization details, but you cannot make changes to the design.

Chapter 6

Plackett-Burman Designs

Chapter Contents

Chapter 6

Plackett-Burman Designs

Chapter Topics

Plackett-Burman designs are screening designs that involve a large number of factors and relatively few runs. They are Resolution 3 designs, so they can estimate only main effects. They are typically used to identify a few significant factors out of a large set. The significant factors are often studied in more detail with follow-up experiments.

Covered in This Chapter

- Defining variables
- Reviewing design details
- Exploring data
  - Using a main-effects plot
  - Using a scatter plot
- Fitting a model
  - Checking fit assumptions
  - Using automatic selection methods
  - Using a Lenth plot
- Entering experiment notes
- Generating a report

Experimental Objective

A quality engineer wants to increase the lifetime of weld-repaired die castings. The engineer is interested in all factors that influence the lifetime of the die castings. Eight factors, shown in Table 6.1, are suspected to have some influence on the lifetime of the castings. Since runs are expensive, a Plackett-Burman design is used for the experiment.

Table 6.1. Factors for Die-Cast Fatigue Experiment

Type	Name	-1 level	$+1$ level	Description
Factor	INITSTR	no treat	β treat	Initial structure
	BEADSIZE	small	large	Bead size
	PTREAT	none	HIP	Pressure treatment
	HTREAT	anneal	solution	Heat treatment
	HOLDTIME	30 sec	600 sec	Holding time
	CRATE	slow	rapid	Cooling rate
	POLISH	chem	mech	Polishing method
	FTREAT	none	peen	Final treatment
Response	LIFETIME			Casting lifetime

The goal of the experiment is to identify the factors that have a significant influence on die-cast lifetime.

Task List

- Create a Plackett-Burman design.
- Explore the data with a main-effects plot and box plots.
- Find active factors by using a combination of ANOVA, Lenth's method, and Bayesian analysis.

Creating a Plackett-Burman Design

Defining Factors and Responses

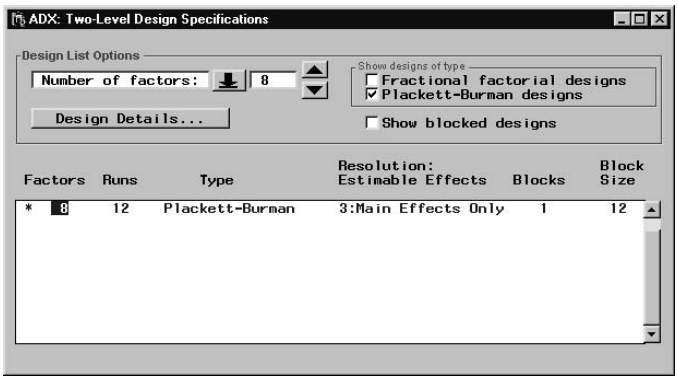
The Die Cast design is an example where this technique has been used. Here, however, you re-create the design so you can learn how to define the variables for a Plackett-Burman Design by following these steps:

1. Select **File** → **Create New Design** → **Two-level** from the ADX desktop to open the main design window.
2. Click **Define Variables**.
3. Click **Add** and select **8** as the number of rows to add. ADX adds one row for each factor and automatically fills in the coded levels for each of the factors.
4. Type a **Factor Name, Low Level, High Level**, and **Factor Label** for each factor as in Table 5.1
5. In a similar fashion click the **Response** tab to enter one response variable.
6. Click **OK** to save the changes.

Selecting the Design

1. In the main design window click **Select Design**.
2. Clear **Fractional factorial designs**.

3. Select the **12** run Plackett-Burman design. The table indicates that this design is Resolution 3, which enables uncorrelated estimation of main effects only.

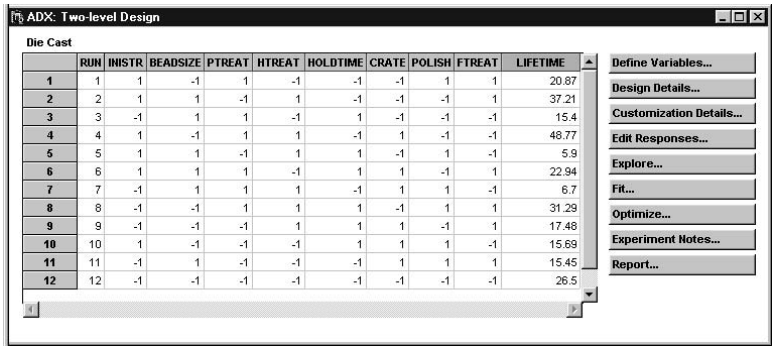


4. Close the window and click **Yes** to use the design.
5. You will be returned to the Two-level Design window, with the new design in the spreadsheet.

Editing the Response Values

In practice, once your experiment is run and the response values are available, you click **Edit Responses** to enter the responses, as explained in the section "Getting Started with a Simple Example" on page 13. Once the responses are entered, the design factors and their levels cannot be changed.

For this example, you can continue by opening the design named Die Cast. This design is the same as the one you just created, but it includes the response values.



	RUN	INISTR	BEADSIZE	PTREAT	HTREAT	HOLDTIME	CRATE	POLISH	FTREAT	LIFETIME
1	1	1	-1	1	-1	-1	-1	1	1	20.87
2	2	1	1	-1	1	-1	-1	-1	1	37.21
3	3	-1	1	1	-1	1	-1	-1	-1	15.4
4	4	1	-1	1	1	-1	1	-1	-1	48.77
5	5	1	1	-1	1	1	-1	1	-1	5.9
6	6	1	1	1	-1	1	1	-1	1	22.94
7	7	-1	1	1	1	-1	1	1	-1	6.7
8	8	-1	-1	1	1	1	-1	1	1	31.29
9	9	-1	-1	-1	1	1	1	-1	1	17.48
10	10	1	-1	-1	-1	1	1	1	-1	15.69
11	11	-1	1	-1	-1	-1	1	1	1	15.45
12	12	-1	-1	-1	-1	-1	-1	-1	-1	26.5

Analyzing a Plackett-Burman Design

The Plackett-Burman design is available complete with response values on the ADX desktop. Close the design you just created and open the design named Die Cast.

The analysis strategy is as follows:

- Examine a main-effects plot to see which main effects are active.
- Examine scatter and box plots to visualize response distributions at different factor levels.
- Apply a variety of effect selection methods to determine which factors significantly affect lifetime.

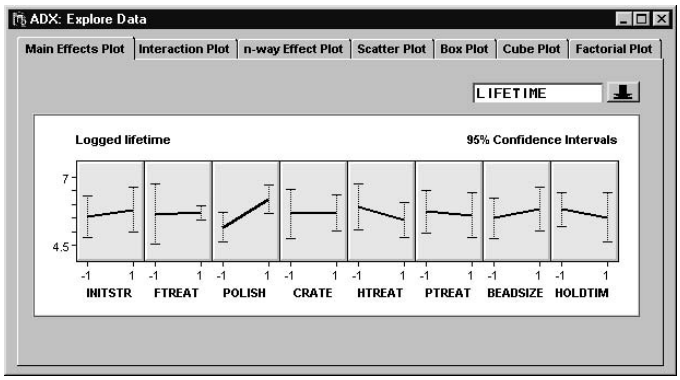
Exploring the Response Data

The main-effects plot, the scatter plot, and the box plot can all be used to visualize the data and to explore the relationship between the factors and the response. Interaction plots, n-way effect plots, cube plots, and factorial plots all have limited usefulness with the Plackett-Burman designs.

Main-Effects Plot

To explore the data in the main-effects plot, follow these steps:

1. Open the Die Cast design from the ADX desktop.
2. Click **Explore**. The main-effects plot can quickly reveal which strains affect lifetime.

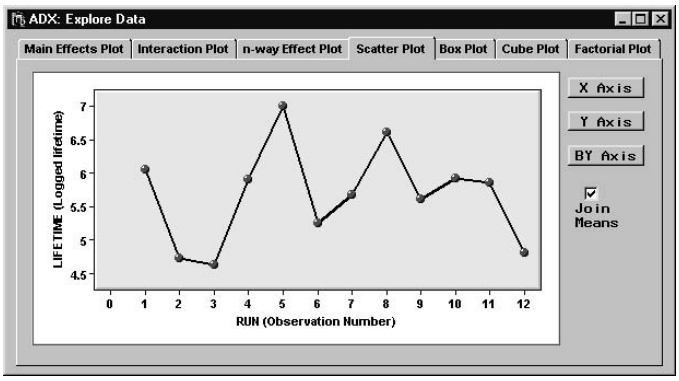


The polishing method (POLISH) seems to have a large effect on lifetime.

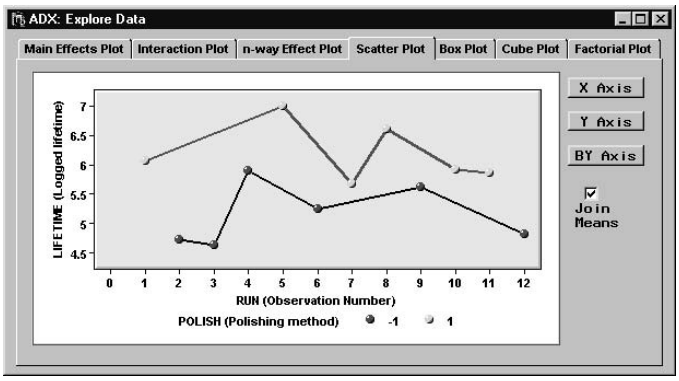
Scatter Plot

A scatter plot with LIFETIME on the Y axis and RUN (observation number) on the X axis might reveal any nonrandom pattern showing a possible effect due to time.

To display a scatter plot, click the **Scatter Plot** tab in the Explore Data window. The default scatter plot is the LIFETIME by Observation Number plot. Selecting **Join Means** connects the points and reveals a pattern that suggests a serial effect.



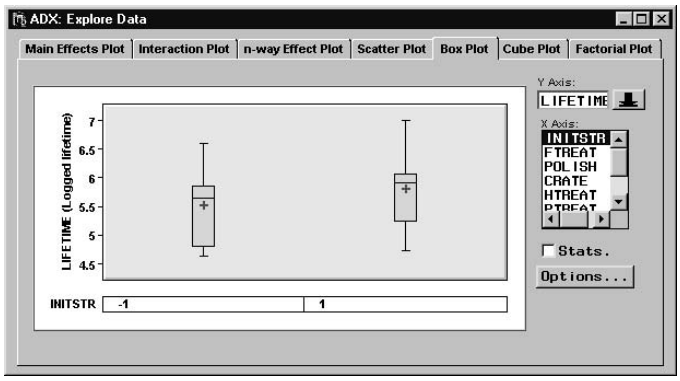
To explore this pattern in more tail, click **BY Axis** and select **POLISH**.



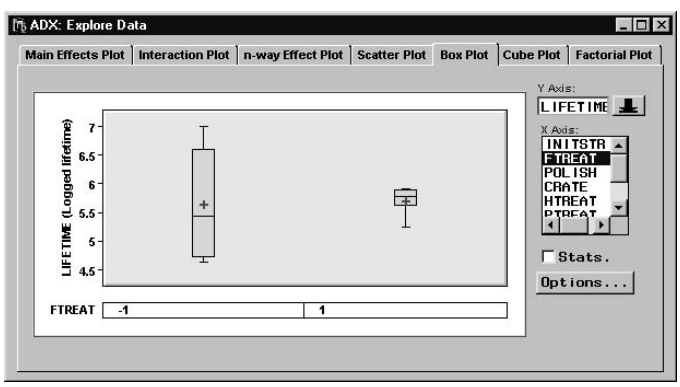
Now there are two groups of runs: one for the high level of POLISH and one for the low level. In this display, there is less evidence of a serial effect.

Box Plot

The box plot displays distributional differences in the response across levels of the factors. To use the box plot, click the **Box Plot** tab in the Explore Data window.

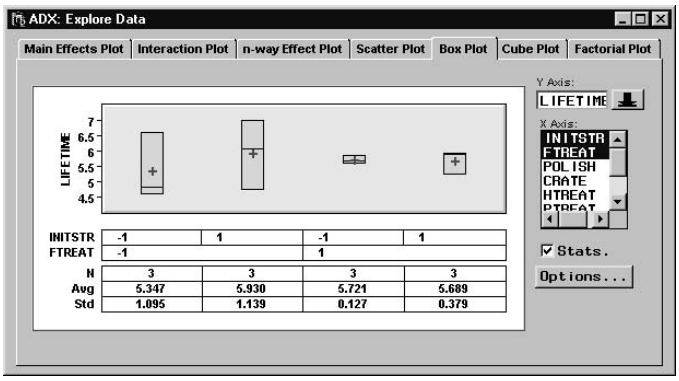


By default, the LIFETIME by INITSTR box plot appears. This provides yet another way of visualizing main effects. You can display important statistics for the response within each factor level by selecting the **Stats** box. The box plot can also indicate possible dispersion effects, or situations where a change in factor level affects the variance of the response. From the list, select **INITSTR** to clear it, and then select **FTREAT** to display a box plot of LIFETIME by FTREAT.

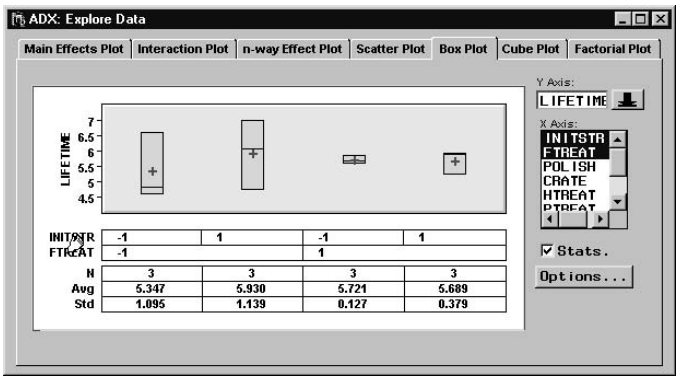


Note that the sizes of the boxes are different. Furthermore, the standard deviation of the LIFETIME at the low level of FTREAT is 1.05, while the standard deviation of the LIFETIME at the high level of FTREAT is 0.25. While there are not enough runs to test the difference of these standard deviations, it might be useful to study this effect with a follow-up experiment. One rough guideline for a significant difference in variances is a ratio of greater than 3 or less than one-third, with more than a factor of 4 between the variances.

The box plot can display response distributions for more than one factor. Select **INITSTR** from the factor list. This time, a box plot with four boxes appears, one for each level combination of the two factors.



You can change the order of the nesting of the factors by clicking and dragging the factor names below the plot (when the arrow changes to a hand).



Finding Significant Effects

ADX provides a variety of methods to identify significant (active) effects and build a model for the response.

Click **Fit**. ADX will open a window with a table of effects, their estimates, and t tests of significance. It also highlights effects that are selected as significant based on an automatic selection method.

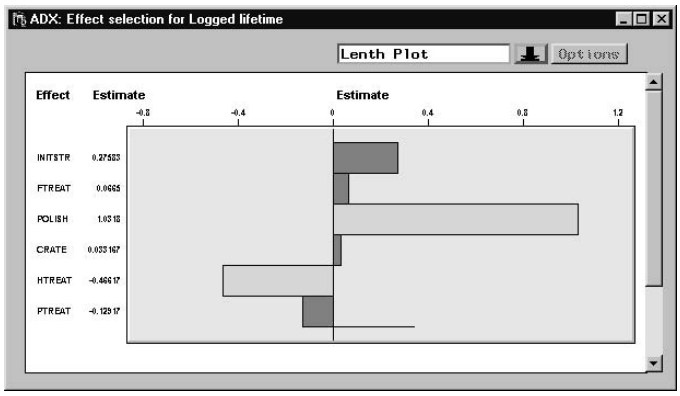
Automatic Selection Methods

By default, ADX uses the ANOVA automatic selection method for this design because three degrees of freedom are available for estimating error. You can choose a different method for selecting active effects with the **Identify** menu. See the section "Analyzing Saturated Designs" on page 72 for more details about which automatic selection methods are used by default.

Lenth's Method and the Lenth Plot

To select effects with Lenth's method and to display a Lenth plot, follow these steps:

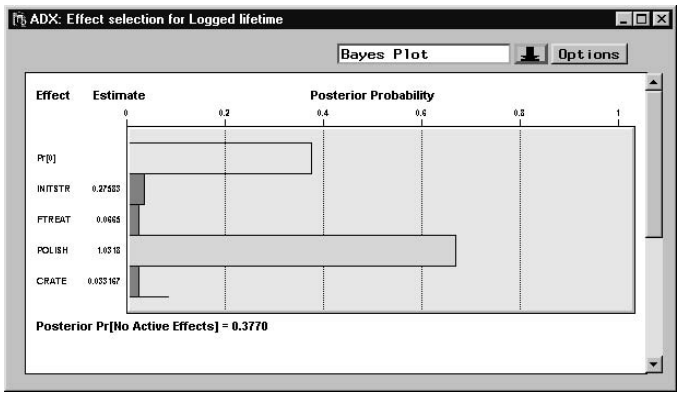
1. Select **Identify** → **Select effects** → **Automatic** → **Lenth**.
2. Change the display to the Lenth plot. The Lenth plot shows the significant effects highlighted at the $\alpha = 0.05$ level. You always have the option of manually selecting or removing factors based on the size and direction of the estimate.



Bayesian Effect Selection

ADX also provides the Bayesian effect selection method described in Box and Meyer (1986), which is a useful supplement to the ANOVA and Lenth methods. Note that the Bayesian and Lenth methods apply to saturated designs, whereas ANOVA does not.

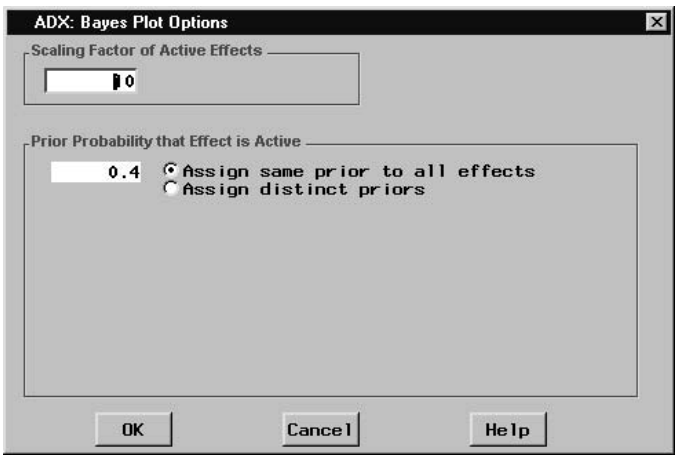
To use the Bayesian method, click the down arrow in the Effect Selection for Logged lifetime window and select **Bayes plot**. A default Bayes plot appears. The default assumes a 0.2 prior probability for an effect to be active, and the bars display the posterior probability that each effect is still active. Bayesian analysis selects the same factors previously identified as significant.



The bar labeled **Pr[0]** indicates the posterior probability that no effects are active given the prior distribution.

Box and Meyer (1986) recommend that effect selection be performed over a range of priors before a final model is fit. To change the prior probability distribution, do the following:

1. Click **Options** while the Bayes plot is displayed.



2. A dialog box will appear with two groups of options. The bottom group affects the prior distribution.
3. If you want to set the prior distribution uniformly for all effects, select **Assign same prior to all effects** and type the prior probability that each individual effect is active. For example, type **0.4** in the text field.
4. Click **OK** to apply the changes to the plot.

If, based on prior experience, you feel that some effects are more likely to be active, you can select **Assign distinct priors** in the Bayes Plot Options dialog box and assign each prior separately.

You can specify the Bayesian method as the default selection method by selecting **Identify** → **Select effects** → **Automatic** → **Bayes cutoff**. By default, an effect will be selected as active if its posterior probability is 0.5 or greater. You can change the cutoff, or click **OK** to apply the effect selection method.

Tying It All Together

The analysis identified the polishing method (POLISH) and heat treatment (HTREAT) as the significant main effects for the lifetime of the die cast.

Points to Remember

- Plackett-Burman designs are two-level screening designs, which estimate many main effects with relatively few runs.
- Main-effects plots are useful for exploring Plackett-Burman designs.
- ADX provides a number of automatic effect selection methods for two-level designs. These include ANOVA, Lenth's method, and Bayesian analysis.
- ADX provides a variety of ways to display selected effects, including Pareto, Lenth, and Bayesian plots.

Chapter 7

Response Surface Designs

Chapter Contents

Chapter 7

Response Surface Designs

Chapter Topics

Response surface designs examine both the linear and the quadratic behavior of the responses over the design region. These designs, which are typically sufficient to fit a quadratic model, enable you to do the following:

- Distribute points in such a way as to provide information about the response throughout the experimental region
- Block runs
- Compute an independent estimate of error
- Use as few runs as feasible
- Estimate model parameters and carry out an analysis of variance
- Fit models that can be used to find optimal factor settings
- Test for model adequacy, including lack of fit

Refer to Myers and Montgomery (1995) for a discussion of response surface designs.

Covered in This Chapter

- Choosing a response surface design
- Fitting a model
  - Performing an ANOVA
  - Performing a model adequacy test
  - Performing canonical and ridge analyses
  - Examining contours for the master and reduced model
- Optimizing a response
  - Using the prediction profiler
  - Defining a desirability function
  - Using a contour plot
  - Using the contour optimizer
  - Performing a numerical optimization

Experimental Objective

An engineer is interested in following up the IC Fabrication Screening experiment in Chapter 5 with a response surface design in order to identify factor settings that optimize the process. This experiment showed that acid flow rate was not significant, so that factor will not be considered here.

Table 7.1 describes the factors and responses of the new experiment with their ranges.

Table 7.1. Factors and Responses of the IC Fabrication Screening Experiment

Type	Name	Low	High	Description
Factors	TEMP	1210	1220	Deposition temp (C)
	FLOW	55	60	Arsenic flow rate
	TIME	10	16	Deposition time
	ETCH	1180	1200	Etch rate
Responses	THCKNESS			Thickness of film
	RESTIVTY			Resistivity of final film layer

The experiment takes three days to run, and each day will be run in a separate block.

The goal of the experiment is to determine factor settings that result in a film thickness of 60 and maximum resistivity.

Task List

- Choose an appropriate response surface design.
- Generate a central composite design (CCD).
- Define factors and responses. The factor library provides a shortcut.
- Explore data and evaluate the regression assumptions.
- Fit a quadratic model.
- Find optimum factor setting levels.

Creating a Response Surface Design

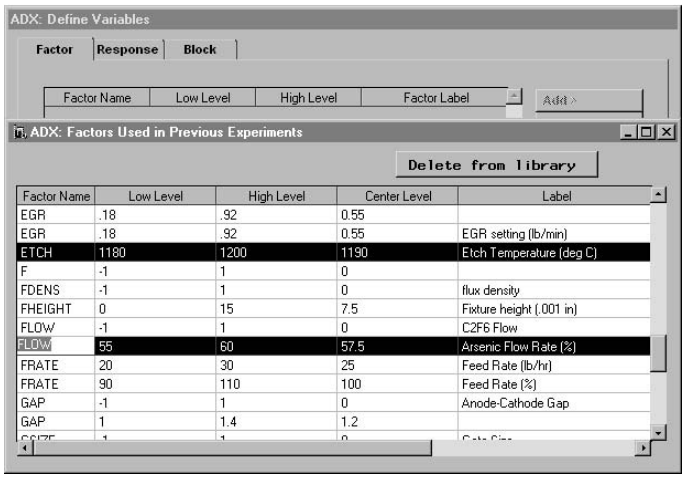
Select **File** → **Create New Design** → **Response Surface** from the ADX desktop to begin creating a response surface design.

Defining Factors, Responses, and Blocks

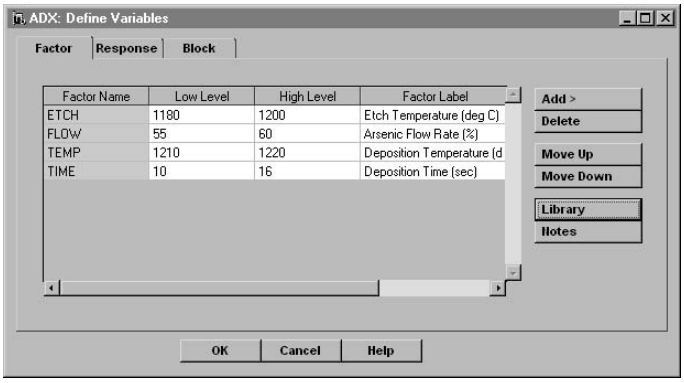
The factor names, levels, and labels from the IC Fabrication Screening experiment have been saved in the factor library. Using the library, you can copy this information over to the new design. Follow these steps:

1. Click **Define Variables** in the main design window.

2. Click **Library** to open the factor library.
3. Hold down the CTRL key and click to select **ETCH**, **FLOW**, **TEMP**, and **TIME**.

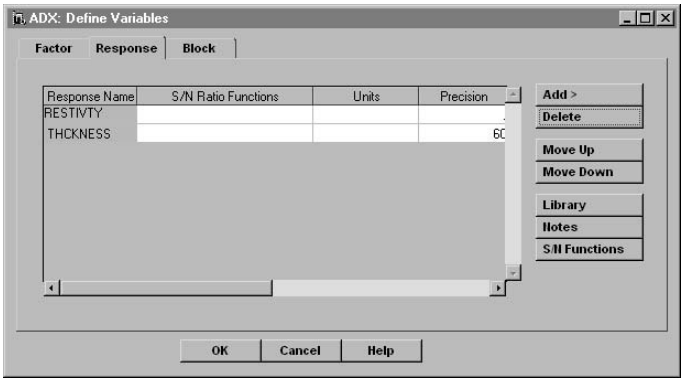


4. Close the Library window.

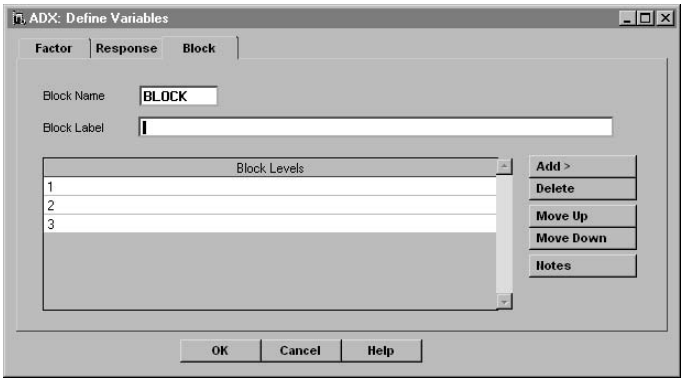


Finish defining the variables:

1. Select the response variables from the Response Library.
2. Select **Y1** and click **Delete** to delete it.



3. Click the **Block** tab.
4. Click **Add** to add two rows so that you have three block levels.

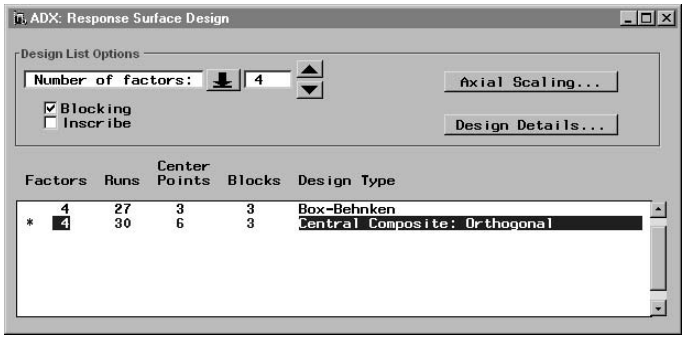


5. Click **OK** and save the changes.

Selecting a Design

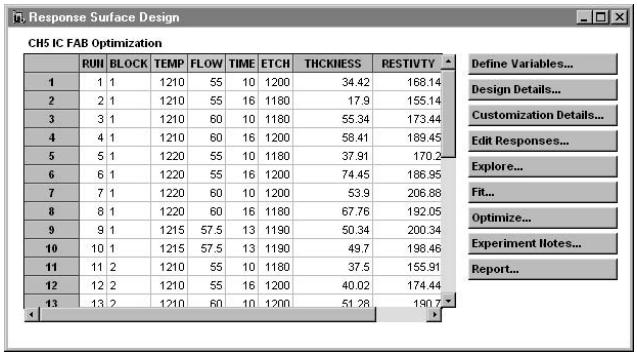
Click **Select Design** in the main design window. Since you defined four factors, ADX will display a list of all the available designs with four factors. The response surface design types available in ADX are described in Appendix A, "Glossary of ADX Terms," and in standard references such as Montgomery (1997), Myers and Montgomery (1995), and Box and Draper (1987). In addition, ADX generates designs described by Hartley (1959), where the factorial portion is a special nonregular fractional factorial. To select the central composite design, do the following:

1. Select the **Central Composite: Orthogonal** design.



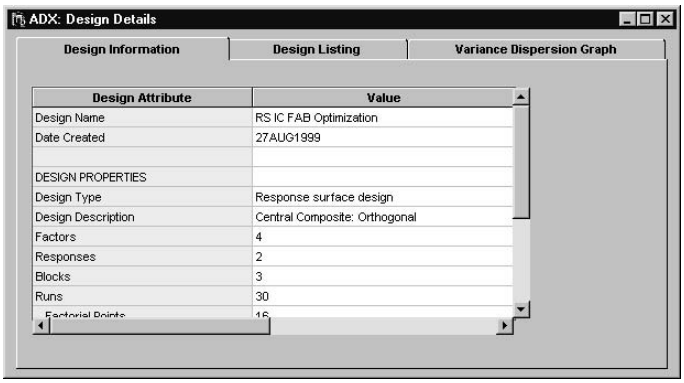
Click **Axial Scaling** to view how the axial runs will be generated. You have four choices: rotatable, orthogonal blocking, face center, or custom scaling. The choice affects the distance of the axial runs from the center of the design region.

2. Click **OK** to select the rotatable axial scaling for this design, and close the window to generate the design.



Viewing Design Details

To view a summary of the design, click **Design Details**. The first tab, **Design Information**, describes how the design was generated.

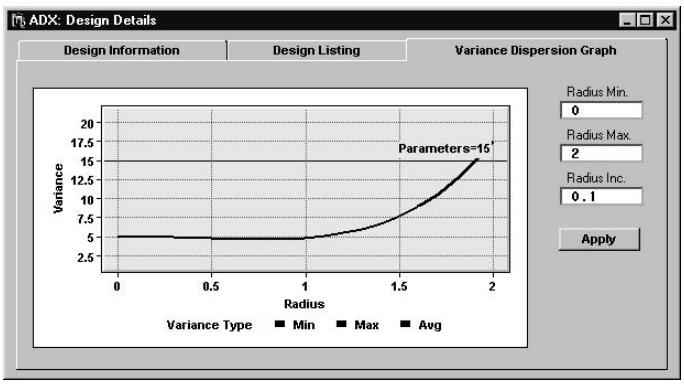


In this case, the design has 30 runs in three blocks. Two of the blocks contain eight factorial runs and two centerpoints each. The remaining block contains eight axial points and two center points. Information about the axial scaling is also provided.

You can view the design points by clicking the **Design Listing** tab.

The **Variance Dispersion Graph** tab generates a graph that is helpful in choosing response surface designs, including the number of center points. The graph displays the prediction variance scaled by the number of runs and the underlying error against the distance away from the center of the experimental region. Refer to Myers and Montgomery (1995, pp. 374ff.) for more information about using variance dispersion graphs.

Close the Design Details window to return to design selection.



A sample design with response values is available on the ADX desktop.

Analyzing a Response Surface Design

Because response surface designs can estimate quadratic effects, the analysis differs from that used for screening designs. ADX automatically provides tools that are appropriate for examining the quadratic effects.

Open the response surface design named IC Fabrication Optimization in the ADXBKV9 folder.

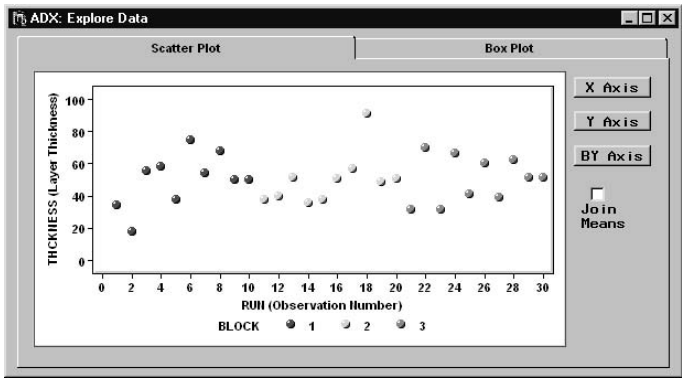
Exploring Data

If you click **Explore**, you will see tabs labeled **Scatter Plot** and **Box Plot**.

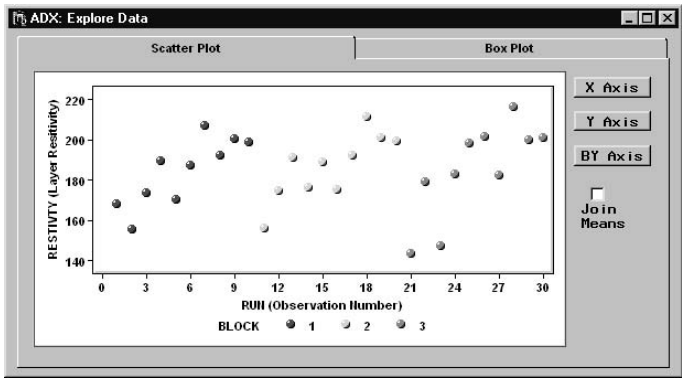
Click **Scatter Plot** to display a default scatter plot. You can change the variables assigned to the X axis and the Y axis, and you can also modify the scatter plot by assigning a BY variable to stratify the display.

To review your design, follow these steps:

1. Change the **X Axis** to **Run** (observation number) and the **BY Axis** to **BLOCK**.
2. Click **Y Axis** and select **THCKNESS** to get the following plot:



3. Click **Y Axis** and select **RESTIVTY** to get the following plot:

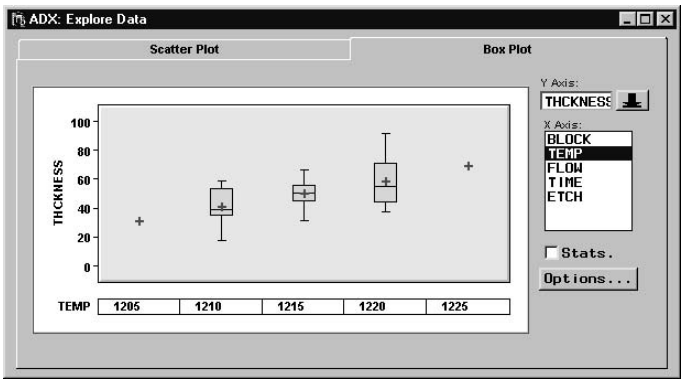


Within each block, resistivity seems to increase. This might be due to a serial effect or lack of randomization.

You can review the scatter plot for each factor.

Box Plot

The use of box plots for response surface data is nearly the same as that for screening designs as described in the section "Box Plot" on page 36. The primary difference is the presence of more boxes, because response surface designs are more complex. The first and last boxes often correspond to distinct single data points because axial runs for each factor occur only once.

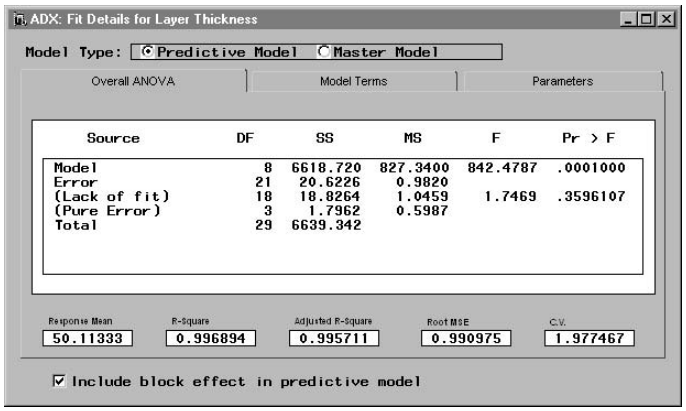


Fitting a Model

Return to the main design window. You can fit a model by clicking **Fit**. Select **THCKNESS**.

To choose the ANOVA method of significant effect selection, select **Identify** → **Select effects** → **Automatic** → **ANOVA**. The only automatic selection methods available for the response surface fit are ANOVA and Stepwise.

To display an ANOVA table, select **Model** → **Fit details**. In the overall ANOVA window, you can review the fitted master model (the full model with all effects) or a smaller model that contains only the effects currently designated as significant in the master model. The overall ANOVA provides descriptive statistics for both models, including the response mean, root mean squared error (RMSE), R square, and the coefficient of variation. ADX will provide a lack-of-fit test whenever sufficient runs are available by splitting total error into pure error and error due to lack of fit. Since the p-value for the lack of fit is large, the conclusion is that this model is adequate.

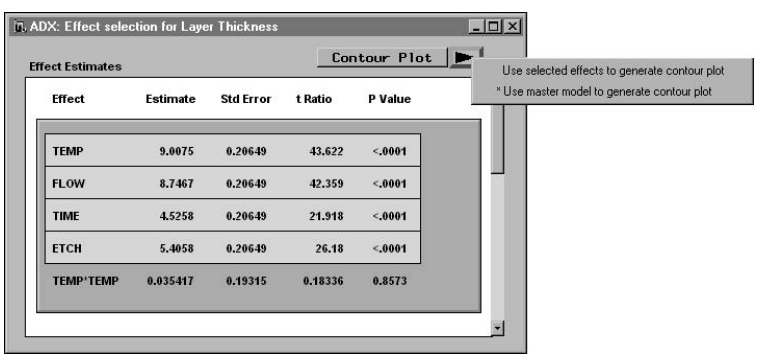


Close the window to return to the Effect Selection for Layer Thickness window.

Viewing Contour Plots from the Fit Window

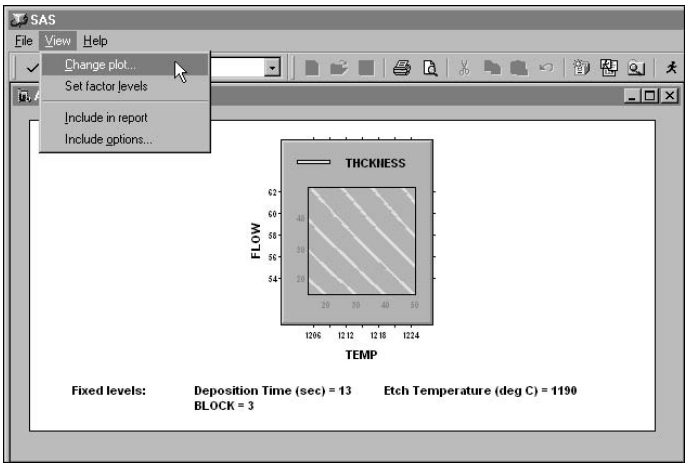
ADX makes a contour plot accessible from the Effect Selection for Layer Thickness window. To view the plot, follow these steps:

1. Click the **Contour Plot** button to select the effects to use for generating the contour plot. You can choose to view the contour plot for the master model or the smaller model containing the selected effects.

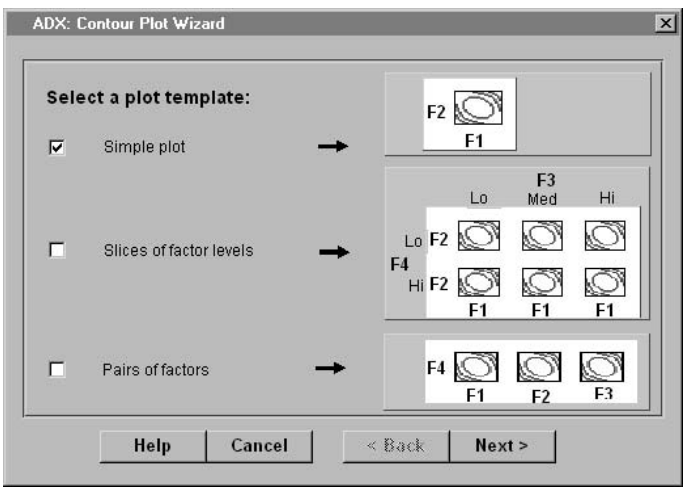


2. Click the arrow beside the **Contour Plot** button and select **Use selected effects to generate contour plot**.

This is a contour plot showing how thickness varies with flow and deposition temperature for the fixed levels of the factors TIME, ETCH, and BLOCK shown at the bottom. The **View** menu enables you to modify the contour plots or include it in a report.

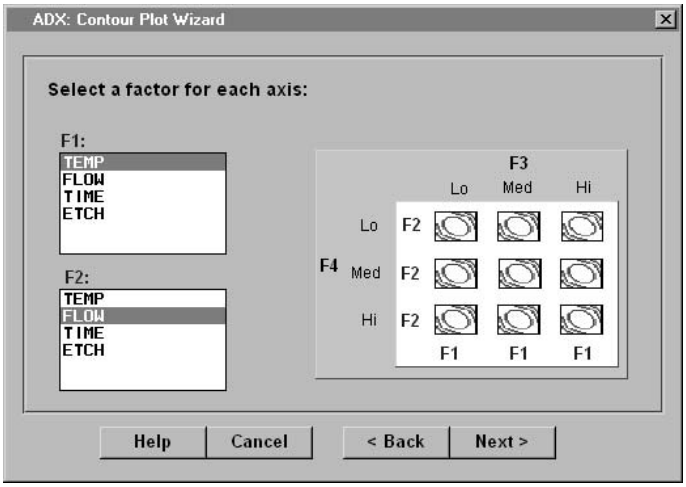


Select **View** → **Change plot** to invoke the Contour Plot Wizard, which provides different options for viewing the contours.

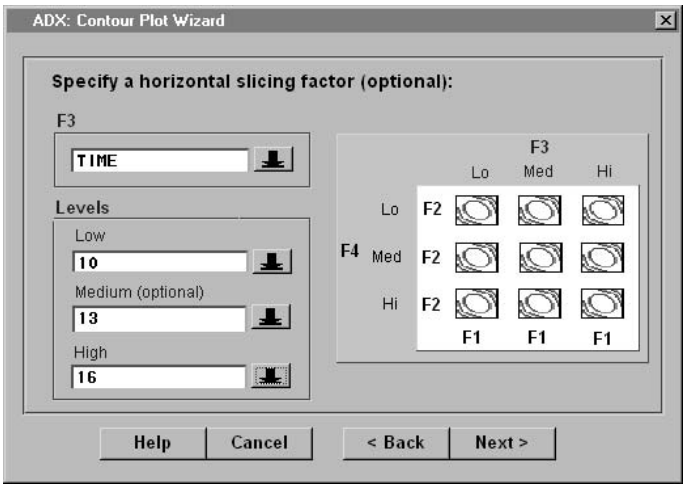


To view FLOW by TEMP contours at low, center, and high values of TIME for Block 2, follow these steps:

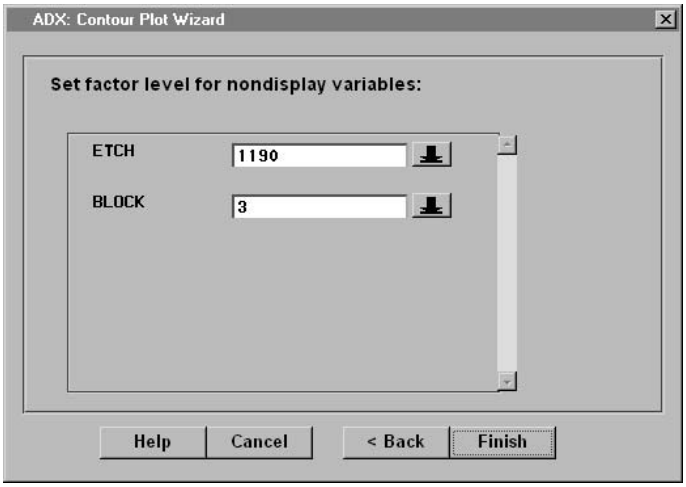
1. Select **Slices of factor levels**.



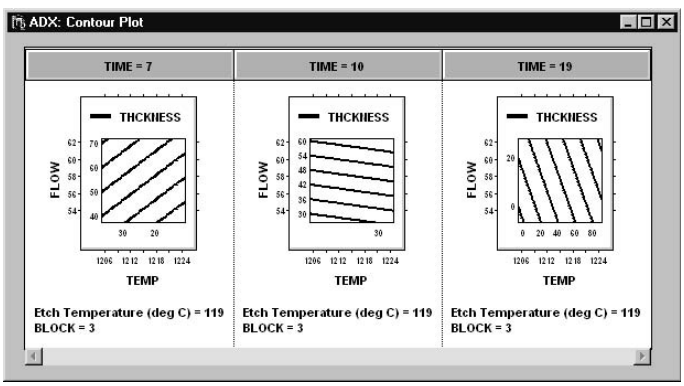
2. Select **F1=TEMP** and **F2=FLOW** from the two lists.
3. Click **Next**.



4. Select **TIME** as the horizontal slicing factor.
5. Use the arrows to change the levels for **Low**, **Medium**, and **High** to **7**, **10**, and **19**, respectively.
6. Click **Next** to set factor levels for nondisplay variables.



7. Click **Finish**. You should see the following display.

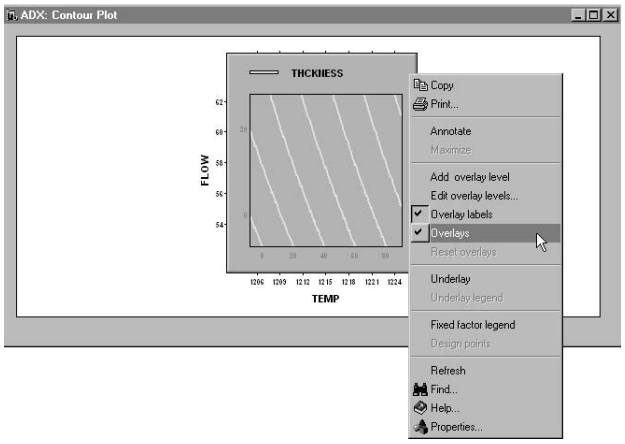


The small labels along the Y and X axes indicate the values of the contours of THCKNESS.

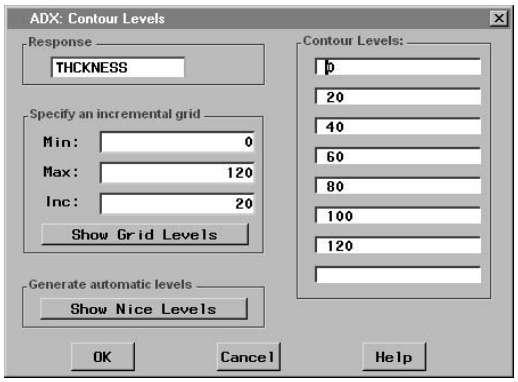
To create a FLOW by TEMP contour plot for THCKNESS at TIME=10, ETCH=1190, and BLOCK=1, click **Change plot** and follow the wizard steps.

To create a FLOW by TEMP contour plot for THCKNESS at TIME=10, ETCH=1190, and BLOCK=1, do the following:

1. Note that contour plots in ADX are highly interactive. Click on a contour line to grab and move contour lines.
2. Right-click to see the options available.

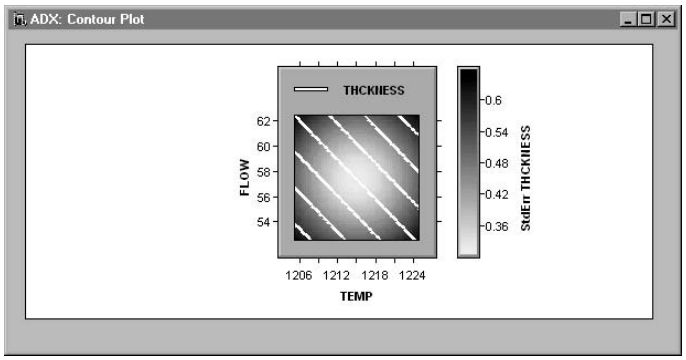


3. Select the **Edit overlay levels** option from the menu to open the Contour Levels window. You can use this window to select which fitted response to overlay, specify the grid, or have ADX generate automatic levels.



4. Click **OK** to close the Contour Levels window.

ADX can also display the standard error of the predicted response by using a shaded underlay. Right-click and select **Underlay**.

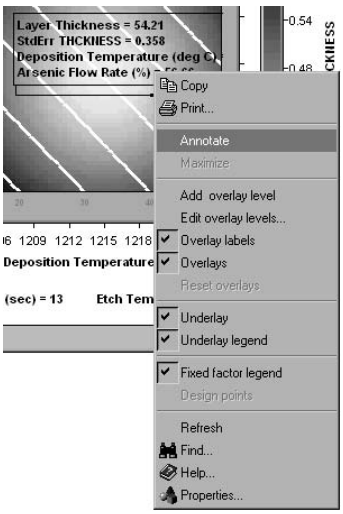


Press the left mouse button and move the mouse pointer over the plot to find those factor combinations that minimize the standard error (StdErr) and achieve a response close to the target of 60. As indicated by the thermometer legend, the lighter shade shows the factor region with the lowest standard error.

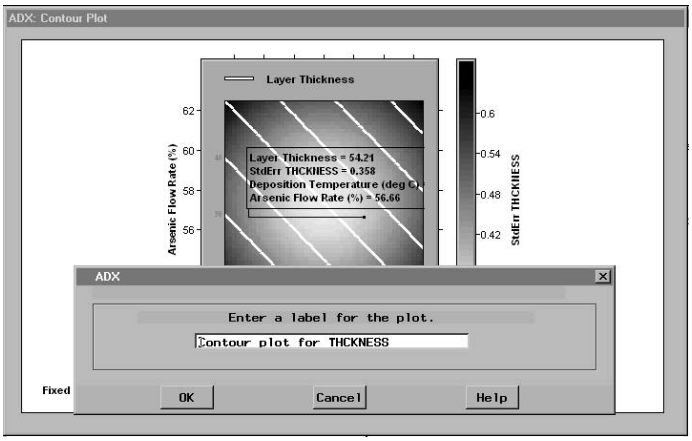
Annotating the Contour Plot

To annotate the contour plot with information about factor settings and to include the display in a report, do the following:

1. Right-click inside the contour plot.
2. Select **Annotate** to annotate the contour plot with the factor settings, response, and standard error of the response.



3. Move your mouse pointer within the contour plot to find the settings.
4. Click a point inside the plot to fix the annotation in place.



To remove the annotation, do the following:

1. Place your mouse pointer within the annotation box and right-click.
2. Select **Annotate**.

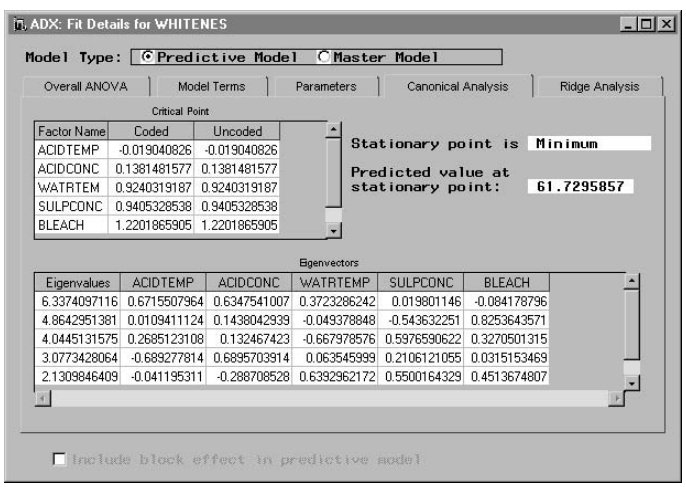
Canonical and Ridge Analyses

ADX performs canonical and ridge analyses for a response surface design when the master model contains all two-factor interactions and second-order polynomial terms, and when the design does not have more than one block. Refer to Myers and Montgomery (1995) for a description of canonical and ridge analyses.

The IC Fabrication design discussed in this chapter has three blocks, so is not a candidate for Canonical and Ridge analyses. The remainder of this section describes the analyses and displays the results for a design that does not have blocks.

To request the canonical analysis, click **Fit** in the main design window and select **Model → Fit Details**. If a canonical analysis is appropriate for a given design, then the **Canonical Analysis** and **Ridge Analysis** tabs will be displayed in the Fit Details window.

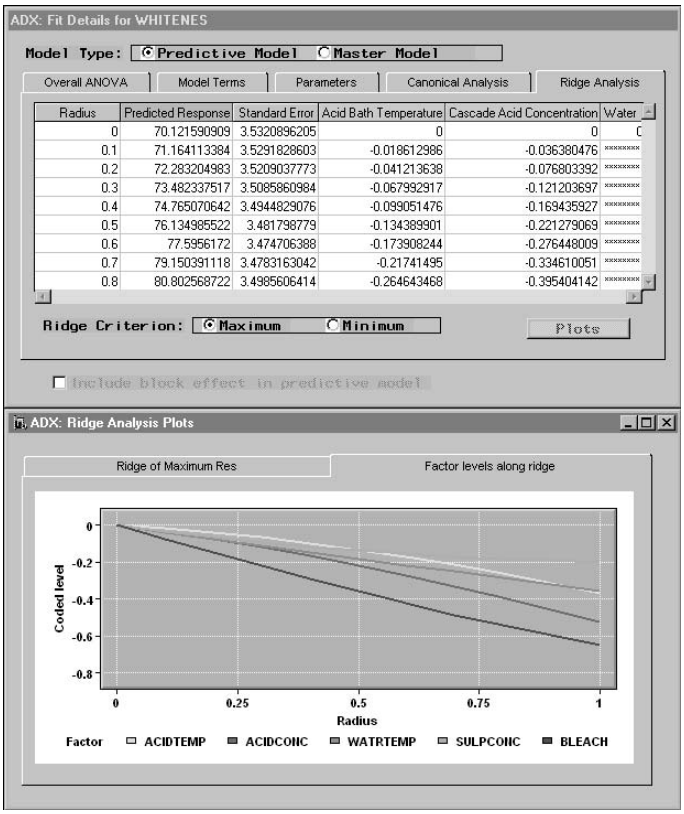
For the canonical analysis, ADX reports the coded and uncoded versions of the factor level settings for the critical (stationary) point and indicates the nature of the critical point (maximum, minimum, saddlepoint). It also reports the predicted response at the stationary point. Finally, it reports the eigenvectors and eigenvalues of the matrix of estimates of the second-order coefficients.



Factor Name	Coded	Uncoded
ACIDTEMP	-0.019040826	-0.019040826
ACIDCONC	0.1381481577	0.1381481577
WATRTEM	0.9240319187	0.9240319187
SULPCONC	0.9405328538	0.9405328538
BLEACH	1.2201865905	1.2201865905

Eigenvalues	ACIDTEMP	ACIDCONC	WATRTEMP	SULPCONC	BLEACH
6.3374097116	0.6715507964	0.6347541007	0.3723286242	0.019801146	-0.084178796
4.8642951381	0.0109411124	0.1438042939	-0.049378848	-0.543632251	0.8253643571
4.0445131575	0.2685123108	0.132467423	-0.667978576	0.5976590622	0.3270501315
3.0773428064	-0.689277814	0.6895703914	0.063545999	0.2106121055	0.0315153469
2.1309846409	-0.041195311	-0.288708528	0.6392962172	0.5500164329	0.4513674807

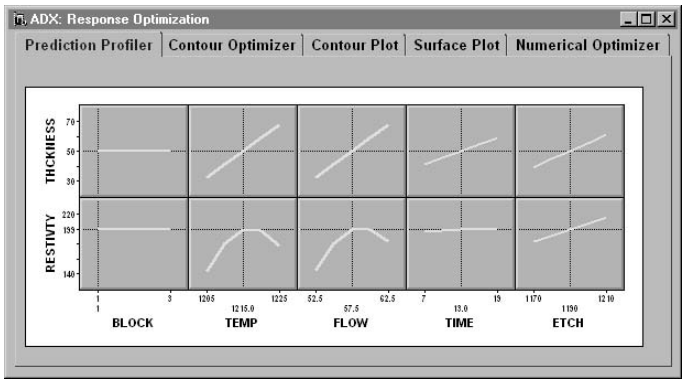
For the ridge analysis, ADX reports predicted values and factor settings along a ridge of optimum response, starting at the origin. Each point shows the factor settings that optimize—either minimize or maximize—the response at a given radius from the origin. A plot of the predicted response against the distance from the origin and a plot of the direction of the different responses along the axis can be requested by clicking **Plots**.



Radius	Predicted Response	Standard Error	Acid Bath Temperature	Cascade Acid Concentration	Water
0	70.121590909	3.5320896205	0	0	0
0.1	71.164113384	3.5291828603	-0.018612986	-0.036380476	********
0.2	72.283204983	3.5209037773	-0.041213638	-0.076803392	********
0.3	73.482337517	3.5085860984	-0.067992917	-0.121203697	********
0.4	74.765070642	3.4944829076	-0.099051476	-0.169435927	********
0.5	76.134985522	3.481798779	-0.134389901	-0.221279069	********
0.6	77.5956172	3.474706388	-0.173908244	-0.276448009	********
0.7	79.150391118	3.4783163042	-0.21741495	-0.334610051	********
0.8	80.802568722	3.4985606414	-0.264643468	-0.395404142	********

Optimizing Factor Settings

Click **Optimize** to find optimal factor settings by using the prediction profiler with a desirability function; see Chapter 3, "Full Factorial Designs," for more details. You can also use numerical optimization and a graphical contour optimizer. Finally, a three-dimensional response surface plot is available to help you visualize the responses. Usually, the best approach to optimization involves a combination of these tools, and you can take advantage of the fact that these interactive tools communicate with each other.



Numerical Optimizer

The numerical optimizer performs a grid search, which is useful for approximating the optimum for small to moderate designs. For this example, the goal is to achieve a target value of 60 for THCKNESS while maximizing RESTIVTY. To begin the optimization, follow these steps:

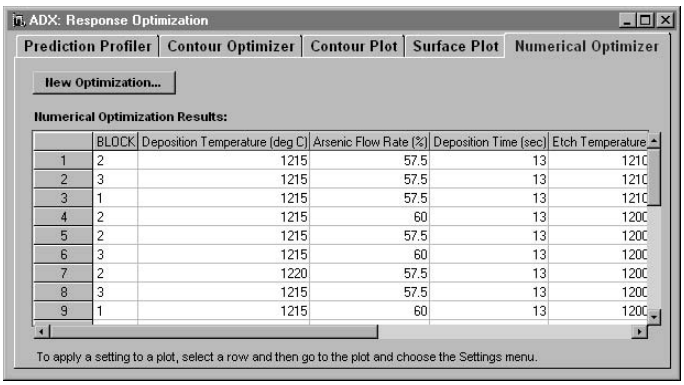
1. Fit a predictive model for THCKNESS and RESTIVTY if you have not done so already.
2. Click **Optimize** to optimize on both factors at the same time.
3. Select **THCKNESS** and **RESTIVTY**.

You can see from the **Prediction Profiler** tab that RESTIVTY is quadratic in TEMP and FLOW.

To perform a numerical optimization, do the following:

1. Click the **Numerical Optimizer** tab.
2. Select **RESTIVTY** as the response to optimize, and select **Maximize** for the objective. Click **Next** to continue.
3. The next screen enables you to specify constraints on THCKNESS. Since this response has a target of 60, set the low limit to **55** and the high limit to **65**. Click **Next** to continue.
4. Set the grid options for each of the factors. The default minimum and maximum are set to the **Min** and **Max** columns in the Quantitative Variables window. These defaults are acceptable, but change the number of grid points for each factor to **10**. Click **Next** to continue.
5. ADX will warn you that you have requested 30,000 grid points, but it is safe to continue in this case. ADX will automatically calculate the response for each level combination in each block. Click **Next**.

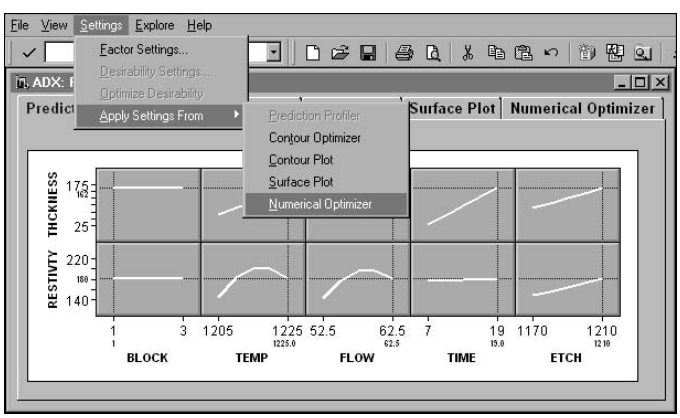
6. After doing a grid search, ADX will return a list of factor levels and their predicted responses, sorted in descending order by RESTIVTY. All level combinations for which THCKNESS response is not within the prescribed limits are filtered out. In this window you can delete infeasible level combinations. Click **Finish** to display the Numerical Optimization Results window.



	BLOCK	Deposition Temperature (deg C)	Arsenic Flow Rate (%)	Deposition Time (sec)	Etch Temperature
1	2	1215	57.5	13	1210
2	3	1215	57.5	13	1210
3	1	1215	57.5	13	1210
4	2	1215	60	13	1200
5	2	1215	57.5	13	1200
6	3	1215	60	13	1200
7	2	1220	57.5	13	1200
8	3	1215	57.5	13	1200
9	1	1215	60	13	1200

In the fifth row (your calculations might differ) is a level combination for which THCKNESS is close to 60 and RESTIVTY is close to the maximum. Select this combination by clicking **5** in the left column.

Return to the prediction profiler by clicking the **Prediction Profiler** tab. Select **Settings** → **Apply settings from** → **Numerical Optimizer**. The prediction profiler will apply the settings of the level combination selected in the numerical optimizer. Note that this gives a response close to the target.



Contour Optimizer and Contour Plot

Now that you have found factor settings that optimize both responses, take a closer look at the response surface with the contour optimizer. The interactive features of the contour optimizer are similar to those of the contour plot described in the section

"Viewing Contour Plots from the Fit Window" on page 109. You can also access contour plots from the Response Optimization window. Follow these steps:

1. Click **Contour Optimizer**.
2. Select **Underlay** to underlay the standard error of THCKNESS on the contours.
3. Select **Overlay** to overlay RESTIVTY contours on the THCKNESS contours.
4. Select **Settings** → **Apply Settings From** → **Prediction Profiler**. This displays the area of the response surface that is optimal for both responses.

You can interact with the contour optimizer as you did for each contour plot earlier.

Right-click and select **Edit overlay levels** to add contour lines. To move a contour, position the mouse pointer over a line. The pointer becomes a hand, which can be used to move the line. Clicking the mouse when the pointer is an arrow shows the factor settings and response values at that location.

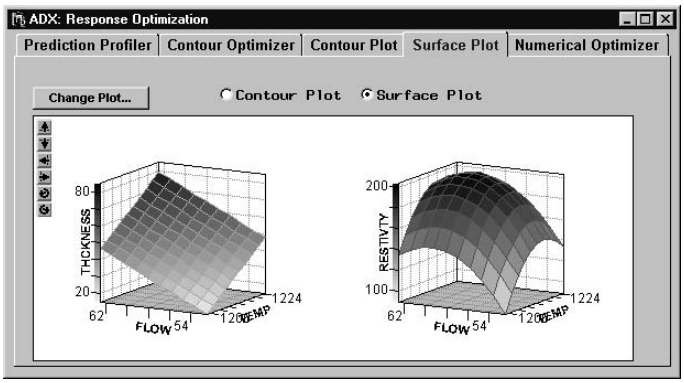
To create a matrix of contour plots, which is especially useful when dealing with more than two significant effects, follow these steps:

1. Click **Contour Plot** → **Change Plot**.
2. Select **Pairs of factors**, and click **Next**.
3. A single response, THCKNESS, is selected for you. Click **Next**.
4. TEMP and FLOW are selected for the horizontal axis, and TIME and ETCH are selected for the vertical axis. Click **Next**.
5. The middle values for factors not displayed are selected by default. Since these values are adequate, click **Finish**.

Surface Plot

In addition to the prediction profiler and contour optimizer, ADX provides surface plots that help you visualize the dependence of a fitted response on two or more factors.

Click the **Surface Plot** tab of the Response Optimization window. The following display appears.



You can use the six buttons in the upper left to rotate the plot. This is useful if the default perspective on the surface is not sufficient to show the salient features.

You can change the properties of the plot, including the presence of the cube and grid, by right-clicking and selecting from the menu.

If there are more than two factors, the factors not displayed will have fixed values that are displayed at the bottom. Optionally, two or more plots with these factors appearing at different levels can be displayed, or two or more plots with different pairs of factors can be displayed. You can change the fixed factors by clicking **Change Plot**, as in the case of the contour plot.

Points to Remember

- ADX provides a number of response surface designs. You can add blocks and choose axial scaling.
- You can use the factor library to define factors, responses, and blocks that you have defined in previous experiments.
- ADX provides interactive contour plots and three-dimensional surface plots to help you visualize the fitted response surface.
- Use the **Model** menu to review ANOVA statistics for the master and reduced models.
- ADX performs a lack-of-fit test whenever it has the data to do so.
- You can use the Contour Plot Wizard to create matrices of contour plots.
- You can display the standard error of the response as an underlay on response contours.
- You can annotate contour plots.
- The prediction profiler, contour optimizer, surface plots, and numerical optimizer help you optimize multiple responses.
- The surface plot helps you visualize the fitted response surface. You can create matrices of surface plots.

Chapter 8

Optimal Designs

Chapter Contents

Chapter 8
Optimal Designs

Chapter Topics

ADX provides a rich variety of standard designs, such as fractional factorial and central composite designs. However, in some cases, standard designs are unsuitable, such as when there are resource limitations or irregular design regions. In such cases, you can create D- and A-optimal designs, which are determined by a numerical optimality criterion.

Covered in This Chapter

- Creating an optimal design
- Defining variables
- Specifying a model
- Specifying the candidate set

Experimental Objective

An engineer needs to examine six factors. Two of the factors have three levels, and four have two levels. All two-factor interactions and the quadratic effects of the three-level factors need to be estimated. No more than two of the two-level factors can be at the $+1$ level.

In this example, you will only create the design. Analysis techniques are similar to those for designs covered earlier and are not repeated.

Task List

- Define the factors.
- Specify a master model.
- Specify a candidate set.
- Specify the optimality criterion and the search method.

Creating the Optimal Design

In this example, you will do the following:

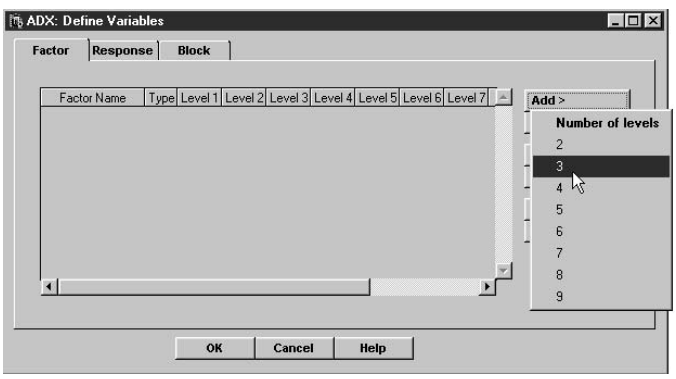
1. Define six factors. Two of the factors are quantitative with three levels each (such as time or temperature variables). The other four are two-level factors.

2. Identify the effects you want to estimate. For this example, you will specify a model with polynomial effects for the two quantitative factors.
3. Specify the candidate set.
4. Choose the number of runs you want in the final design. This cannot be less than the number of effects you want to estimate.

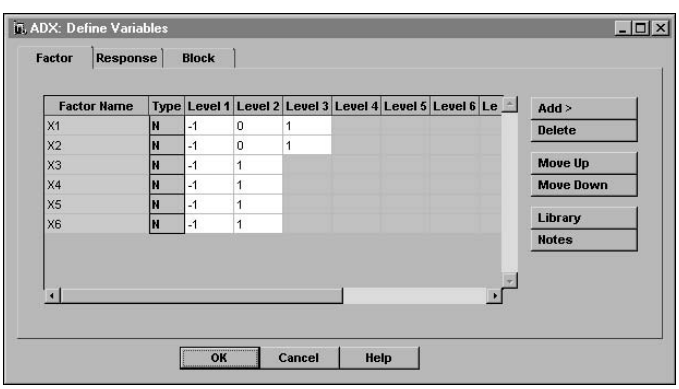
Defining Factors

ADX can generate optimal designs for factors having two to nine levels. You specify the number of levels for a factor when you define it. Follow these steps:

1. Select **File** → **Create New Design** → **Optimal** from the ADX desktop.
2. Click **Define Variables**.
3. Click **Add** and select **Add quantitative factorial variable** → **Number of levels** → **3**.



4. Repeat step 3 to add another three-level variable.
5. Click **Add** and select **Add quantitative factorial variable** → **Number of levels** → **2**.
6. Repeat step 5 four times to add the two-level factors X3, X4, X5, and X6.



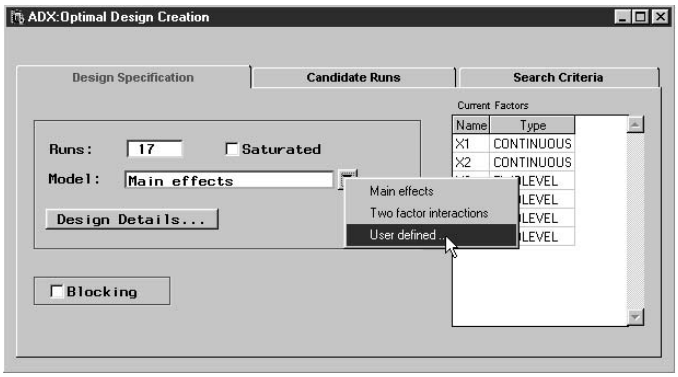
7. Click **OK** and then **Yes** to save the changes.

Optimal designs can be created with qualitative and quantitative factors having between two and nine levels.

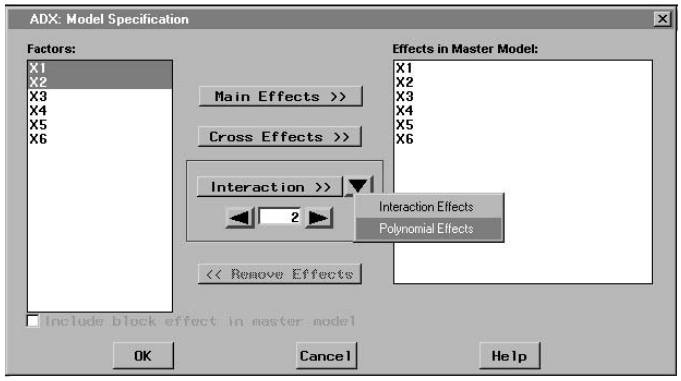
Specifying a Model

Once you have defined the factors, you need to specify the master model. Do the following:

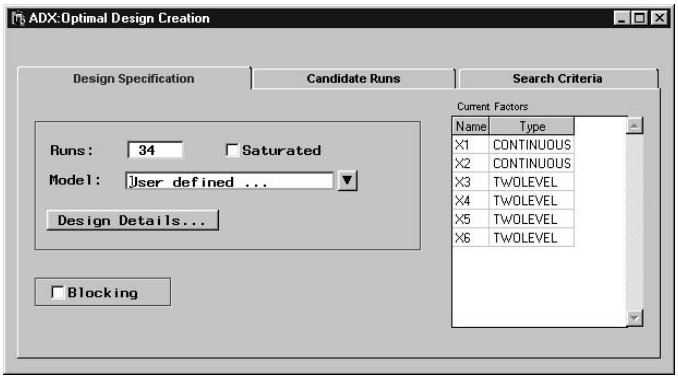
1. Click **Select Design**.



2. In the Design Specification window, click the arrow and select **User defined** from the menu.
3. Select **X1** and **X2** and change **Interaction Effects** to **Polynomial Effects** with the arrow, and then click **Polynomial** to add quadratic effects to the model.



4. Select **X1** through **X6**, change **Polynomial Effects** back to **Interaction Effects**, and click **Interaction** to add all the two-way interaction effects to the model.
5. Click **OK**. ADX determines that 34 runs are needed for the design.

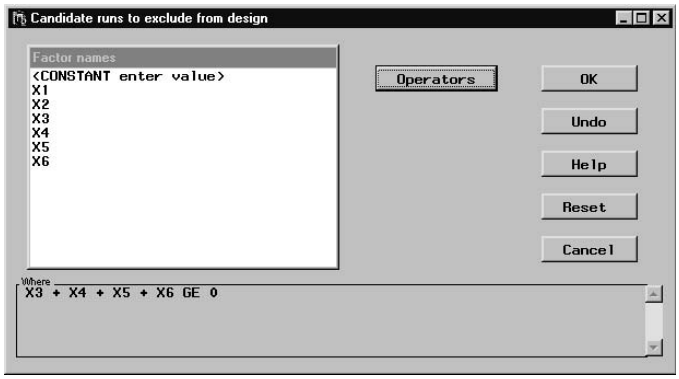


By default, ADX will pick 10 more runs than the number needed to make a saturated design. You can choose a different number of runs, select **Saturated** to generate the minimum number of runs given the model, or select **Blocking** to specify the number of blocks and the number of runs within each block.

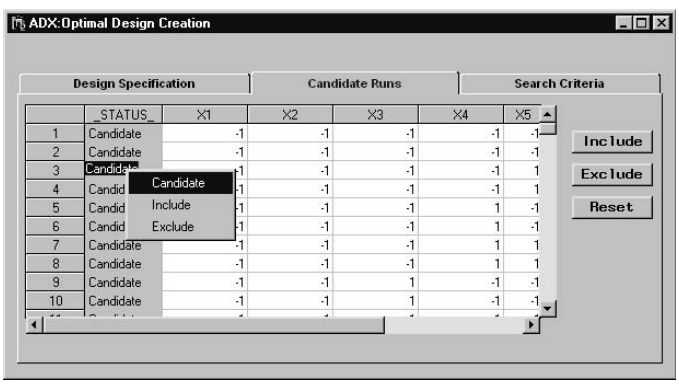
Specifying a Candidate Set

Click the **Candidate Runs** tab to specify the candidate set. In this example, the design region excludes runs where more than two of the two-level factors are at the $+1$ level. Because these factors have $(-1, +1)$ encoding, points where the sum of the levels of X3, X4, X5, and X6 is greater than zero are excluded. Follow these steps:

1. Click **Exclude**.
2. Select **X3** from the list.
3. The **Operators** menu will automatically appear. Select the **+** operator.
4. Select **X4** and then select **+**.
5. Select **X5** and then select **+**.
6. Select **X6** and then select **GT**. GT stands for "Greater Than."
7. Select **<CONSTANT enter value>** from the list and type **0**.
8. Click **OK** to accept the value.



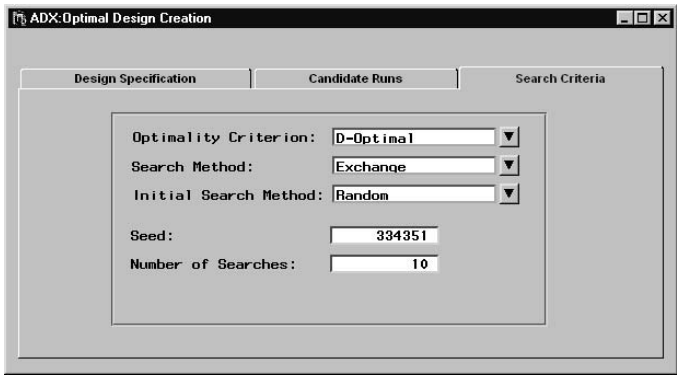
You can also include or exclude a particular candidate point by clicking in the appropriate row of the **Status** column and selecting **Candidate**, **Include**, or **Exclude** from the menu.



You can click **Reset** to set all points to be candidate points.

Choosing the Search Method

You can choose the optimality criterion and search method on the **Search Criteria** tab. The defaults in ADX usually return designs close to optimal.

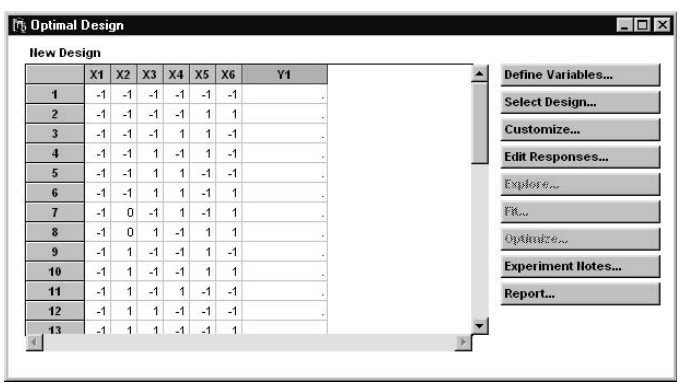


This window is an interface to the OPTEX procedure, which ADX uses for finding the optimal design. In this case, the OPTEX procedure searches for a D-optimal design by using the exchange algorithm and a random initial search. For more information, refer to the chapter on the OPTEX procedure in the *SAS/QC 9.1 User's Guide* (2003) and the references therein.

Close the window to create the design.

The Optimal Design

Using the specified optimality criterion, ADX searches the given candidate runs to find an optimal design that meets the design search criteria. For this example ADX constructs an optimal design with 34 runs that can estimate all the main effects and two-factor interactions.



	X1	X2	X3	X4	X5	X6	Y1
1	-1	-1	-1	-1	-1	-1	.
2	-1	-1	-1	-1	1	1	.
3	-1	-1	-1	1	1	-1	.
4	-1	-1	1	-1	1	-1	.
5	-1	-1	1	1	-1	-1	.
6	-1	-1	1	1	-1	1	.
7	-1	0	-1	1	-1	1	.
8	-1	0	1	-1	1	1	.
9	-1	1	-1	-1	1	-1	.
10	-1	1	-1	-1	1	1	.
11	-1	1	-1	1	-1	-1	.
12	-1	1	1	-1	-1	-1	.
13	-1	1	1	-1	-1	1	

Analyzing an Optimal Design

To do the analysis and optimization of an optimal design, perform steps in the Fit, Explore, and Optimize windows similar to those for other designs. For exploring the data, the scatter and box plots are available. For automatically selecting effects, ANOVA and stepwise regression are available. For finding optimal factor settings,

the prediction profiler, contour optimizer, contour plot, surface plot, and numerical optimizer are all available.

Points to Remember

- Optimal designs provide a way of planning experiments that do not fall into the standard categories of two-level, response surface, mixed level, and mixture designs. Often, optimal designs are used when the design region is irregular or when the number of runs required by a standard design exceeds the available resources.
- To create an optimal design in ADX, you must click **Define Variables** to create a candidate set of runs from which to choose.
- You must specify the model, using the Design Specification window, for the effects you want to estimate.
- You can specify the number of runs you want in an optimal design, but you must be sure to specify enough runs to estimate the effects you have specified in your model.

Chapter 9

Mixed-Level Designs

Chapter Contents

Chapter 9
Mixed-Level Designs

Chapter Topics

Taguchi (1978) and Taguchi and Wu (1980) proposed a class of experimental designs for quality improvement, which are known as Taguchi-type designs, crossed-array designs, or product designs. Because these designs involve a crossproduct of two designs, one based on control factors and one based on noise factors, they tend to have more runs than fractional factorial and response surface designs. The control factor designs are typically small orthogonal arrays. These are not intended to (nor are they able to) investigate interactions. Refer to Dehnad (1989) and Phadke (1989) for discussions of product designs.

In ADX, these small orthogonal arrays are referred to as "mixed-level designs" because they usually involve factors with varying numbers of levels. However, if all your factors have two levels, you should use a two-level design because more tools are available.

Control factors are factors whose levels can easily be fixed in a laboratory setting and in the field. Noise factors are factors whose levels can be fixed for purposes of experimentation but not in the field. Noise factors are assumed to account for the variation in the quality characteristics of interest. The design for the control factors is called the inner array, and the design for the noise factors is called the outer array.

The Taguchi approach also involves signal-to-noise ratios, which combine deviation from the target with variation around the target into a single measure. These quality characteristics reflect the idea that not only should the expected outcome be optimized, but the variation around the optimum should be minimized as well.

Covered in This Chapter

- Creating a mixed-level design
- Defining an outer array
- Choosing a response function or signal-to-noise ratio
- Exploring data
- Fitting a model
- Optimizing a response function or signal-to-noise ratio

Experimental Objective

Table 9.1. Factors and Responses for Nylon Experiment

Variable	Name	Levels	Description
Control Factors	INTERFER	Low, Medium, High	Difference between outer width of tubing and inner width of connector
	WALL	Thin, Medium, Thick	Connector wall thickness
	IDEPTH	Shallow, Medium, Deep	Depth of insertion of tubing into connector
	ADHESIV	Low, Medium, High	Amount of glue in connector pre-dip
Noise Factors	TIME TEMPERAT HUMIDTY	24,120 72, 150 0.25, 0.75	Time for assembly Temperature Relative humidity
Response	FORCE		Force to pull tubing from connector

The example here was reported by Byrne and Taguchi (1986) and performed by researchers at Baylock Manufacturing Corporation. The researchers were investigating the strength of nylon tubing connections, and they identified the following control factors, noise factors, and response for the experiment, shown in Table 9.1.

The goal of the experiment is to find factor settings that maximize the pull-off force and minimize variation in pull-off force among tubing connections.

Task List

- Set up the mixed-level inner array.
- Set up the outer array.
- Create a signal-to-noise response function for force.
- Fit best models for FORCE and for the signal-to-noise ratio.
- Optimize the signal-to-noise ratio.

Creating a Mixed-Level Design

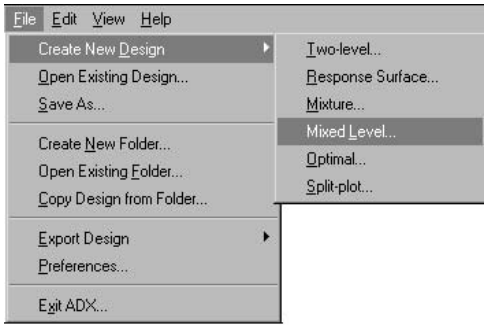
To create a mixed-level design, follow these steps:

1. Create the design for the inner array (control) factors.
2. Create the design for the outer array (noise) factors by modifying the design for the inner array.
3. Determine the appropriate signal-to-noise ratio, and create a separate response for it.

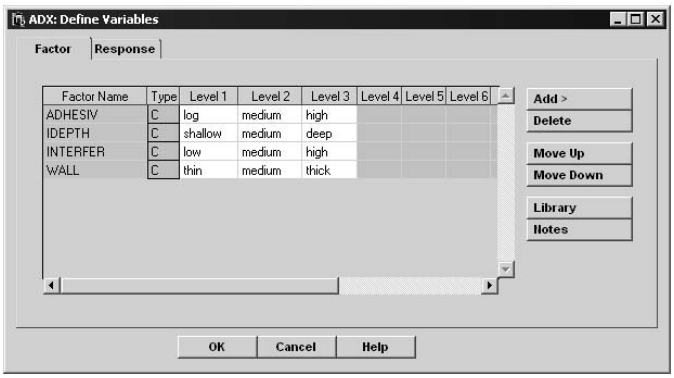
Creating an Inner Array Design

Use a mixed-level design for the control factors, since there are three levels for each of the four control factors. Follow these steps:

1. Select **File** → **Create New Design** → **Mixed Level** from the ADX desktop or click the **Mixed-Level Design** icon on the toolbar.



2. In the Mixed-Level Design window, click **Define Variables**.
3. Click **Add** and select **Add qualitative factor variable** → **3**.
4. Repeat step 3 three more times to add the remaining factors.
5. Type in the factor names and levels from Table 9.1. Your Define Variables window should look as follows:

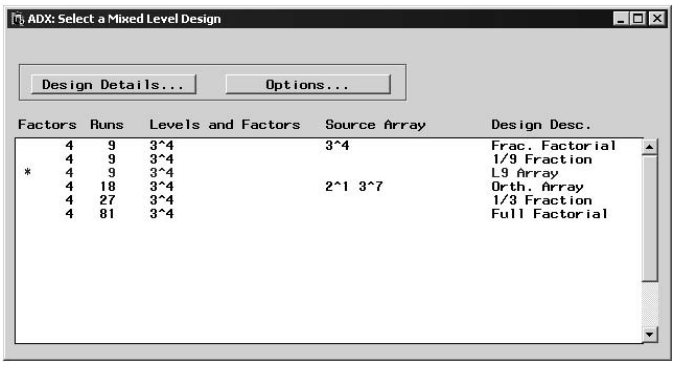


6. Click **OK** to return to the Mixed Level Design window.

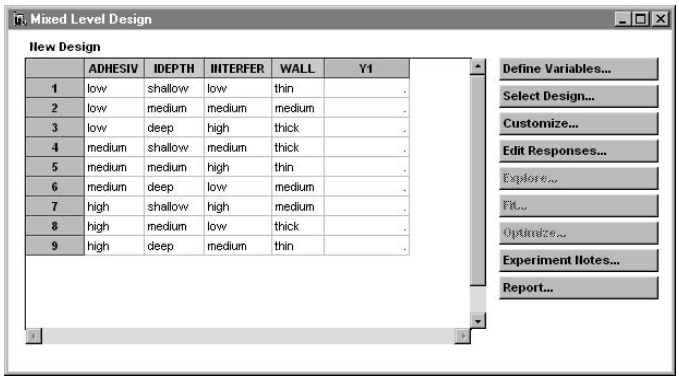
To add the response, click the **Response** tab. Change the name of **Y1** to **Force** and return to the main design window.

To select the design, follow these steps:

1. Click **Select Design**.
2. Select the **L9 Array** design for **4** factors, all with **3** levels.



Close the Create Mixed Level Design window. The design for the inner array will be displayed in the Mixed Level Design design window.

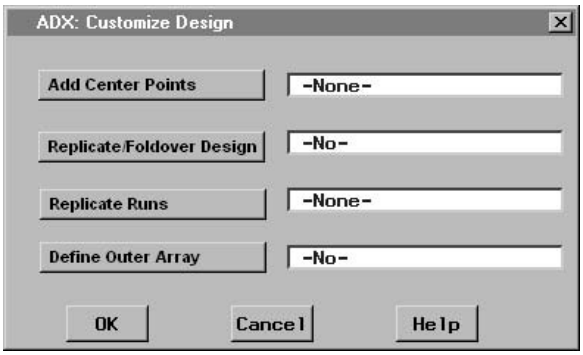


	ADHESIV	IDEPTH	INTERFER	WALL	Y1
1	low	shallow	low	thin	.
2	low	medium	medium	medium	.
3	low	deep	high	thick	.
4	medium	shallow	medium	thick	.
5	medium	medium	high	thin	.
6	medium	deep	low	medium	.
7	high	shallow	high	medium	.
8	high	medium	low	thick	.
9	high	deep	medium	thin	.

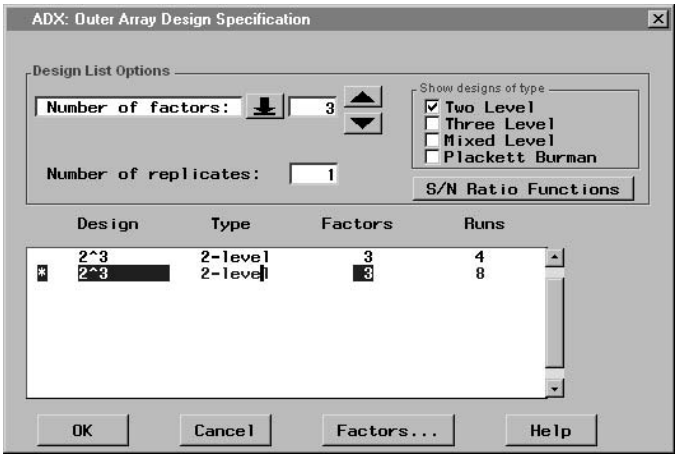
Creating an Outer Array Design

To create the outer array, you customize the current design you created for the inner array. Follow these steps:

1. Click **Customize**.

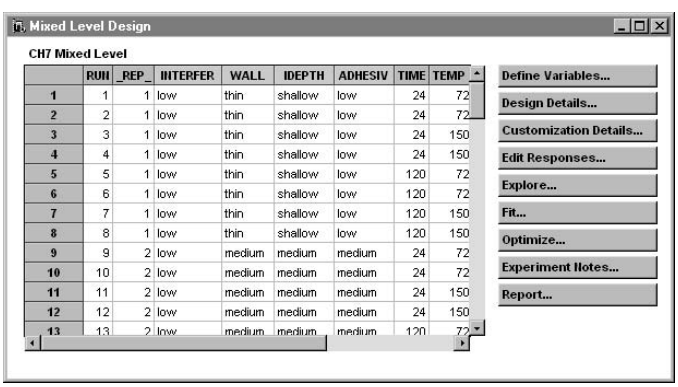


2. Click **Define Outer Array** to open the Outer Array Design Specification window.
3. Change the number of factors to **3**.
4. Select the **2-level** design with **3** factors and **8** runs. You can show only two-level designs by selecting **Two Level** and clearing the other check boxes.



5. Click **Factors** to define the TIME, TEMPERAT, and HUMIDITY noise factor names and levels for the outer array.
6. Click **OK** to accept this design for the outer array. ADX indicates the outer array design in the Customize window.
7. Click **OK**.

The complete product design, shown in the Mixed Level Design window, will have 72 runs.



	RUN	_REP_	INTERFER	WALL	IDEPTH	ADHESIV	TIME	TEMP
1	1	1	low	thin	shallow	low	24	72
2	2	1	low	thin	shallow	low	24	72
3	3	1	low	thin	shallow	low	24	150
4	4	1	low	thin	shallow	low	24	150
5	5	1	low	thin	shallow	low	120	72
6	6	1	low	thin	shallow	low	120	72
7	7	1	low	thin	shallow	low	120	150
8	8	1	low	thin	shallow	low	120	150
9	9	2	low	medium	medium	medium	24	72
10	10	2	low	medium	medium	medium	24	72
11	11	2	low	medium	medium	medium	24	150
12	12	2	low	medium	medium	medium	24	150
13	13	2	low	medium	medium	medium	120	72

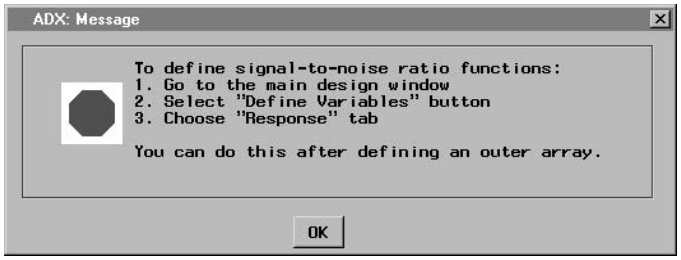
Creating a Signal-to-Noise Ratio Response

You can define the following response functions in ADX:

- Mean: the response mean at each control factor design point over the noise array
- Standard Deviation: the response standard deviation at each control factor point
- Variance: the response variance at each control factor point

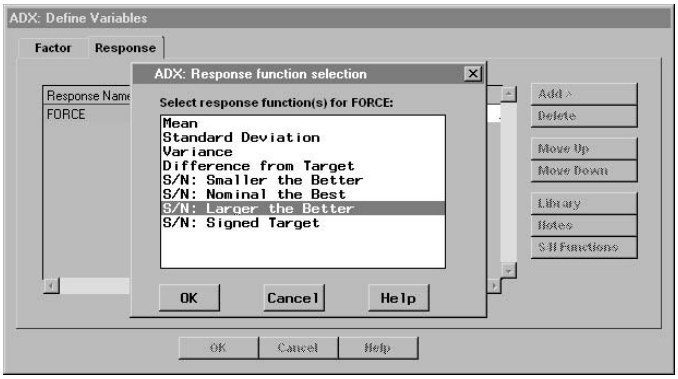
- Difference from Target: the difference between the average response and a user-specified target at each control factor point
- S/N: Smaller the Better: The "smaller-the-better" signal-to-noise ratio, which increases as the response mean decreases and variation around the mean decreases
- S/N: Nominal the Best: The "nominal-the-best" signal-to-noise ratio, which increases as the response mean gets closer to a user-specified target and variation around the mean decreases
- S/N: Larger the Better: The "larger-the-better" signal-to-noise ratio, which increases as the response mean increases and variation around the mean decreases.
- S/N: Signed Target: The "signed target" signal-to-noise ratio, which is a -10 times the logarithm of the response variance at each inner array design point. This increases as the variation around the mean decreases.

If you click the **Signal-to-Noise** button in the Outer Array Design Specification window, an ADX message appears that explains how to define the signal-to-noise ratio.



To define the signal-to-noise, follow these steps:

1. Go to the main design window.
2. Click **Define Variables**.
3. Click the **Response** tab.
4. Click **FORCE** to select the FORCE row.
5. Click **S/N Functions**.
6. Select **S/N: Larger the Better** since a higher pull-off force means a better quality of nylon tubing; also select **Mean** since Taguchi (1978) suggested that you should always analyze the mean.



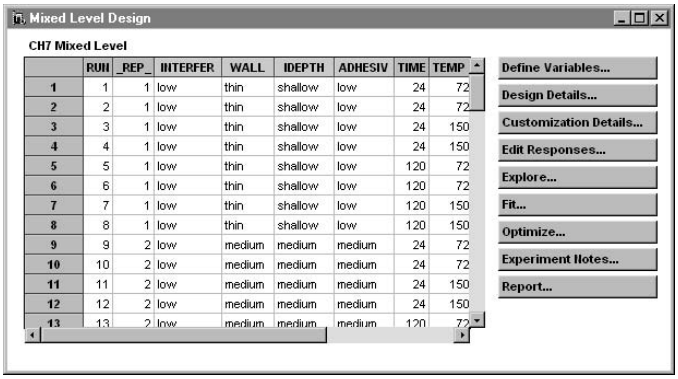
7. Click **OK** to define the signal-to-noise ratio.
8. Click **OK** in the Define Variables window to return to the Mixed Level Design window.

At this point, you have completed all the steps required to create the product design for the pull-off force experiment. To proceed, close this design and open the sample design named pull-off force, which is identical to the design you just created and contains the response values.

Reviewing a Mixed-Level Design

The design and data for the design described previously are already on the ADX desktop. Review the details of the design before creating your own design. To review design details, do the following:

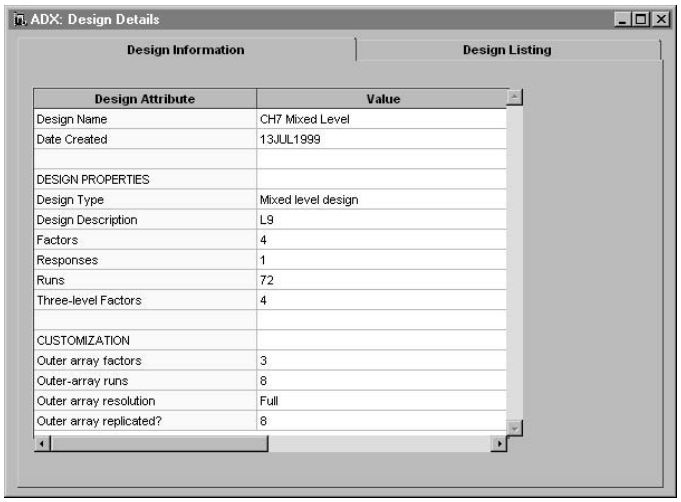
1. Open the ADXBKV9 folder (or the folder in which you placed the book designs).
2. Open the Pull-off Force design.



	RUN	_REP_	INTERFER	WALL	IDEPTH	ADHESIV	TIME	TEMP
1	1	1	low	thin	shallow	low	24	72
2	2	1	low	thin	shallow	low	24	72
3	3	1	low	thin	shallow	low	24	150
4	4	1	low	thin	shallow	low	24	150
5	5	1	low	thin	shallow	low	120	72
6	6	1	low	thin	shallow	low	120	72
7	7	1	low	thin	shallow	low	120	150
8	8	1	low	thin	shallow	low	120	150
9	9	2	low	medium	medium	medium	24	72
10	10	2	low	medium	medium	medium	24	72
11	11	2	low	medium	medium	medium	24	150
12	12	2	low	medium	medium	medium	24	150
13	13	2	low	medium	medium	medium	120	72

ADX differentiates inner array (control) factors from outer array (noise) factors by coding the column headings with different colors.

Click **Design Details** to review the design information for this design.



Design Attribute	Value
Design Name	CH7 Mixed Level
Date Created	13JUL1999
DESIGN PROPERTIES	
Design Type	Mixed level design
Design Description	L9
Factors	4
Responses	1
Runs	72
Three-level Factors	4
CUSTOMIZATION	
Outer array factors	3
Outer-array runs	8
Outer array resolution	Full
Outer array replicated?	8

The **Design Properties** section describes the design for the control factors of the inner array. The **Customization** section describes the design for the noise factors of the outer array. Close the Design Details window.

Analyzing a Mixed-Level Design

To fit a model, click **Fit** in the main design window. ADX presents a window asking you to specify a response for which a model should be fit. Select **SNRL(FORCE)** and click **Run**.

Note that the only effects shown are the main effects of the control factors. You cannot select noise factors as significant. Because you are analyzing a signal-to-noise ratio, ADX collapses the design into the inner array.

None of the effects are automatically selected because the inner array design is saturated, and the only available automatic effect selection methods are ANOVA and stepwise regression.

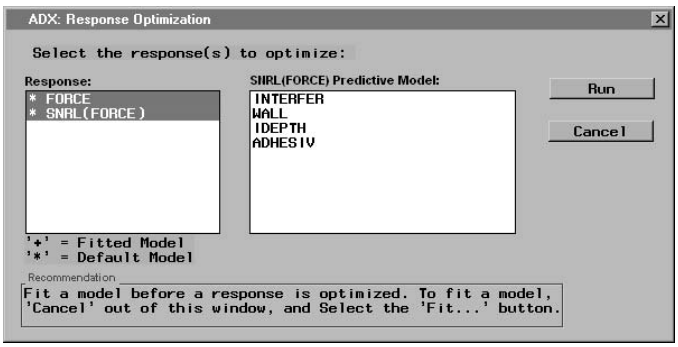
Close the Effect Selection for SNRL(FORCE) window. After the changes are saved, a message dialog box appears asking whether to continue. Click **Yes** to return to the main design window.

Fit a model for MEAN(FORCE). There are no significant effects. Close the fit window and click **OK**. ADX will estimate the parameters of the master model, which includes just the main effects, and use this in optimization.

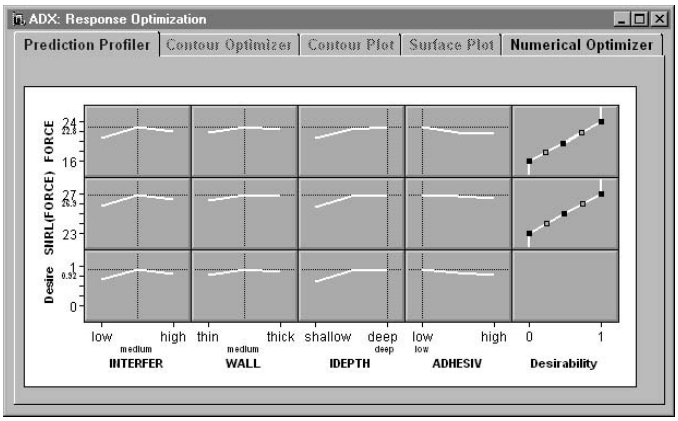
Optimizing a Response

The goals of this experiment are to determine the levels of the control factors that bring MEAN(FORCE) to target and to minimize variability around that target. A high SNRL indicates small variability, so maximizing SNRL is part of the goal. With the desirability function in the prediction profiler, you can maximize SNRL at the same time that you optimize the control factor settings. Follow these steps:

1. Click **Optimize**.
2. Since ADX has not selected any significant effects for either FORCE or SNRL(FORCE), it uses the master model to optimize responses. Select **FORCE** and **SNRL(FORCE)** and click **Run**.



3. Select **View** → **Show Desirability** to view desirability functions and traces.
4. Define desirability functions to maximize MEAN(FORCE) and SNRL(FORCE).
5. Move the factor settings to maximize overall desirability. Alternatively, you can select **Settings** → **Optimize desirability**.



Tying It All Together

MEAN(FORCE) and SNRL(FORCE) are maximized when INTERFER is set at medium, WALL at medium, IDEPTH at deep, and ADHESIV at low. However, IDEPTH and ADHESIVE do not affect the desirability as much as INTERFER.

Points to Remember

- A mixed-level design that uses the Taguchi (1978) approach is characterized by two sets of factors: control factors and noise factors.
- The experimental design for the control factors is called an inner array and is often chosen as a mixed-level design.
- The Taguchi (1978) approach with mixed-level designs does not typically consider interactions.
- You can use the Customize Design window to define the outer array for the noise factors.
- The **Response** tab of the Define Variables window is used to create a signal-to-noise response ratio.
- You can use the ADX optimization tools on the fitted master model when analyzing mixed-level designs by using the Taguchi (1978) approach if the inner array design is saturated.

Chapter 10

Mixture Designs

Chapter Contents

Chapter 10
Mixture Designs

Chapter Topics

Mixture designs are a special class of experimental designs in which the factors are the relative amounts of components in a blend. For example, the factors might be the proportions of chemicals in a mixture for coating wafers in semiconductor manufacturing. Since the levels of the mixture components must sum to one (or 100%), both the design and the analysis of the experiment differ from the design and analysis of screening and response surface experiments.

Covered in This Chapter

- Creating a mixture design
  - Defining variables by using the factor library
  - Selecting a mixture design
- Exploring data
- Fitting a Scheffé model
  - Checking regression assumptions
  - Transforming the response
- Optimizing the response
  - Using the prediction profiler
  - Using the contour optimizer

Experimental Objective

This classic mixture example was discussed by Cornell (1990). A yarn is manufactured by blending three different materials, and the investigators are interested in the best blend for creating a fiber with maximum elongation. They use a simplex-lattice mixture design for the experiment. The investigators identified the following variables for the experiment shown in Table 10.1.

Table 10.1. Responses and Factors for Yarn Elongation Experiment

Variable	Name	Description
Factors	PRO	Polypropylene proportion
	ETH	Polyethylene proportion
	STY	Polystyrene proportion
Response	ELONG	Yarn elongation

The goal of the experiment is to maximize elongation and minimize prediction variance.

Task List

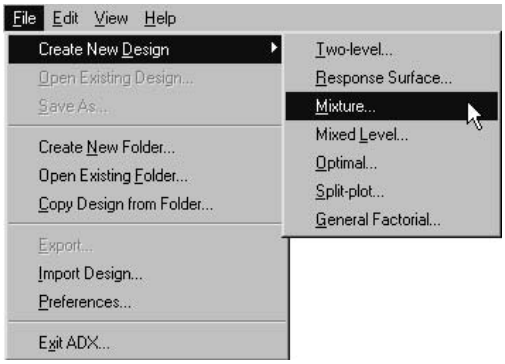
- Create a simplex-lattice mixture design.
- Fit a Scheffé model to the elongation response.
- View the prediction profiler and contour plot to find optimum blend.

Creating a Simplex-Lattice Mixture Design

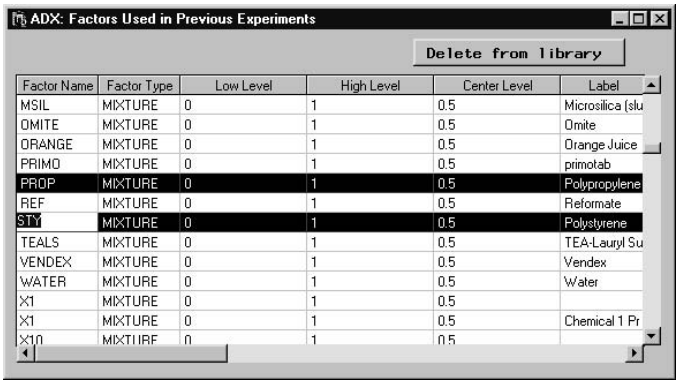
Defining Variables

To define the mixture factors, follow these steps:

1. Select **File** → **Create New Design** → **Mixture** from the ADX desktop or click the **Mixture** tool button .



2. Click **Define Variables**.
3. Click **Library** on the **Mixture Variables** tab to take advantage of the fact that the factors are already defined in the factor library. Otherwise, you would need to enter the factor information directly in the Define Variables window.
4. Select **PROP**, **STY**, and **ETH**.



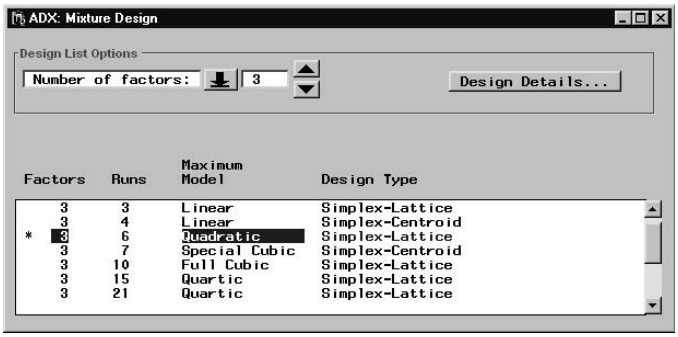
Factor Name	Factor Type	Low Level	High Level	Center Level	Label
MSIL	MIXTURE	0	1	0.5	Microsilica (slu
OMITE	MIXTURE	0	1	0.5	Omite
ORANGE	MIXTURE	0	1	0.5	Orange Juice
PRIMO	MIXTURE	0	1	0.5	primotab
PROP	MIXTURE	0	1	0.5	Polypropylene
REF	MIXTURE	0	1	0.5	Reformate
STY	MIXTURE	0	1	0.5	Polystyrene
TEALS	MIXTURE	0	1	0.5	TEA-Lauryl Su
VENDEX	MIXTURE	0	1	0.5	Vendex
WATER	MIXTURE	0	1	0.5	Water
X1	MIXTURE	0	1	0.5	
X1	MIXTURE	0	1	0.5	Chemical 1 Pr
X10	MIXTURE	0	1	0.5	

5. Close the Factors Used in Previous Experiments window.
6. Click the **Response** tab in the Define Variables window.
7. Select the **Y1** cell and type **ELONG**.
8. Click **OK** to close the Define Variables window, and click **Yes** to save the changes.

Selecting the Design

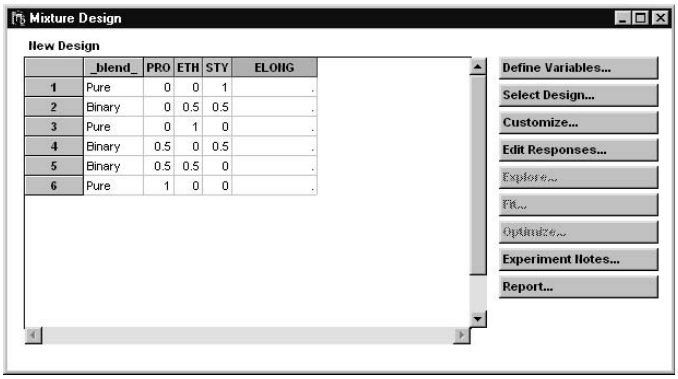
To select an appropriate design, follow these steps:

1. Click **Select Design** from the main design window.
2. The table lists available mixture designs for three factors. Select the **6** run **Quadratic Simplex-Lattice** design.



	Factors	Runs	Maximum Model	Design Type
	3	3	Linear	Simplex-Lattice
	3	4	Linear	Simplex-Centroid
*	3	6	Quadratic	Simplex-Lattice
	3	7	Special Cubic	Simplex-Centroid
	3	10	Full Cubic	Simplex-Lattice
	3	15	Quartic	Simplex-Lattice
	3	21	Quartic	Simplex-Lattice

3. Close the design window and click **Yes** to use the design.

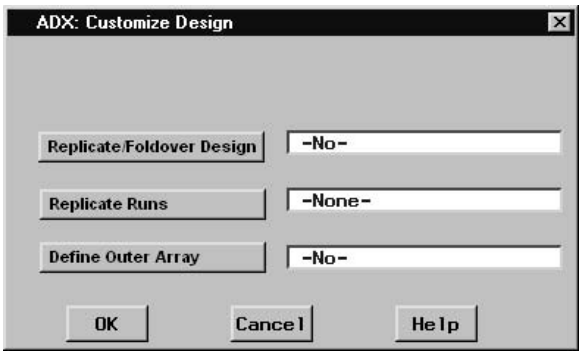


For mixture designs, ADX provides a descriptive column, called **blend**, which indicates the composition of the blend for each run. A pure blend consists of only one factor. A binary blend is a mixture of two factors.

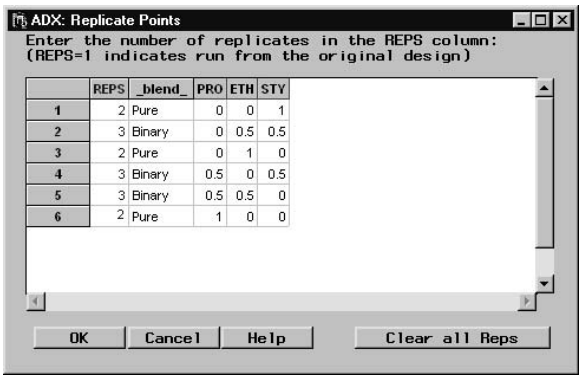
Customizing the Design

To complete this design as described by Cornell (1990), add one replicate for each pure blend and two replicates for each binary blend. Follow these steps:

1. Click **Customize** from the main design window.

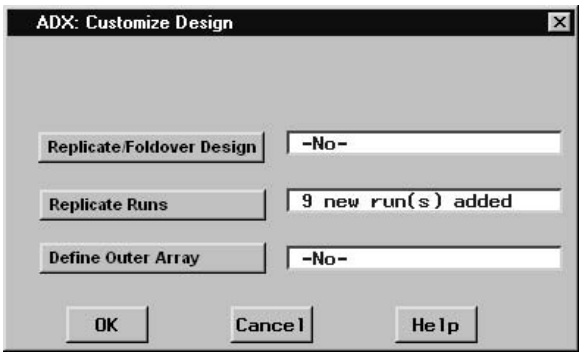


2. Click **Replicate Runs**.
3. For each pure blend run, type **2** for REPS. For each binary blend run, type **3** for REPS.



	REPS	_blend_	PRO	ETH	STY
1	2	Pure	0	0	1
2	3	Binary	0	0.5	0.5
3	2	Pure	0	1	0
4	3	Binary	0.5	0	0.5
5	3	Binary	0.5	0.5	0
6	2	Pure	1	0	0

4. Click **OK**. ADX reports the number of runs added.



5. To accept the customization, click **OK**.

The design customization adds 9 runs. The complete design has 15 runs and is ready for the response data to be entered. Instead of entering the responses by hand, close the design you just created and open the sample design named Yarn Elongation, which contains the response values.

Analyzing a Simplex-Lattice Mixture Design

You can use the **Fit** button to examine significant effects and to obtain a predictive model. To use the prediction profiler and contour optimizer to find the optimal blend, you can use the **Optimize** button. The prediction profiler displays the relationship between factor setting and predicted response. The contour optimizer provides a triangular plot for graphically determining the optimal blend for obtaining maximum elongation.

Fitting a Model

To fit a Scheffé model, click **Fit** in the main design window. The Effect Selection window displays the fitted master model and highlights the significant effects. ADX does not allow you to exclude the main effects from the predictive model in the mixture designs since all components need to be present in the mixture. Hence ADX always highlights the main effects in the Effect Selection window regardless of significance; two- and three-factor interaction effects are highlighted according to the automatic selection criterion. Effects highlighted in the Effect Selection for Yarn elongation window are incorporated into the predictive model, which is subsequently used to compute the predicted response values in optimization.

As with other design types, the Check Fit Assumptions window and the automatic effect selection methods are available from the Effect Selection main menu. The only two methods available for automatic effect selection are ANOVA and stepwise regression. Many of the plots and charts provided for other design types do not apply to mixture designs.

The Prediction Profiler

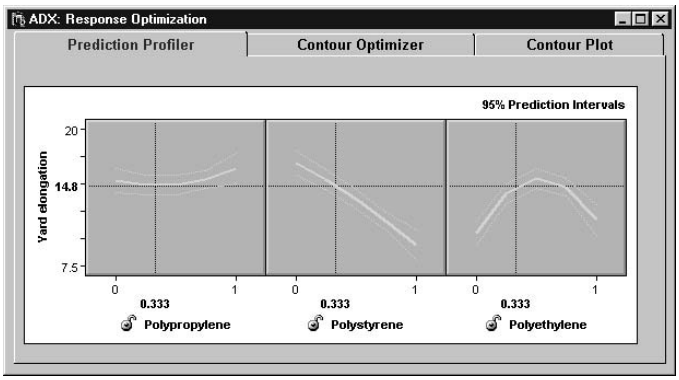
In a factorial design a factor can be set independently of the other factors. However, in a mixture design the factor settings must sum to one. Consequently, the prediction profiler for mixture designs is modified to satisfy this constraint. Click **Optimize** in the main design window to display the prediction profiler.

The prediction profiler is initially displayed with the factors at the centroid of the simplex region. Moving a factor setting will affect the other factor settings, which will be changed in such a way that the following occur:

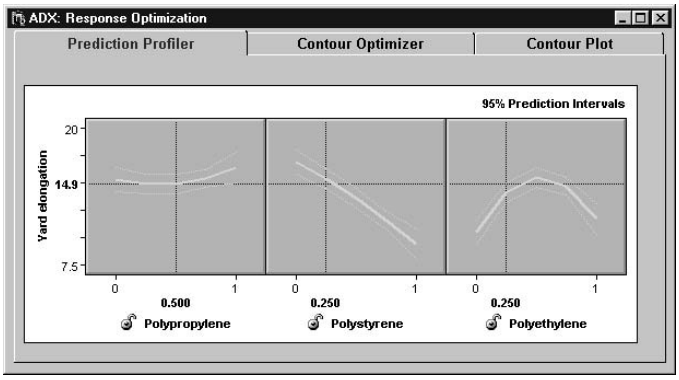
- The sum of the factor settings is always one.
- The new settings are at the centroid of the simplex region subject to the constraints imposed by the factor setting just made and any locked factors. Initially, no factor settings are locked.

The current predicted response line (the horizontal line) will move to intersect the prediction line for the current factor at the new factor setting. Note that the prediction lines will not move.

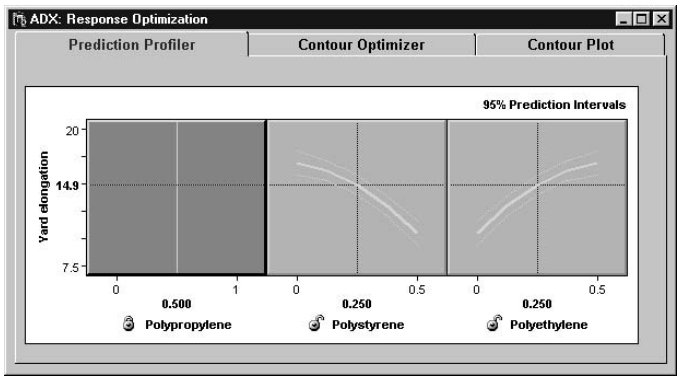
Locking a factor will prevent ADX from changing its setting when you change other factor settings. You can lock or unlock a factor setting by clicking the lock icon.



For example, the prediction profiler for the Yarn Elongation design will open with the PRO, STY, and ETH settings at (1/3, 1/3, 1/3), the centroid of the original simplex. If the PRO setting is moved to 1/2, the factor settings will change (1/2, 1/4, 1/4) because that is the centroid of the region of the original simplex constrained to PRO=1/2. The predicted response will be 14.89.



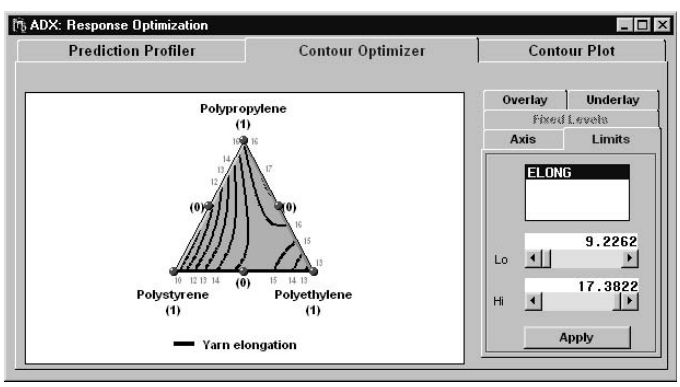
Click the lock beside Polypropylene to fix its level at 1/2. The region changes color, and the other two prediction lines change. Moving another factor —say, Polystyrene —will no longer cause the Polypropylene to move. However, the Polyethylene factor will still move to keep the sum of the factors at 1. Note that after Polypropylene is locked, you cannot set any other factor higher than 1/2, because then the factor settings would sum to a value greater than one.



When only two factors are unlocked, their prediction traces are symmetric. Moving one factor in one direction is equivalent to moving the other factor in the opposite direction.

The Contour Optimizer

The contour optimizer accommodates the unique issues surrounding mixture designs. The triangle is a cross section of a cube through the three corners where one coordinate is one and the rest are zero. This corresponds to the two-dimensional region where the factors sum to one. In general, if there are n factors, the simplex will have the dimension $n - 1$.

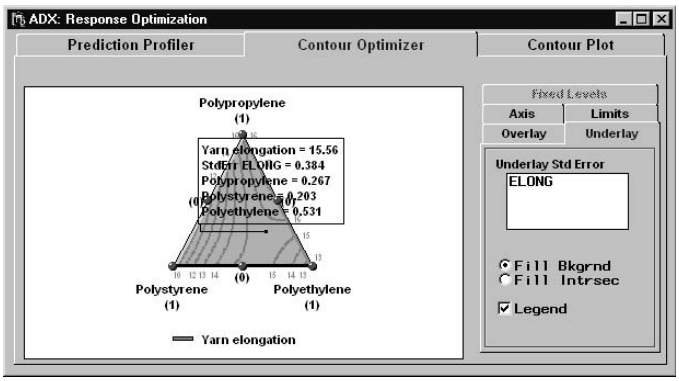


The coordinate system for a mixture design is a simplex coordinate system. The vertices correspond to pure blends, and the triangle edges correspond to binary blends. The contours of the predicted response are plotted on the face of the triangle. The symbol markers indicate design points.

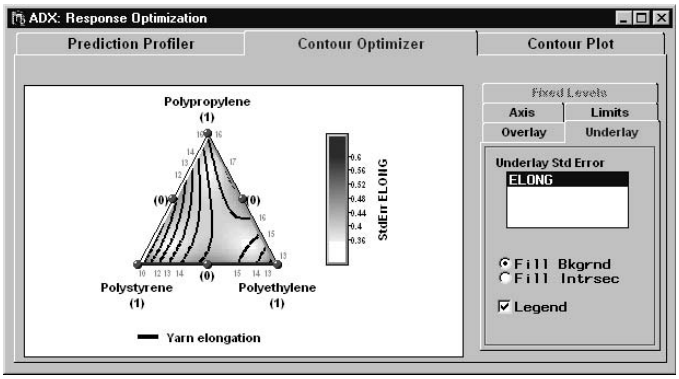
You can interact with the contour optimizer, just as with other contour plots:

- Click on a contour line to label it.
- Click in the background to create an annotation.

- Right-click and select **Annotate** from the menu to create or delete a permanent annotation.
- Grab a contour line to move it.



You can also underlay the standard deviation of the response under the contour lines. In this example the goal is to maximize the predicted elongation while minimizing the prediction variance.



To add a standard error underlay, follow these steps:

1. Click the **Underlay** tab.
2. Select **ELONG**. The legend indicates that the lightest areas are those with the lowest standard error.
3. Maximize the Contour Plot window to make it easier to interact with the plot.

Click between the contour lines near the top of the triangle to see factor, response, and standard error values at that area of the plot. For two-factor blends, click near the midpoints of the sides of the triangle.

For a pure blend, with minimal standard error and maximum yarn elongation, you can use PROP to achieve a predicted elongation of 17. For a binary blend, you can use a mixture of ETH and STY to achieve an elongation of around 15.

Note that you can select additional options for the contour plot, including colors and fonts, by right-clicking and selecting **Properties** from the menu.

Tying It All Together

In a mixture design, all main effects are considered to be significant. Second- and higher-order interactions are selected through ANOVA or stepwise regression.

The prediction profiler and contour optimizer provide two graphical methods for optimizing the response.

You can incorporate additional linear constraints on the factors in a mixture design, and you can incorporate process variables. This will be discussed in Chapter 11, "More on Mixture Designs."

Points to Remember

- Mixture design factors are components in a blend.
- The levels of the components in a mixture must sum to one, so you need to make special considerations when designing and analyzing a mixture experiment. Refer to Cornell (1990) for details.
- Mixtures can be pure (one factor) or a blend of factors.
- You can use the interactive features of the prediction profiler and contour optimizer to find optimal mixtures.
- You can underlay the standard error of the prediction as a shaded gradient so that you can find the minimum prediction error for your response.

Chapter 11

More on Mixture Designs

Chapter Contents

Chapter 11
More on Mixture Designs

Chapter 10 introduced the simplest kind of mixture design, in which the only constraint is that the factors sum to one. In practice, you are rarely able to conduct a mixture experiment throughout the region defined by this constraint, which is referred to as a simplex. Cost, infeasibility of some levels of particular components, and difference in behavior of the mixture near some edges of the simplex might require that you restrict the runs to a particular region within the simplex.

Furthermore, factors that are not part of the blend might have some significant influence on the response of interest. For example, the blends might be studied at different temperatures. Such factors, called process variables, are not part of the Scheffé model used in Chapter 10. ADX can include process factors in analysis and optimization of mixture designs.

Creating a Constrained Mixture Design

ADX eanbles you to place linear constraints on the factors in addition to the basic constraint that the factors sum to one. Each linear constraint can involve one or more factors.

Since there is no standard design covering all situations for constrained mixtures, ADX uses the optimal design interface for the creation of these designs. This interface chooses runs from the vertices of the constrained region, the centers of the edges, the centroids of the faces, and the overall centroid. You can choose a design for a linear, quadratic, special cubic, full cubic, or quartic model, depending on how many factors are present in the model.

Fitting a model to a constrained mixture design involves the same steps as fitting a model to an unconstrained mixture design. Furthermore, the optimization tools available in analyzing an unconstrained mixture design are also available for the constrained design. The only difference is that ADX marks the feasible region defined by the linear constraints and prevents factor settings outside the bounds of those constraints.

The following sections show how to create a mixture design with three factors, X1, X2, and X3, with the following constraints:

- $X1 \geq 0.1$
- $X2 \geq 2\ X3$

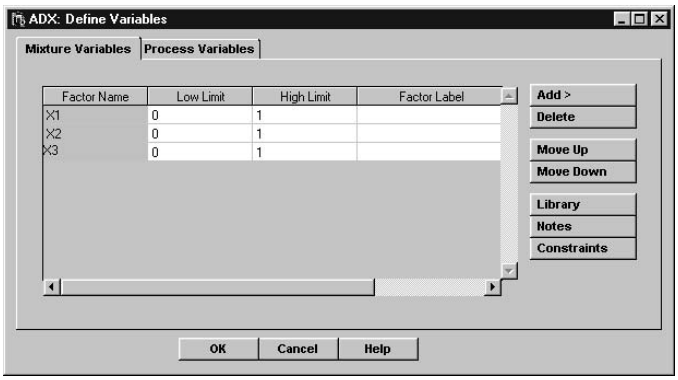
A quadratic model will be used.

Defining Variables and Constraints

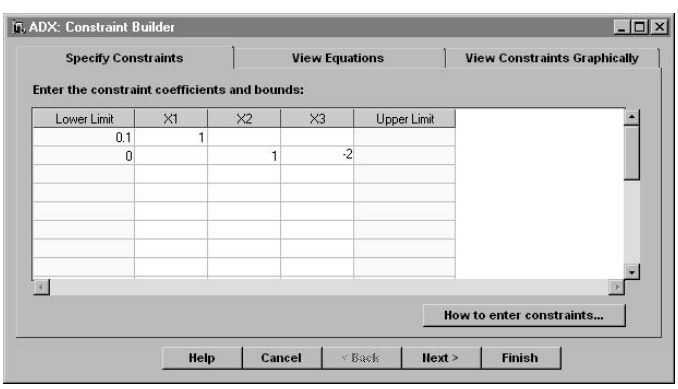
To create the design, select **File** → **Create New Design** → **Mixture** from the ADX desktop. The main design window will open.

Define the variables and constraints for the new mixture design by following these steps:

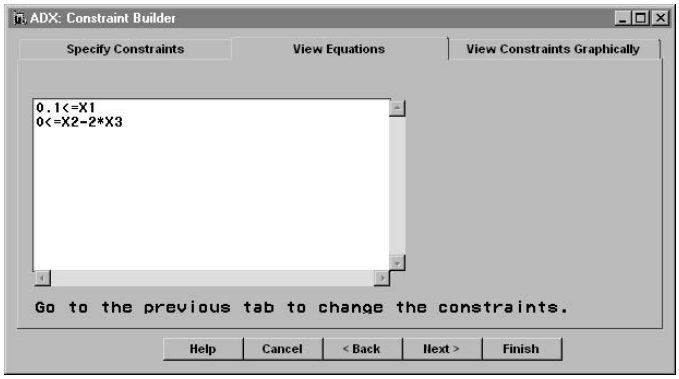
1. Click **Define Variables** and add three variables by clicking **Add** and selecting **3** from the pop-up menu.



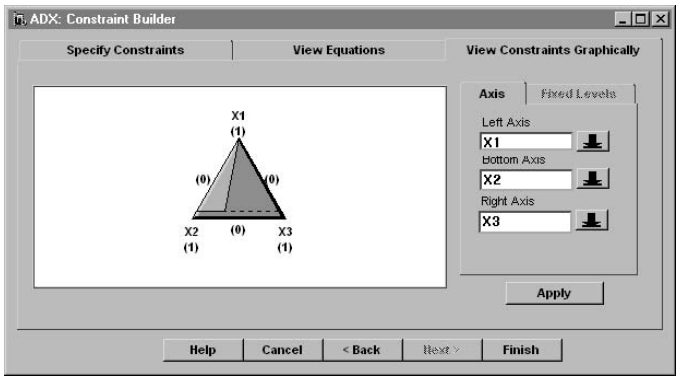
2. Click the **Constraints** button. The Constraint Builder window will appear, with the **Specify Constraints** tab selected.
3. To add the constraint X1 $\geq$ 0.1, note that this is the same as 0.1 $\leq$ X1. Type **.1** in the first box in the **Lower Limit** column of the table, and type **1** in the first box in the **X1** column. Here, 1 is the coefficient of X1.
4. To add the constraint X2 $\geq$ 2 X3, note that this is the same as requiring that X2 $-$ 2 X3 $\geq$ 0. Type **0** in the **Lower Limit** column, **1** in the **X2** column, and $-$**2** in the **X3** column. Here, 1 and -2 are the coefficients of X2 and X3, respectively. When you are finished, the window should look as follows:



5. You can view the constraints in equation form by clicking the **View Equations** tab or clicking **Next**.



6. You can view the region defined by the constraints by clicking the **View Constraints Graphically** tab or by clicking **Next** when viewing the equations.



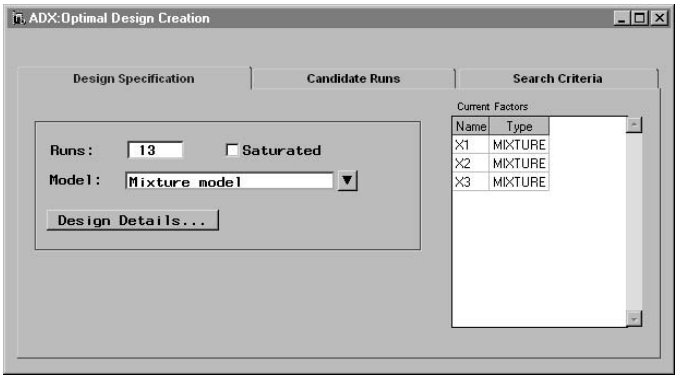
7. Click **Finish** and then **Yes** in the confirmation dialog box to save the constraints.
8. Click **OK** in the Define Variables window and then click **Yes** in the confirmation dialog box to save the variable definitions.

For more information about how to enter constraints, click **How to enter constraints** in the Constraint Builder window.

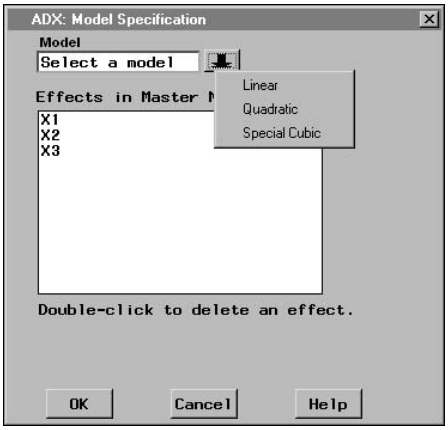
Creating the Design

Now, to create the constrained mixture design, do the following:

1. Click **Select Design** in the main design window.
2. The Optimal Design Creation window will appear. The main difference between this window and the optimal design windows in Chapter 8 is that the type of model you can choose here is tailored to the unique requirements of your mixture design.



3. To change the model, click the down arrow beside **Mixture model**. There is only one choice, **Mixture model**, on the pop-up menu; select it.
4. The Model Specification window will appear. The list indicates which factors are present in the model; by default, the model is linear. Click the down arrow beside **Select a model** to choose the model. Here only linear, quadratic, and special cubic models are available because there are only three factors. Select **Quadratic**.



5. The list will automatically be updated with the new effects. Click **OK** to return to the Optimal Design Creation window.
6. As discussed in Chapter 8, ADX chooses 10 more runs than the number of parameters to estimate. You can specify the number of runs or select **Saturated** to generate the minimum possible number of runs for the previously selected model.
7. You can review the design details, the candidate points, and the search criteria by clicking the appropriate button or tab.
8. Close the window and click **Yes** in the confirmation dialog box to generate the design.

The optimal design will be displayed in the main design window. You can now randomize the run order or enter responses.

Analyzing and Optimizing a Constrained Mixture Experiment

Analyzing and optimizing a constrained mixture experiment with ADX is exactly the same as analyzing and optimizing an unconstrained mixture experiment. ADX automatically adjusts the prediction profiler and contour optimizer to guarantee that any optimal factor settings you find are within the feasible region.

Creating a Mixture Design with Process Variables

Sometimes a mixture experiment will involve factors that are not a component of the blend. Temperature and blend time are two examples of such factors.

Analysis of a mixture experiment with process variables involves the same tools as for any mixture design. However, the usage must be adjusted to account for the process variables.

In this section, you will create and analyze a mixture experiment including process variables.

Experimental Task

The following experiment examines quality characteristics of drug tablets based on the levels of certain excipients, the mixing time of the compound, and the load in the tablet compression, as shown in Table 11.1.

Table 11.1. Factors and Responses for PV Tablet Formulation Mixture

Variable	Name	Levels	Description
Mixture Factors	ALPHA BETA PRIMO	0–1 0–1 0–1	Alpha-lactose monohydrate Beta-lactose monohydrate Primotab
Process Factors	MIXTIME COMPLOAD	2, 10 1, 2	Mixing time Compression load
Responses	CRUSHSTR DISSRATE		Crushing strength Dissolution rate

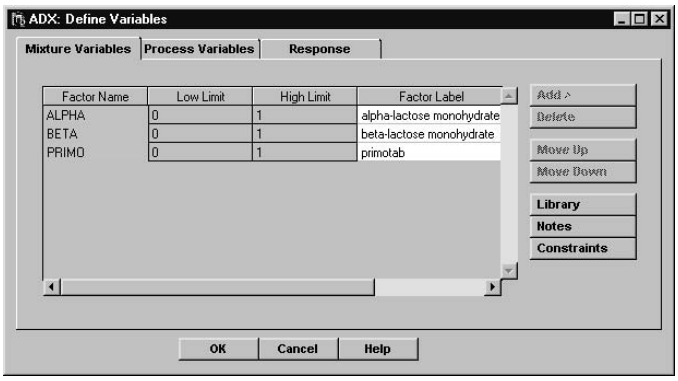
A high crushing strength and low dissolution rate are desirable.

Defining Variables

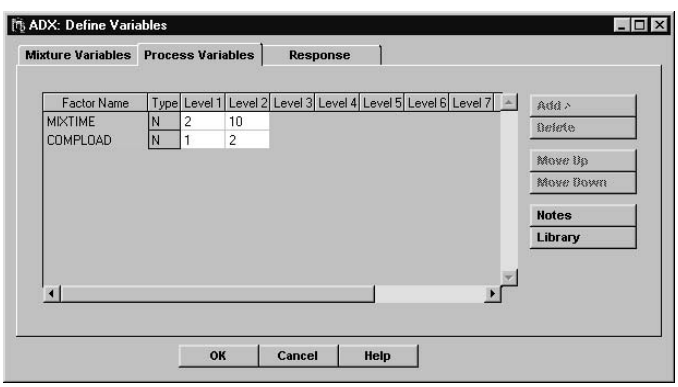
Select **File** → **Create New Design** → **Mixture** from the ADX desktop. Define the variables for the design by doing the following:

1. Click **Define Variables**.
2. Create the mixture variables just as in any other mixture experiment. In this case, click **Add** and select **3**.

3. Change the names of the mixture variables to **ALPHA**, **BETA**, and **PRIMO**.



4. Click the **Process Variables** tab. You will see a factor definition interface similar to that in the Define Variables window in Chapter 8, "Optimal Designs."
5. Click **Add** and select **Add quantitative factorial variable** → **2**. This creates a new process variable named Z1 with two levels.
6. Create a second two-level quantitative process variable named Z2.
7. Change the **Factor Name** of Z1 to **MIXTIME**. Set the low level to **2** and the high level to **10**.
8. Change the name of Z2 to **COMPLOAD**, the low level to **1**, and the high level to **2**.

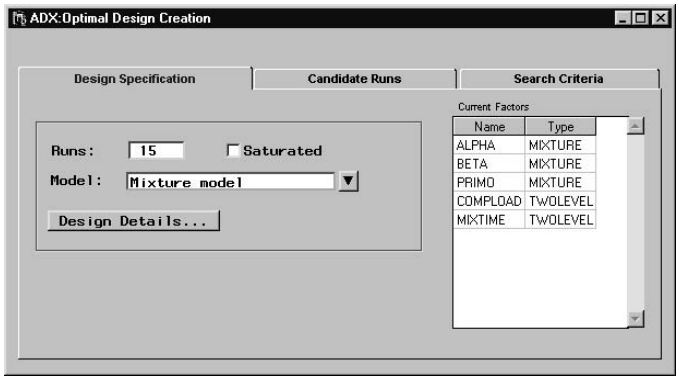


9. Click the **Response** tab and change the name of the response to **CRUSHSTR**.
10. Add a second response variable, and change the name to **DISSRATE**.
11. Click **OK** and then **Yes** to save the factor definitions.

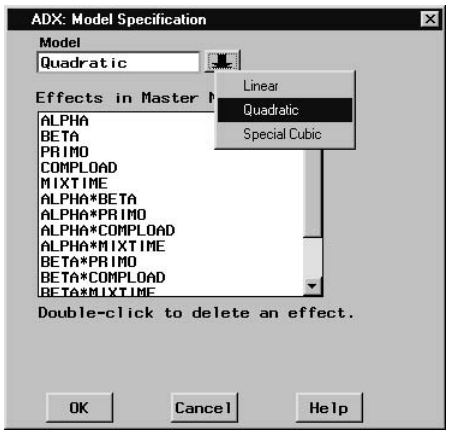
Creating the Process Mixture Design

Since there are few standard designs accommodating mixture experiments with process variables, ADX uses the optimal design interface to construct the design. To generate the runs, do the following:

1. Click **Select Design** from the main design window.
2. The Optimal Design Creation window appears in place of the standard Design Selection window.

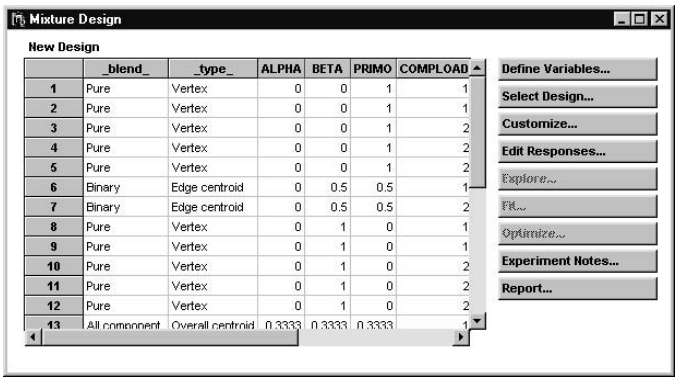


3. Select the model you want to use by clicking the down arrow beside **Model**. Select **Mixture model**, the only item on the menu.
4. The Model Specification window appears. Click the down arrow beside **Select a model**.
5. The pop-up menu lists all the possible choices for the number of factors you defined. Select **Quadratic**.



6. Click **OK** to change the model.
7. Change the number of runs to **25**, if necessary.

8. You can review the candidate set or alter options in the design search algorithm, just as you did in Chapter 8, "Optimal Designs." However, the defaults are satisfactory in this case.
9. Close the Optimal Design Creation window and click **Yes** to generate the design. ADX searches for a D-optimal design based on the model you defined.



	blend	_type_	ALPHA	BETA	PRIMO	COMPLOAD
1	Pure	Vertex	0	0	1	1
2	Pure	Vertex	0	0	1	1
3	Pure	Vertex	0	0	1	2
4	Pure	Vertex	0	0	1	2
5	Pure	Vertex	0	0	1	2
6	Binary	Edge centroid	0	0.5	0.5	1
7	Binary	Edge centroid	0	0.5	0.5	2
8	Pure	Vertex	0	1	0	1
9	Pure	Vertex	0	1	0	1
10	Pure	Vertex	0	1	0	2
11	Pure	Vertex	0	1	0	2
12	Pure	Vertex	0	1	0	2
13	All component	Overall centroid	0.3333	0.3333	0.3333	1

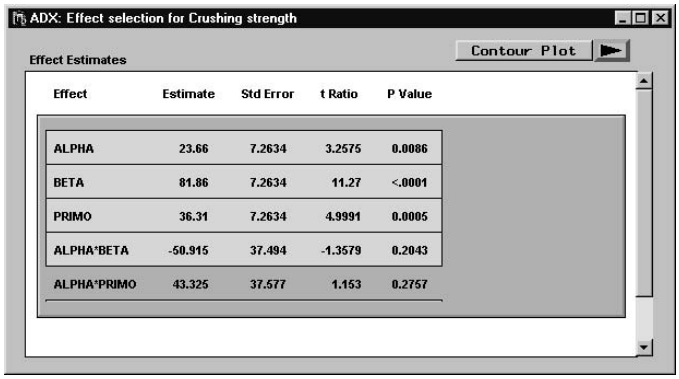
At this point, you can enter the responses. Instead, close the design you just created and open an identical sample design called Tablet Formulation Mixture, which contains the responses.

Analyzing the Mixture Experiment

Analyzing a mixture experiment with process variables is much like analyzing other designs, except that you cannot select or deselect the process variables. ADX automatically includes them in the analysis and optimization, and they can influence which mixture effects are significant. ADX requires you to include all main effects of mixture factors in the fitted model.

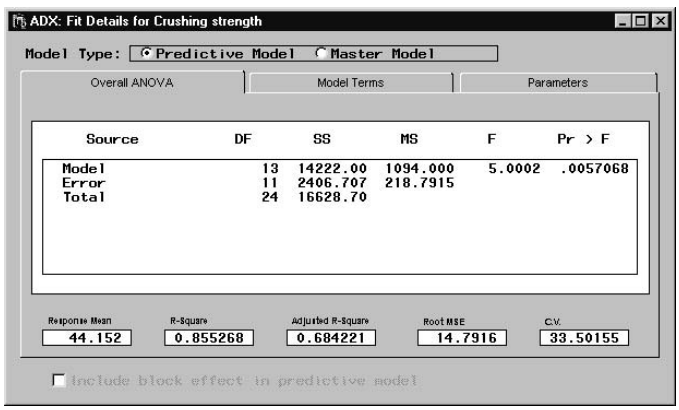
To fit a model, do the following:

1. Open the Tablet Formulation Mixture design.
2. Click **Fit**.
3. After you select a response, the Check Fit Assumptions window appears. To analyze the untransformed data, close the Check Fit Assumptions window.
4. The Effect selection for Crushing strength window appears. Note that all main effects are selected whether they are significant or not. In addition, some significant interaction effects are selected.



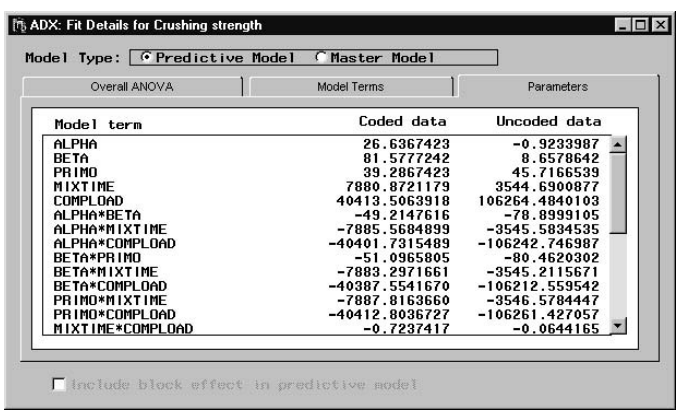
Effect	Estimate	Std Error	t Ratio	P Value
ALPHA	23.66	7.2634	3.2575	0.0086
BETA	81.86	7.2634	11.27	<.0001
PRIMO	36.31	7.2634	4.9991	0.0005
ALPHA*BETA	-50.915	37.494	-1.3579	0.2043
ALPHA*PRIMO	43.325	37.577	1.153	0.2757

5. Select **Model** → **Fit Details**. The overall ANOVA appears.



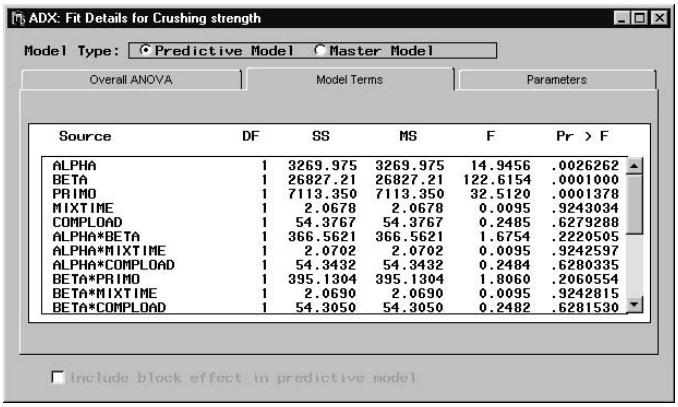
Source	DF	SS	MS	F	Pr > F
Model	13	14222.00	1094.000	5.0002	.0057068
Error	11	2406.707	218.7915		
Total	24	16628.70			

6. To view the parameter estimates for the process variables, click the **Parameters** tab. The parameter estimates for both coded and uncoded data appear in the list.



Model term	Coded data	Uncoded data
ALPHA	26.6367423	-0.9233987
BETA	81.5777242	8.6578642
PRIMO	39.2867423	45.7166539
MIXTIME	7880.8721179	3544.6900877
COMPLOAD	40413.5063918	106264.4840103
ALPHA*BETA	-49.2147616	-78.8999105
ALPHA*MIXTIME	-7885.5684899	-3545.5834535
ALPHA*COMPLOAD	-40401.7315489	-106242.746987
BETA*PRIMO	-51.0965805	-80.4620302
BETA*MIXTIME	-7883.2971661	-3545.2115671
BETA*COMPLOAD	-40387.5541670	-106212.559542
PRIMO*MIXTIME	-7887.8163660	-3546.5784447
PRIMO*COMPLOAD	-40412.8036727	-106261.427057
MIXTIME*COMPLOAD	-0.7237417	-0.0644165

7. To see which effects in the ANOVA are significant, click the **Model Terms** tab. Keep in mind that all mixture main effects and process variables are always included in the fitted model, whether they are significant or not.



Source	DF	SS	MS	F	Pr > F
ALPHA	1	3269.975	3269.975	14.9456	.0026262
BETA	1	26827.21	26827.21	122.6154	.0001000
PRIMO	1	7113.350	7113.350	32.5120	.0001378
MIXTIME	1	2.0678	2.0678	0.0095	.9243034
COMPLOAD	1	54.3767	54.3767	0.2485	.6279288
ALPHA*BETA	1	366.5621	366.5621	1.6754	.2220505
ALPHA*MIXTIME	1	2.0702	2.0702	0.0095	.9242597
ALPHA*COMPLOAD	1	54.3432	54.3432	0.2484	.6280335
BETA*PRIMO	1	395.1304	395.1304	1.8060	.2060554
BETA*MIXTIME	1	2.0690	2.0690	0.0095	.9242815
BETA*COMPLOAD	1	54.3050	54.3050	0.2482	.6281530

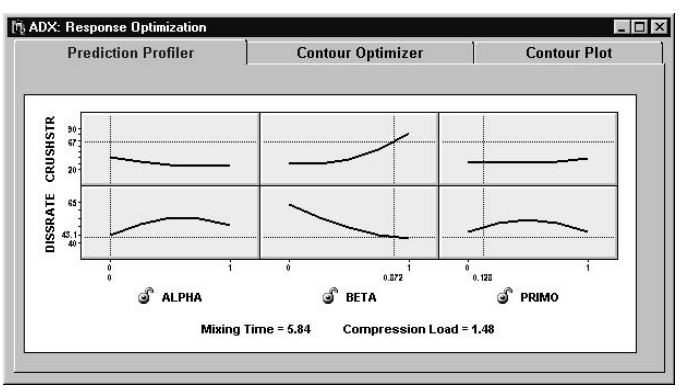
8. Close the Fit Details for Crushing strength window to return to the Effect selection for Crushing strength window.
9. Close the Effect selection for Crushing strength window and click **OK** to save the fitted model.

Optimizing the Mixture Design with Process Variables

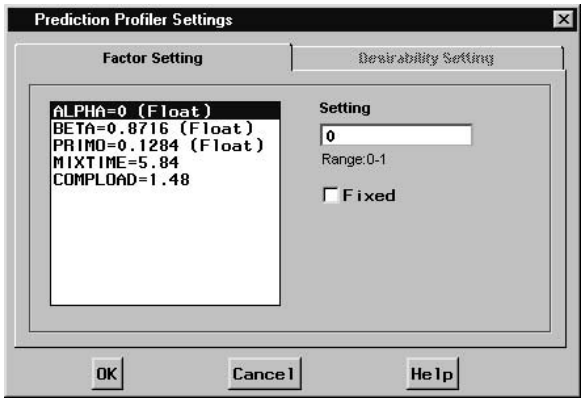
Optimizing mixture designs with process variables is similar to optimizing other mixture designs, except that the process variables are held at fixed levels.

The following steps illustrate how you work with process variables in the prediction profiler:

1. Click **Optimize**.
2. Select both responses in the list and click **Run**. The Prediction Profiler in the Response Optimization window appears.



3. Set the mixture variable levels as described in Chapter 10.
4. Select **Settings** → **Factor Settings**.

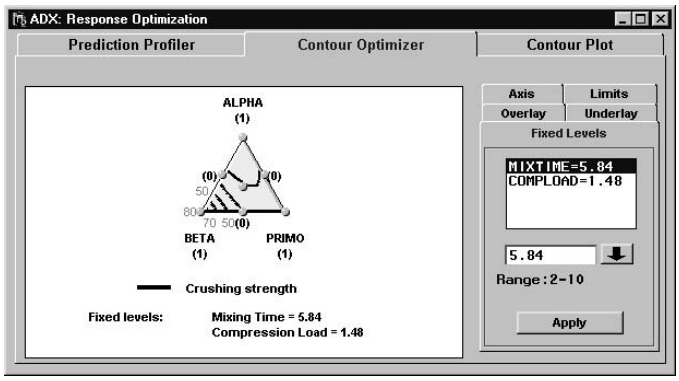


5. Click **MIXTIME** in the list, and set its level to **2**.
6. Change the level of **COMPLOAD** to **1**.
7. Click **OK** to apply the changes.

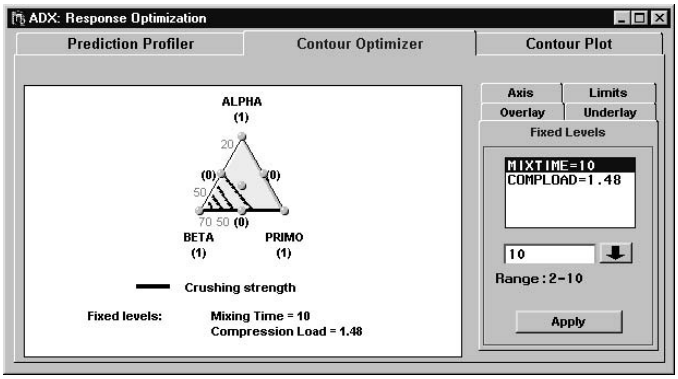
You can set as many different combination levels as you want to view.

To optimize a mixture design by using the contour optimizer, do the following:

1. Click the **Contour Optimizer** tab.
2. Click the **Fixed Levels** tab to the right of the plot.



3. All variables whose levels are fixed, including the process variables, are included in the list. Click **MIXTIME** and type **10** in the text field below the list.
4. Click **Apply** and note how the contour plot changes.



5. Change the level of **COMPLOAD** to **2** and click **Apply**.

In all other respects, the contour optimizer behaves the same as when only mixture factors are involved.

Points to Remember

- You can define linear constraints on the variables in mixture experiments.
- Because no standard set of designs covers all possible linear constraints, ADX generates D-optimal designs by using the vertices and centroids of the constrained region. The optimization tools automatically accommodate the constraints.
- ADX can generate, analyze, and optimize mixture experiments (both unconstrained and constrained) with process variables.
- ADX generates D-optimal designs for mixture experiments with process factors.
- ADX automatically includes process variables in the fitted model.
- You can set the levels of the process variables in the **Prediction Profiler** or on the **Fixed Levels** tab in the **Contour Optimizer**.

Chapter 12
Split-Plot Designs

Chapter Contents

Chapter 12
Split-Plot Designs

Chapter Topics

In many experiments, treatments are applied to different sizes of experimental material. This occurs, for example, when some treatment levels are hard to change or when different batch preparation methods are studied. Some treatments are randomized on large units of material, called *whole plots*, while others are randomized on smaller units, called *split plots* or *subplots*. *Split-plot designs* are used to carry out such experiments.

Split-plot designs collect information from both whole plots and subplots, with corresponding nominal levels of noise. This is modeled by treating whole-plot errors as random effects. Therefore, ADX uses a mixed-models formulation to analyze these experiments.

Covered in This Chapter

- Creating a split-plot design
- Reviewing design details
- Exploring data
  - Using the scatter plot
  - Using the box plot
- Fitting a model
- Generating a report

Experimental Objective

This example revisits the tablet production scenario in Chapter 3, "Full Factorial Designs," with an alternate analysis suggested by Fossceco (1999). The tablet production process has several stages, which include batch mixing, where ingredients are combined and mixed with water, and pellet production, where the batch is processed into pellets that are compressed to form tablets. It is more convenient to mix batches and randomize the treatments within each batch than to mix a new batch for each run. Thus, this experiment calls for a standard two-stage split-plot design.

The moisture content and mixing speed for the batch constitute whole-plot factors, while the factors that control the variety of ways that pellets can be produced from a single batch are subplot factors. The responses of interest are measured on the final tablets. Table 12.1 shows all the variables involved and the stage with which they are associated.

Table 12.1. Factors and Responses in the Tablet Formulation Experiment

Variable	Name	Low Level	High Level	Description
Whole Plot	FLUID	90	115	Moisture content (%)
	MIX	15	45	Mixing time (min)
Split Plot	EXTRUDER	36	132	Extruder speed (rpm)
	SCREEN	0.6	1.0	Screen size (mm)
	RESID	2	5	Residence time (min)
	DISK	450	900	Disk speed (rpm)
Response	MPS			Mean particle size (micron)

The goal of the experiment is to determine which effects are significant. The researcher is interested in both whole-plot factors and subplot factors.

Task List

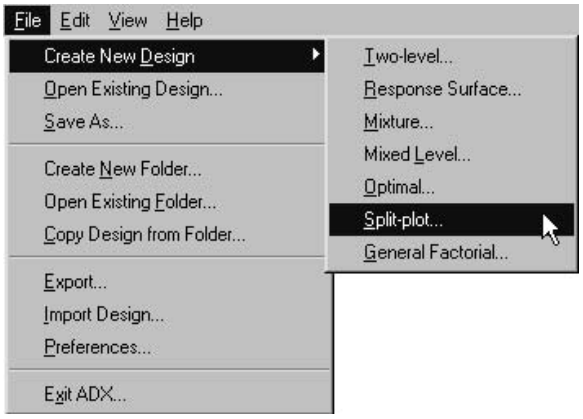
- Create the split-plot design.
- Explore the response data with scatter plots and box plots.
- Estimate all main effects and as many two-factor interactions as possible between the factors.

Creating a Split-Plot Design

In ADX, creating a split-plot design is similar to creating a two-level design. To create a split-plot design for tablet formulation experiment, follow these steps:

1. Create a new split-plot design.
2. Define the two whole-plot and four subplot factors.
3. Select the design with the right defining contrasts. This example uses a full factorial split-plot design.

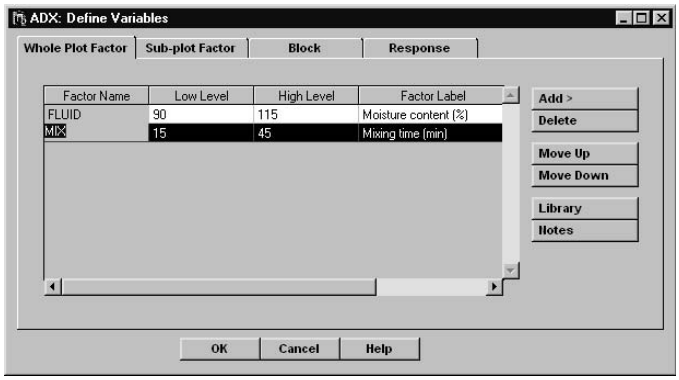
To create a split-plot design, select **File** → **Create New Design** → **Split-plot** from the ADX desktop. Alternatively, you can click the **Split-Plot Design** icon on the toolbar. The main design window will appear.



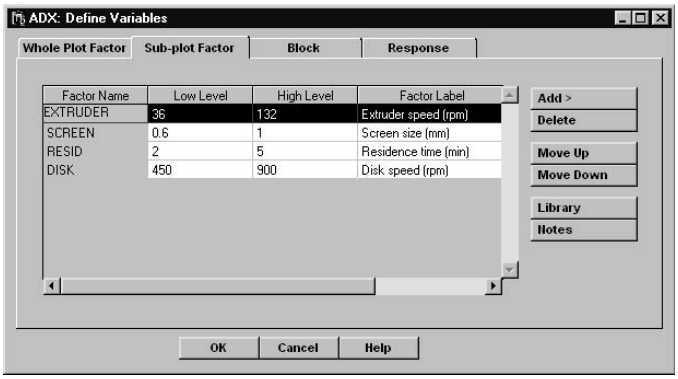
Defining Variables

To define the variables in this experiment, do the following:

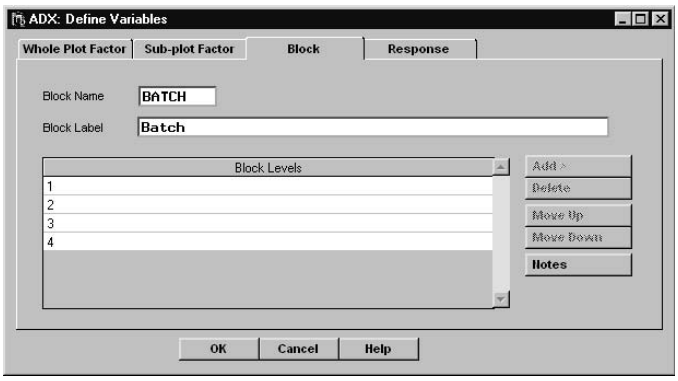
1. Click **Define Variables**. The Define Variables window will appear, and the **Whole Plot Factor** tab will already be selected.
2. Define the whole-plot factors.
   (a) Create two new factors by clicking **Add** and selecting **2**.
   (b) Enter the factor names given in the whole-plot section of Table 12.1.



3. Define the subplot factors.
   (a) Click the **Sub-plot Factor** tab.
   (b) Create four new factors by clicking **Add** and selecting **4**.
   (c) Enter the factor names given in the subplot section of Table 12.1.



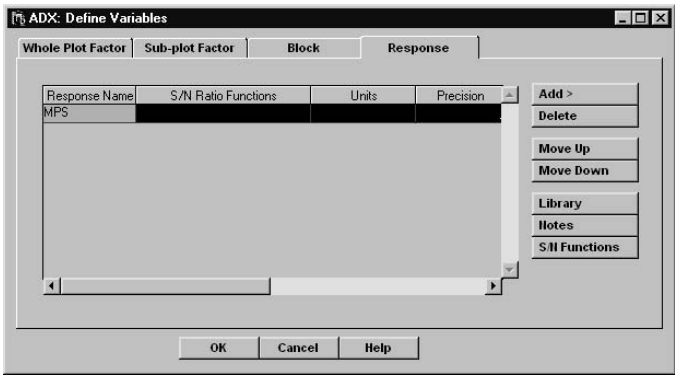
4. Click the **Block** tab. ADX will assign a unique block level to each whole plot when it generates the design, so you do not need to specify the number of block levels. Change the block name to **BATCH**, since each whole plot is a batch of material.



5. Enter the response information.

   (a) Click the **Response** tab.

   (b) Change the name of the default response to **MPS** and its label to **Mean Particle Size (microns)**.



6. Click **OK** to accept the variable definitions.

Selecting a Design

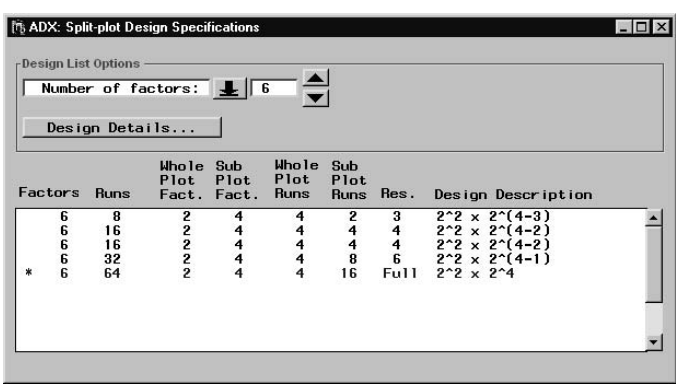
This example uses a $2^2 \times 2^4$ split-plot design. This notation indicates the following:

- two whole-plot factors, each with two levels
- full factorial in whole-plot factors
- four split-plot factors, each with two levels
- full factorial in split-plot factors

This is equivalent to the $2^{(2+4)-(0+0)}$ notation used by Bingham and Sitter (2001). The second part of the exponent refers to the degree of fractionation. The 0's indicate that this is a full factorial design in both the whole-plot and split-plot factors.

To select this design, click **Select Design** in the main design window. The Split-Plot Design Specifications window will appear. Select the $2^2 \times 2^4$ row in the list.

Close the Split-Plot Design Specification window and click **Yes** to generate the design. The design has 64 runs, the same as a 2^6 factorial design.



	Factors	Runs	Whole Plot Fact.	Sub Plot Fact.	Whole Plot Runs	Sub Plot Runs	Res.	Design Description
	6	8	2	4	4	2	3	2^2 x 2^(4-3)
	6	16	2	4	4	4	4	2^2 x 2^(4-2)
	6	16	2	4	4	4	4	2^2 x 2^(4-2)
	6	32	2	4	4	8	6	2^2 x 2^(4-1)
*	6	64	2	4	4	16	Full	2^2 x 2^4

Close the design you just created. Open the Tablet Formulation Split-Plot design, which is identical to the design you just created and contains response values.

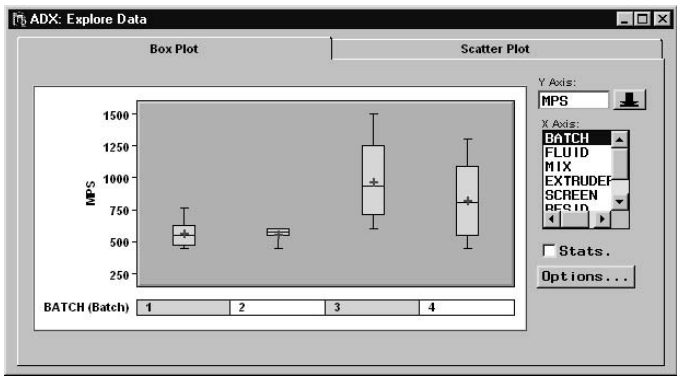
Analyzing a Split-Plot Design

ADX uses a mixed model approach to analyze split-plot designs. Basic split-plot designs have two sources of error, the *whole-plot error* and the *subplot error*. A mixed model analysis for a split-plot design estimates fixed effects and compares them to the appropriate estimate of error.

Exploring Response Data

Before fitting a mixed model, click **Explore** in the main design window. Both box plots and scatter plots are available. Box plots help you visualize the differences in response distribution across levels of different factors, both random and fixed. Scatter plots show the individual responses broken down by factor level or run and can also be used to investigate time dependence.

The box plot is the first graph that is displayed. You can explore the distribution of the response broken down by each of the factors or batches that make up the whole plot.



Close the window to return to the main design window.

Specifying Fixed and Random Effects

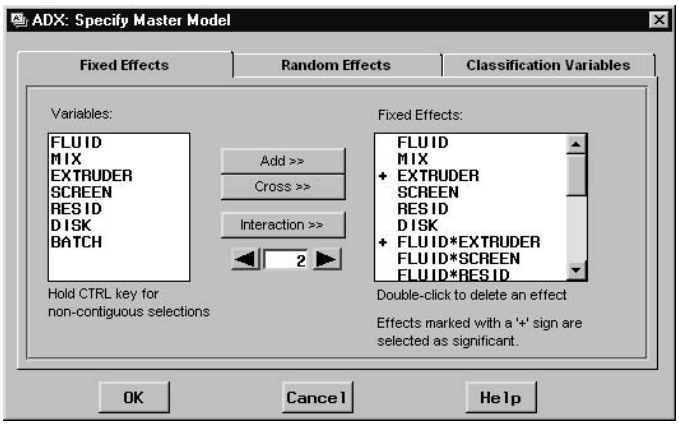
ADX does not generate a default master model for a split-plot design, so you must do so before fitting. Click **Fit** in the main design window. The Fit Details for MPS window will open. It has sections to define fixed and random effects and classification variables.

The fixed effects in a split-plot design are, as usual, the main effects and interactions of interest between the factors. The split-plot structure of the experiment determines the choice of random effects, which in turn determines the proper error term for each fixed effect.

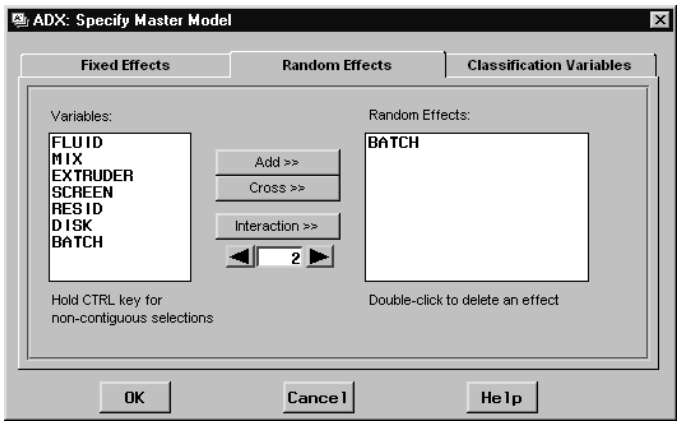
The modeling objectives of a split-plot design are in principle the same as those of a standard screening design. You want to estimate as many effects as possible involving the factors and determine which ones are significant. When this design was analyzed as a standard full factorial in Chapter 3, the 64 runs provided enough degrees of freedom to estimate effects and interactions of all orders. However, FLUID and MIX are whole-plot effects and apply only to batches. Therefore, with respect to these two factors, the experiment has only four runs (the four batches). The interaction between the whole-plot effects will estimate the whole-plot error, so this interaction is not included as a fixed effect.

Click **Fit** in the main design window. Select **Model** → **Change master model** to open the Specify Master Model window. On the **Fixed Effects** tab, specify the following as fixed effects:

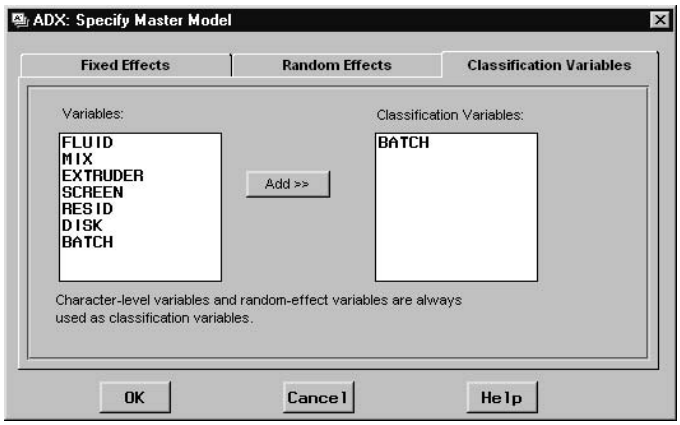
- All main effects. Click and drag or hold down the CTRL key and click to select the FLUID, MIX, EXTRUDER, SCREEN, RESID, and DISK variables. Then click **Add**.
- All two-factor interactions except FLUID*MIX. Select all six factors and click **Interaction**. Double-click FLUID*MIX in the list on the right to remove it from the master model. (You might have to scroll to find it.)



Next, click the **Random Effects** tab. Here you specify the whole-plot error, which is BATCH. Select BATCH and click **Add**.



Examine the **Classification Variables** tab. BATCH is automatically entered because it is a random effect. If there were categorical fixed effects, you would enter them on this tab.



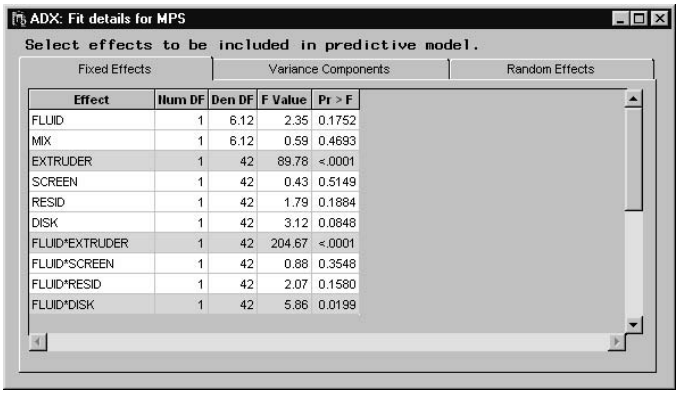
Click **OK** to close this window and fit the master model.

Fitting a Model

ADX uses the MIXED procedure to estimate the fixed and random effects and variance components of the model.

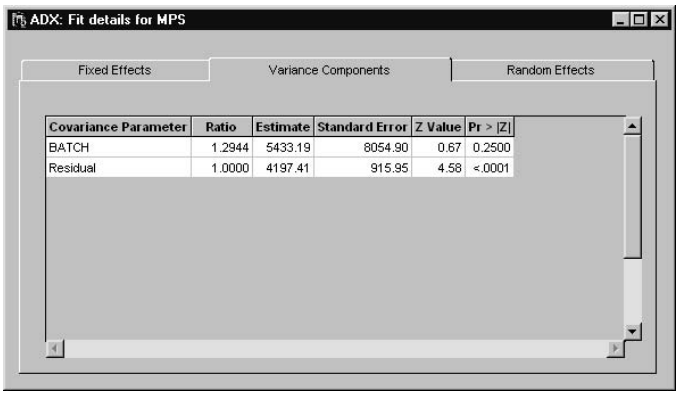
After specifying the model, you will see the Fit Details for MPS window. There are three tabs:

- The **Fixed Effects** tab is similar to the Effects Selector for other designs. The table lists Type 3 tests of the fixed effects. Click an effect to toggle the selection of significant effects.



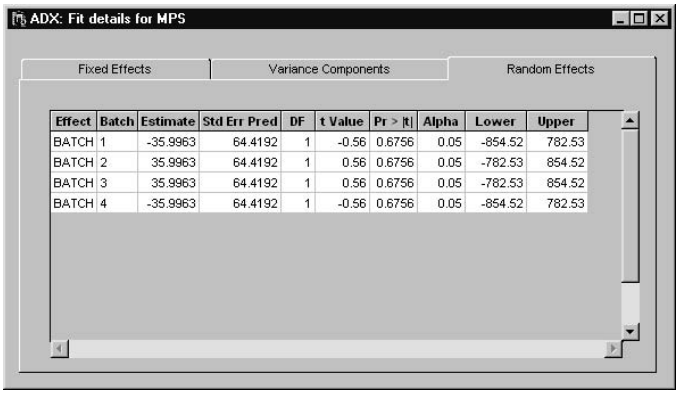
Effect	Num DF	Den DF	F Value	Pr > F
FLUID	1	6.12	2.35	0.1752
MIX	1	6.12	0.59	0.4693
EXTRUDER	1	42	89.78	<.0001
SCREEN	1	42	0.43	0.5149
RESID	1	42	1.79	0.1884
DISK	1	42	3.12	0.0848
FLUID*EXTRUDER	1	42	204.67	<.0001
FLUID*SCREEN	1	42	0.88	0.3548
FLUID*RESID	1	42	2.07	0.1580
FLUID*DISK	1	42	5.86	0.0199

- The **Variance Components** tab provides estimates of the variance of each random effect, including the residual error. The approximate confidence limits for variance components can be calculated easily from this information.



Covariance Parameter	Ratio	Estimate	Standard Error	Z Value	Pr > |Z|
BATCH	1.2944	5433.19	8054.90	0.67	0.2500
Residual	1.0000	4197.41	915.95	4.58	<.0001

- The **Random Effects** tab lists the random effects broken down by level (for interactions, these are broken down by each combination of levels). These are empirical best linear unbiased predictors (EBLUPs) of the observed random effects. You can use them to screen for unusual whole plots and to assess the normality assumption of the model.



Effect	Batch	Estimate	Std Err Pred	DF	t Value	Pr > |t|	Alpha	Lower	Upper
BATCH	1	-35.9963	64.4192	1	-0.56	0.6756	0.05	-854.52	782.53
BATCH	2	35.9963	64.4192	1	0.56	0.6756	0.05	-782.53	854.52
BATCH	3	35.9963	64.4192	1	0.56	0.6756	0.05	-782.53	854.52
BATCH	4	-35.9963	64.4192	1	-0.56	0.6756	0.05	-854.52	782.53

Optimization

In SAS 9.2, ADX does not offer an optimization strategy for split-plot designs. However, an analysis of the box plots of the response by the significant factors can offer some insight into the best level combinations. Keep in mind, though, that it is difficult to predict the response because of random effects.

More on Mixed Models

The approach used by ADX to analyze split-plot designs involves the use of mixed models. This is in contrast to the analysis of variance approach presented in classical texts, such as Cochran and Cox (1992) or Montgomery (1997).

For a full discussion of these approaches, refer to the *SAS System for Mixed Models* (Littell, Milliken, Stroup, and Wolfinger 1996). Chapter 2 of that book presents an extensive discussion of the theory of mixed models for split-plot designs.

Fractional Factorial Split-Plot Designs

Huang, Chen, and Voelkel (1998) described a class of minimum-aberration fractional factorial split-plot designs. In SAS 9.2, ADX can generate these designs. You still analyze these designs with the mixed-model paradigm by deciding on an appropriate whole-plot error term (usually the block variable automatically created in ADX) and entering that as a random effect.

Points to Remember

- ADX uses the mixed-model approach to analyzing split-plot designs, with a random effect for the whole plots.
- The Explore Data window provides box plots and scatter plots for visualizing split-plot design data.
- The Fit Details window provides information about significant fixed effects, random effects, and variance components determined from the mixed-model analysis.

Chapter 13
Special Topics

Chapter Contents

Chapter 13
Special Topics

Overview

In this chapter, topics are included that have not been discussed earlier or that cannot fit into a new chapter individually. There are some design techniques that are extremely useful in practical circumstances but cannot be categorized as any of the ones discussed so far.

Covered in This Chapter

- Augmenting a design
  - Folding over a design
  - Adding optimal runs to break specific alias links
  - Augmenting a screening design to a response surface design
  - Dropping inactive factors and projecting into a higher-resolution design
- Creating nonstandard designs
  - Choosing a nonprincipal fraction in a fractional factorial design
  - Constructing a user-specified-model-based design by using the FACTEX procedure
  - Constructing a factorial design from a user-specified SAS program
- Analyzing the mean and variance of a response variable by using the dual-response approach

Design Augmentation

In some situations, it is statistically useful and more economical to augment an existing design rather than to perform a completely new experiment. You should consider design augmentation in the following situations:

- The optimum factor settings are within the original experimental region, so that a screening design can be augmented to a response surface.
- The initial fractional factorial experiment cannot distinguish between aliased significant effects, and so it must be augmented to break certain alias strings.
- Conducting an additional experiment would be too expensive, so you want to reuse information from an initial screening experiment.

Covered in This Section

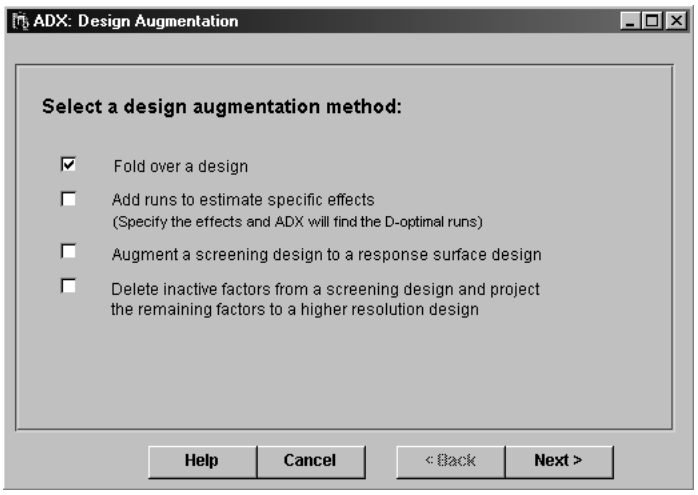
- Folding over a Resolution 3 design
- Adding optimal runs to break alias strings
- Adding axial runs and center points to create a central composite design
- Deleting inactive factors and projecting into a higher resolution design

Augmenting Designs

In some cases, a two-level design might not yield enough information to optimize the factor settings, or you might have reason to believe that higher-order effects are present after the preliminary experiment has been run. ADX provides a design augmentation facility to accommodate these situations:

1. From the ADX desktop, select the design you want to augment.
2. Right-click on the design and select **Augment**.

ADX presents four techniques for augmenting designs, as shown in the following Design Augmentation window:



The augmentation methods are as follows:

1. Fold over the design.
2. Add runs to estimate certain effects.
3. Augment a screening design to a response surface design.
4. Delete inactive factors.

For each augmentation method, you are given the opportunity to review important details and the design listing for the augmented design. You will also have the option to add the new runs in a block, which is useful, for example, if a new batch has to be prepared for the new runs, or if the runs are done on a different day or a different machine.

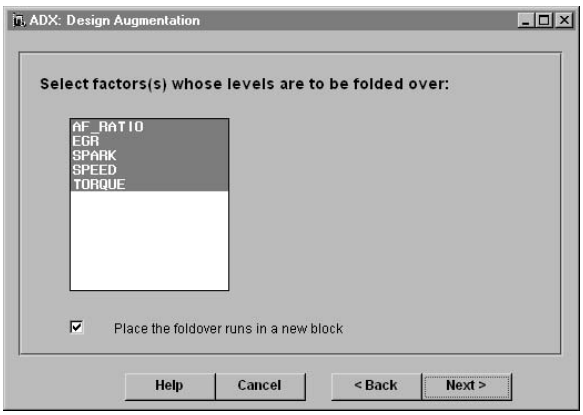
The original unaugmented design is untouched and remains unaffected by the augmentation process. The augmented design, consisting of a copy of the original design together with the new runs, will be saved as a new design. The name of the new design will be the old design name with the suffix "(Augmented)." Double-click the new design and click **Edit Responses** to add the response values for the new runs.

For folded-over designs and designs augmented through the optimal design interface, and also for designs with some factors deleted, the exploration, analysis, and optimization of the new design are the same as for the old design. For a design augmented to a response surface design, the tools for response surface analysis are available as if it were a newly created response surface design.

Folding Over a Design

Design folding is a technique used to increase the resolution of a Resolution 3 two-level fractional factorial design by adding runs that are taken from the fraction opposite the original fraction of the corresponding full factorial design. In other words, for each run in the original design, a run is added in which the coded factor levels are switched in sign. Fully folding over a design doubles the number of runs.

This technique is recommended if you notice the potential significance of two-factor interactions but are still interested only in the main effects. Since folding over increases the resolution to 4, the main effects in the augmented design can be estimated independently of the two-factor interactions. You can select any or all factors to fold over.



Adding Optimal Runs

If the two-level design is not Resolution 3, or if folding over a design is infeasible, you can use the optimal design approach to add the runs needed to break particular alias strings. This technique requires you to be familiar with the alias strings of the design; see Chapter 4 for more information. You should also know which effects are active before adding optimal runs.

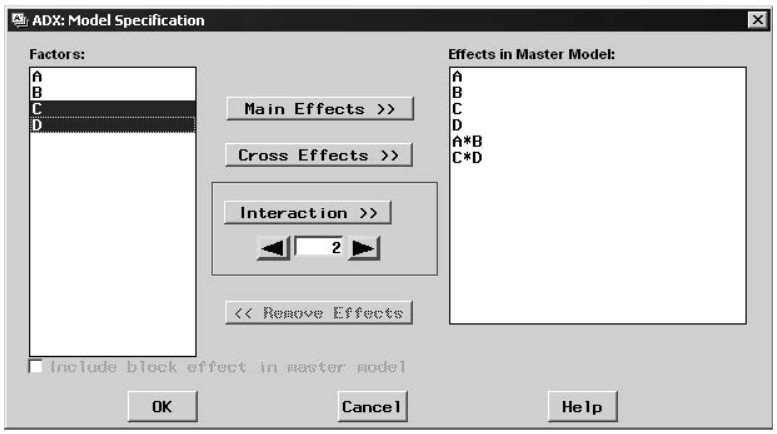
The advantages of this approach are its flexibility (you can choose exactly which effects to free) and its efficiency (the least number of runs possible are used). The disadvantage is the danger of unnoticed influences from effects that are still aliased. You should use this technique with caution.

An example of a 2^{4-1} design named Design Augmentation Example is included with the sample designs. As described by Barker (2001), the response for this experiment follows the deterministic model $Y = 200 + 10A + 5B + 2C + 3D + 4CD + 2AB$.

Open the example, and click **Design Details**. The **Alias Structure** tab shows that the six two-factor interactions are paired in three alias strings. One of the strings includes $AB + CD$. If you suspect that one or both of these effects are active, then you need to augment the design to break this alias string, as follows:

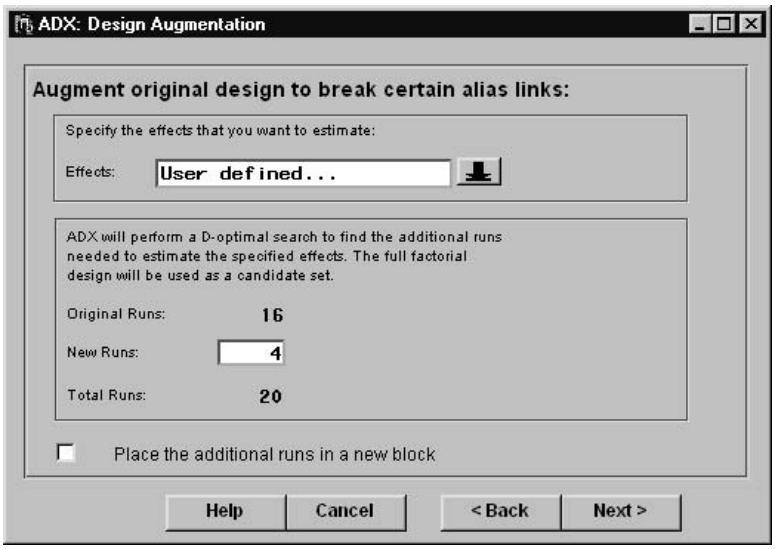
1. Close the design to return to the ADX desktop.

2. Click the **Design Augmentation Example** design, right-click, and select **Augment** to open the Design Augmentation wizard.
3. Select **Add runs to estimate certain effects** and click **Next**.
4. The wizard now shows the design details you saw before. Continue to the next page of the wizard.
5. The third page shows the original design. Continue to the next page of the wizard.
6. The fourth page directs you to select the model you want to fit. To disentangle selected effects, click the down arrow and select **User defined** from the list.

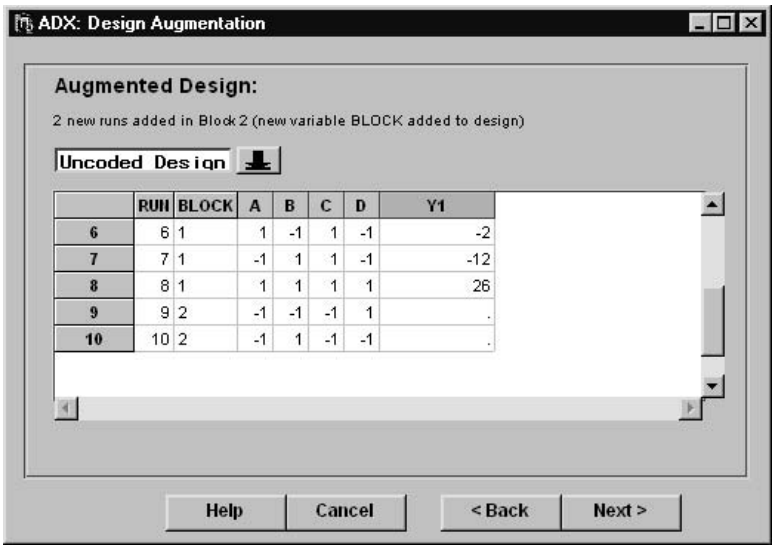


7. Now select the interaction effects (AB and CD) you want to disentangle:
   - Select A and B by holding down the CTRL key and clicking, and then click **Cross Effects**. This adds the AB interaction to the model.
   - Select C and D by holding down the CTRL key and clicking, and then click **Cross Effects**. This adds the CD interaction to the model.
   - Click **OK** to return to the Design Augmentation wizard.

   Since only two additional runs are needed to disentangle the two interactions, change the number of **New Runs** from **4** to **2**. Finally, clear **Place the foldover runs in a new block**. Continue to the next page of the wizard.



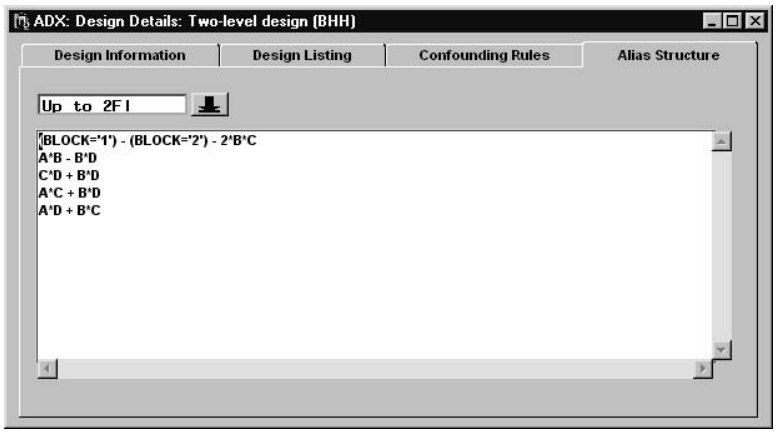
8. The next page shows the new design. Continue to the next page of the wizard.



	RUN	BLOCK	A	B	C	D	Y1
6	6	1	1	-1	1	-1	-2
7	7	1	-1	1	1	-1	-12
8	8	1	1	1	1	1	26
9	9	2	-1	-1	-1	1	.
10	10	2	-1	1	-1	-1	.

9. The last page of the augmentation wizard directs you to name the new design. Augmentation leaves your original design untouched. Click **Finish** to save the new design on the ADX desktop.

Open the new design and click **Design Details**. Click the **Alias Structure** tab. Notice that AB and CD are now on separate lines.



The alias structure of a nonorthogonal design such as this one is not as easy to interpret as that of an orthogonal design. ADX shows the expected value of the estimate of the first effect in each string. The expected value of the estimate of AB in the original design was $AB + CD$ (in the absence of three or more factor interactions). Now, since BD and all higher-order interactions are inactive in the underlying model, the expected value of the estimate of AB is the effect AB. Likewise, for CD the expected value of the estimate of CD is CD.

Before running the augmented design, make sure that its aliasing structure is appropriate.

Augmenting to a Response Surface Design

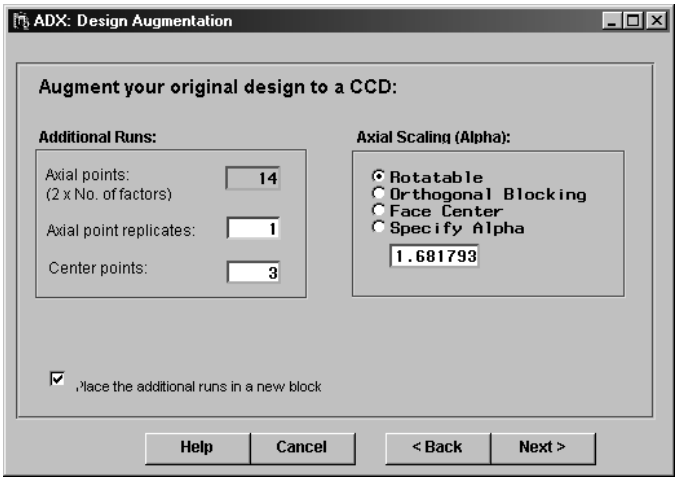
Montgomery (1997) provides the following guidelines for using screening designs and response surface designs:

1. Use a two-level screening design to identify significant effects.
2. Add runs along the gradient of the surface of the predicted response and fit a second-order curve.
3. Find the optimum point (minimum or maximum) on the curve and use this information to determine new factor ranges for the response surface design. The new ranges should be small enough to investigate the surface in detail in the area.
4. Conduct a response surface design experiment to find the optimum factor level.

Sometimes, due to the cost of runs or to irregularities in the response for the two-level design, it is preferable to augment the two-level design into a response surface design rather than running a completely new response surface experiment.

The augmented design is a central composite design. ADX enables you to specify the number of center points, the number of times you want to replicate all the axial

points, and whether you want a rotatable, orthogonally blocked, face center, or custom design. As with the other augmentation methods, the new runs can be put into a new block.



Deleting Inactive Factors

After you run and analyze a two-level full factorial or fractional factorial experiment, you might discover that some factors are not statistically significant and have no bearing on the outcome of the response variables. In such cases you can drop the inactive factors permanently from the experiment and project the design in the subset of the remaining factors. This greatly increases the power of your design with no additional resources. Suppose the original design is an unreplicated 2^k full factorial design and r factors are discarded. Then the projected design becomes a 2^{k-r} replicated factorial design with 2^r replicates.

For example, let's suppose the original design is a 2^{7-2} quarter-fraction factorial, Resolution 4, design and you find after fitting a model and analyzing the data that two of the factors are not important and these two factors are not involved in any significant interactions. So you choose to delete those two factors and project it into a full factorial 2^5 design. The augmented design can now estimate all two-factor interactions. Montgomery (1997) suggests that the conclusions drawn from designs of this type of augmentation should be considered tentative and subject to further analysis.

Points to Remember

- Design augmentation is performed from the ADX desktop by selecting a design, right-clicking, and selecting from the menu.
- Augmentation methods include folding over, adding runs to break specific alias strings, adding runs to create a central composite design, and design projection.

Creating Nonstandard Designs

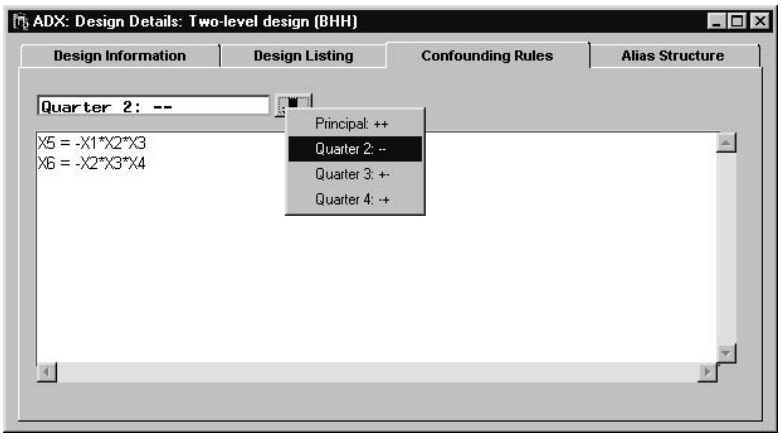
ADX provides you with a wide variety of standard designs, which are recommended for the vast majority of experiments that require fractionation. However, there are certain circumstances that call for nonstandard fractional factorial designs. You can use the design selection facility in ADX to select nonprincipal fractions. In situations requiring even greater flexibility, this facility provides advanced users with an interface to the FACTEX procedure and the SAS programming language. If you need a D- or A-optimal design, see Chapter 8.

Creating a Nonprincipal Fraction Design

By default, ADX creates the principal fraction of a fractional factorial design, meaning that the product of the coded levels of the factors in each defining contrast is 1. In some cases, however, you might want to use a nonprincipal fraction. Follow these steps:

1. Click **Select Design** from the main design window.
2. Select the design according to the number of factors and the number of runs you want.
3. Click **Design Details** and then click the **Confounding Rules** tab.
4. Click the down arrow to open a pop-up menu.

5. Select the fraction you want to use. Note how the confounding rules change when you select a nonprincipal fraction.

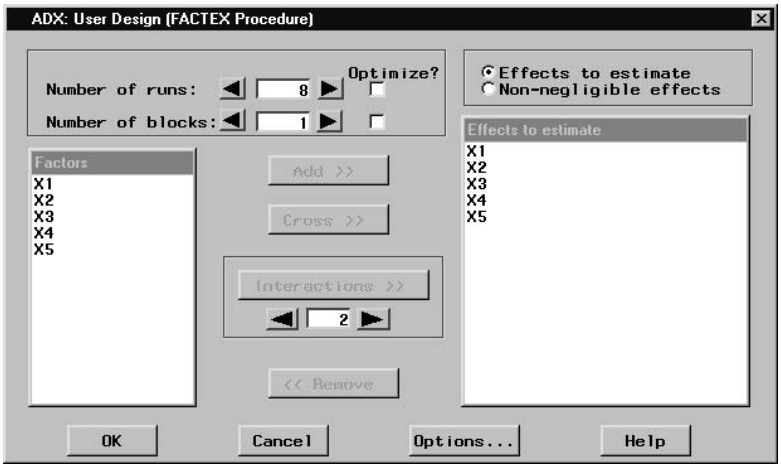


6. Close the window to return to the design selection window. The design you selected is still highlighted.
7. Close the window and click **OK** to create the design.

Creating a Design with the FACTEX Procedure

To create a custom design with the FACTEX procedure, follow these steps:

1. From the main design window, click **Select Design** to open the Two-Level Design Specifications window.
2. Select the number of factors you want. For example, type **5** in the text field beside **Number of factors**.
3. Click on a design in the list of designs that most closely fits your needs . For example, choose a **1/4 Fraction** design.
4. Select **Create**→ **User Design**→ **from FACTEX procedure**.
5. The User Design (FACTEX Procedure) dialog box will appear.



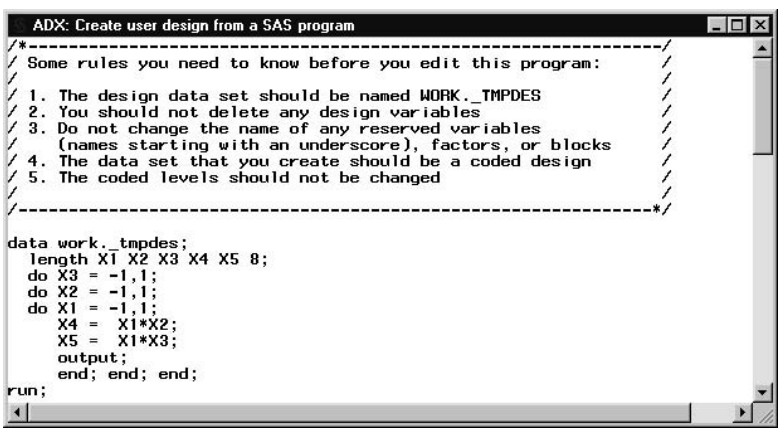
6. Select the number of runs and the number of blocks you want. Alternatively, you can have the FACTEX procedure select the optimum for these by selecting the appropriate check box under **Optimize?**
7. Select the effects to estimate by clicking the factors in the list on the left and clicking **Add**.
8. You can also select interaction effects by holding down the CTRL key and clicking to select multiple effects, selecting the order of interaction you want, and clicking **Interactions**. For example, to add all two-factor interactions, select all effects, select **2** for the order, and click **Interactions**.
9. You can remove effects by selecting the effect in the list on the right and clicking **Remove**.
10. Select the nonnegligible effects by selecting the **Non-negligible effects** option and performing the same effect selection procedure. **Note:** Nonnegligible effects are effects that you do not want to estimate but that might be active. The FACTEX procedure will avoid aliasing these effects with effects you do want to estimate.
11. If you want a minimum aberration design, click **Options** and click **Minimum aberration design** in the resulting dialog box. Click **OK** to dismiss the dialog box.
12. Click **OK** to return to the Two-Level Design Specifications window. A new line with the design type **User Design** will be added to the design list and will be selected automatically.
13. Close the window and click **Yes** to create the custom design.

CAUTION: This facility can create designs so small that they do not have enough runs to check assumptions. Use these designs with care.

Creating a Design with a SAS Program

If you have a strong background in design of experiments and need to create a completely customized design with a SAS program, you can follow these steps:

1. From the main design window, click **Select Design** to open the Two-Level Design Specifications window.
2. Select the number of factors you want. For example, type **5** in the text field beside **Number of factors**.
3. Click on a design that most closely fits your needs in the list box of designs. For example, choose a **1/4 Fraction** design.
4. Select **Create**→ **User Design**→ **from SAS program**.
5. A program editor will appear with the SAS program that creates the design selected in the Two-Level Design Specifications window. Some guidelines for creating the design are listed in comments in the program.



6. Modify the program to suit your needs. For example, you can modify the confounding rules used to create the design. Note that you can use the FACTEX or OPTEX procedure instead of a DATA step, as long as you follow the guidelines.
7. Press the **F3** key or click the **Submit** button  to create the design.
8. ADX will return to the Two-Level Design Specifications window. A new line with the design type User Design will be added to the design list and will be selected automatically.
9. Close the window and click **Yes** to create the custom design.

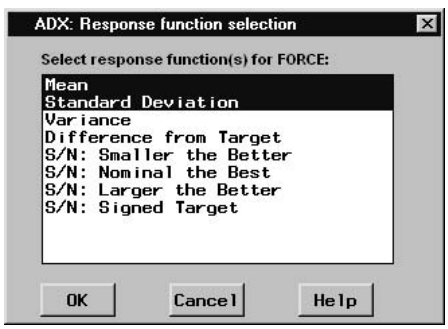
This approach is recommended only if the standard designs available in ADX do not fit the circumstances. If you want to create D- or A-optimal designs, see Chapter 8 for information about the ADX optimal design interface.

The Dual-Response Approach

Some researchers prefer to analyze the mean and variance of the response directly at an inner array design point rather than define a signal-to-noise ratio. You can select the mean and variance, or the mean and standard deviation, as response functions and fit models to them. Then you can use the prediction profiler to optimize the mean while controlling the variance. For more information about the "dual response" approach, refer to Vining and Myers (1990).

To perform a dual response analysis for the Pull-off Force design, do the following:

1. On the **Response** tab of the Define Variables window, select **FORCE** and click **S/N Functions**. (Alternatively, you can click the **S/N Functions** cell in the FORCE row.)
2. Select **Mean** and **Standard Deviation**.



3. Fit a model to both the MEAN(FORCE) and SDEV(FORCE) response functions. Note that no effects are selected because the inner array design is saturated, and ADX cannot apply any automatic effect selection methods.
4. Use the prediction profiler to maximize the mean while controlling the standard deviation, or use the numerical optimizer to find the factor settings that maximize the mean while holding the standard deviation under a specified level.

Chapter 14

Useful Techniques

Chapter Contents

Chapter 14
Useful Techniques

Overview

In this chapter some techniques are discussed that give the user more flexibility. These techniques help the user to handle the data better and use ADX more effectively.

Covered in This Chapter

- Managing your designs
- Importing and exporting data

Managing Your Designs

ADX enables you to organize your designs in a system that maintains factor and response values, as well as notes, graphical displays, and statistical results. This chapter describes the use of ADX folders, as well as moving, copying, and backing up ADX folders.

Covered in This Section

- Using folders
  - Creating folders
  - Changing the current folder
  - Copying designs
  - Deleting and renaming designs and changing preferences
- Moving and copying design folders

Using Folders

You can use folders to organize your designs by study, project, group, or any other aspect of your experimental activity.

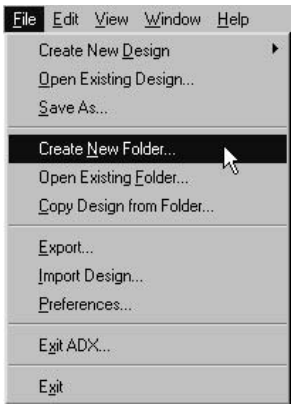
Creating Folders

By default, the ADX Interface stores sample designs in a folder named ADXPARM. You will want to manage your designs by using a different folder for each study.

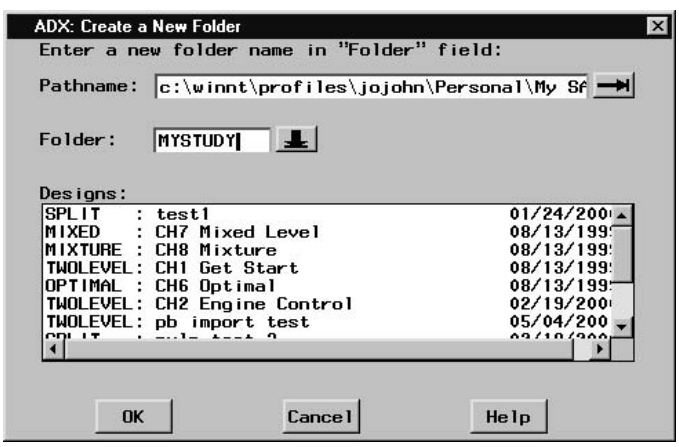
To create a new folder, follow these steps:

1. Make sure that you are viewing the ADX desktop.

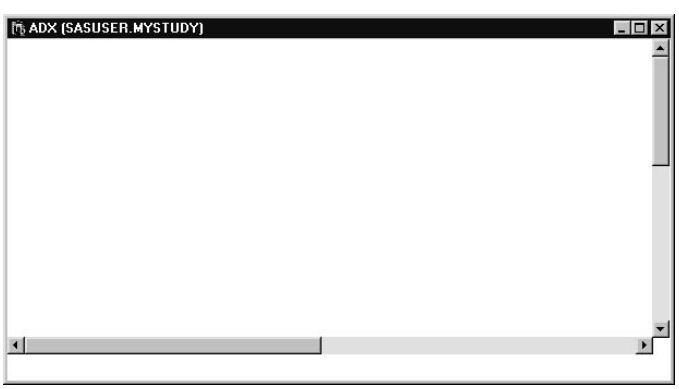
2. Select **File** → **Create New Folder** from the ADX desktop, or click the **Create New Folder** icon .



3. Type **MYSTUDY** in the **Folder** field.



4. Click **OK**, and ADX switches to the folder named MYSTUDY, which is currently empty.



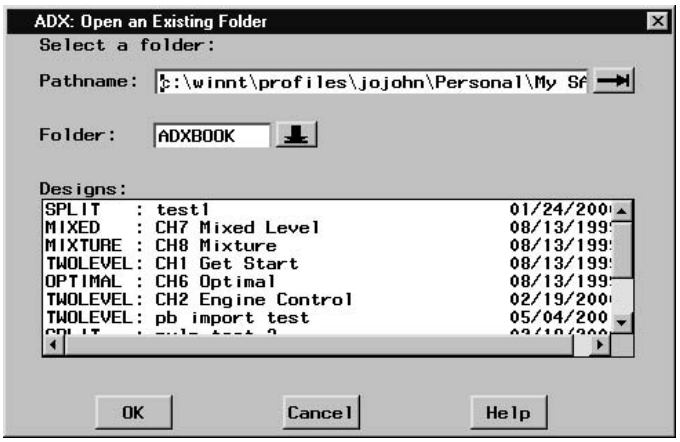
Any design you create and save will be stored in the current folder. For example, if you create the folder MYSTUDY before creating a series of designs for a particular study, they will all be saved in MYSTUDY.

Note: ADX has only one level of folders.

Changing the Current Folder

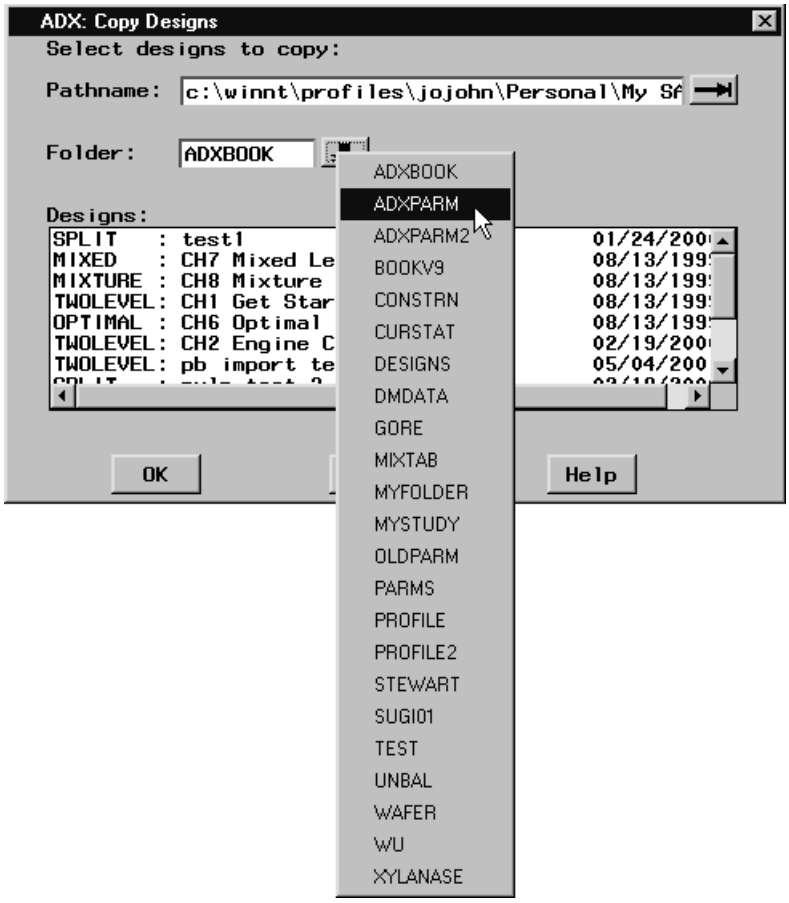
When managing different studies, you will need to switch between the study folders. To change the current folder to MYSTUDY, do the following:

1. Open the Open an Existing Folder window by selecting **File** → **Open Existing Folder** from the ADX desktop or clicking the **Open Existing Folder** icon .
2. The **Pathname** field displays the directory path of your current working design folder. Type the directory path (or click the right arrow button to choose the directory) where the MYSTUDY folder exists. By default, ADX puts all design folders in the directory that the SAS System refers to as the SASUSER library. (You can usually skip this step unless your MYSTUDY folder exists in a directory other than the one where the SASUSER library exists.)



3. Click the down arrow beside **Folder**.
4. A menu listing all the ADX folders in the SASUSER directory will appear. In this case, select **MYSTUDY**.
5. All designs in the folder will be listed.
6. Click **OK** to change the folder. (The **Cancel** button will return you to the ADX folder from which you started.)

Copying Designs



If you have saved a design, you can move it to a different folder. For example, if you want to move the two different tablet formulation designs to MYSTUDY, do the following:

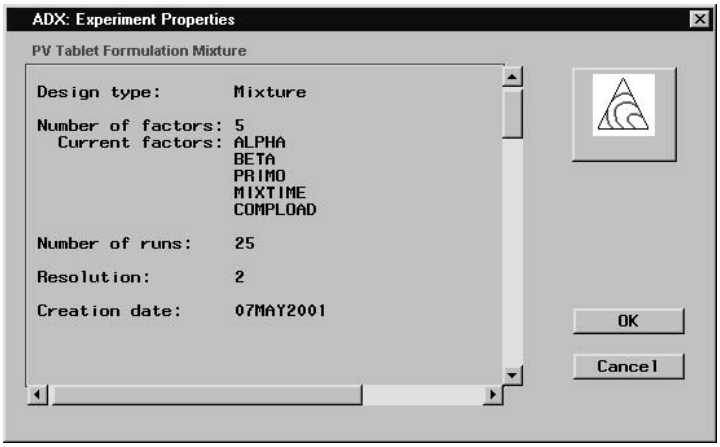
1. Create the folder MYSTUDY, if you have not done so already.
2. Open the folder MYSTUDY.
3. Select **File** → **Copy Design from Folder** to call the Copy Designs window.
4. Change the pathname, if necessary.
5. Click the down arrow beside **Folder**.
6. A menu listing all the ADX folders will appear. Select **ADXPARM**.
7. All the designs in ADXPARM will appear in the list box. Hold down the CTRL key and click to select the **Tablet Formulation** and **Tablet Formulation Mixture** designs.
8. Click **OK**. (The **Cancel** button aborts the copy.)
9. The two designs appear on the desktop in the MYSTUDY folder.

Other Operations on Designs

In addition to managing folders, ADX enables you to manage designs within a folder. To access these features, click on a design and then right-click.

A menu appears with the following commands:

- **Open**, which opens a design (this is the same as double-clicking on a design icon)
- **Duplicate**, which copies a design
- **Rename**, which changes the name of a design
- **Delete**, which removes a design permanently
- **Move**, which enables you to change the position of a design icon on the ADX desktop
- **Export**, which is discussed in Chapter 14
- **Augment**, which is discussed in Chapter 13
- **Properties**, which opens the Experiment Properties window showing the summary of a design and enables you to change the icon associated with it (to change the icon, click on the icon in the Properties window).



Moving and Copying Design Folders

Sometimes you need to transfer designs to other computers or to share a design with another ADX user. For example, you might need to transfer designs from a laptop to a desktop computer or send a design to a colleague. In order to do this, you need to know how ADX stores the design files so that you can move or copy these files. ADX designs are grouped into folders, which are stored as SAS catalogs.

By default, all ADX catalogs are stored in the SASUSER library. To find the path name to the SASUSER library, do the following:

1. Open the SAS Program Editor.
2. Type the following into the SAS Program Editor and submit it to SAS:

```
proc contents data=SASUSER._ALL_ directory nods;
run;
```

3. Bring the SAS Output window to the front and scroll to the beginning of the output.
4. Read the output associated with the line **Physical Name**.

You can navigate to this folder with the operating system to copy, back up, or move the design folders. The name of the design folder ends with .sas7bcat. For example, the default ADX folder has a filename of adxparm.sas7bcat.

To use a design folder with ADX on another computer of the same platform, copy this file to the SASUSER library on the other computer and simply use the **Open Folder** command in ADX. If you are transporting the file to another platform, use PROC CPORT and PROC CIMPORT to create a transport file. Refer to the *Base SAS Procedures Guide* for more information.

If you need to access a design folder that is not in the SASUSER directory, repeat the preceding steps for opening a folder, and open the Open an Existing Folder window by selecting **File** → **Open Existing Folder** or clicking the **Open Existing Folder** icon on the ADX desktop. Then click the right arrow beside **Pathname** in the Open an Existing Folder window and use the system dialog box to navigate to the directory that contains the design folder.

Points to Remember

- You can create folders to organize designs by any aspect of your experimental activity.
- Within ADX, you can move designs between folders.
- Design folders are SAS catalogs, which you can copy, back up, or move to other computers.

Importing and Exporting Data

In many applications, an individual experiment is part of a large study or quality improvement system. Management of the experimental data for the entire study might involve the use of a data warehouse, a specialized database, or a collection of SAS data sets. ADX can export and import data from these sources. In addition, ADX can export metadata such as design summary information.

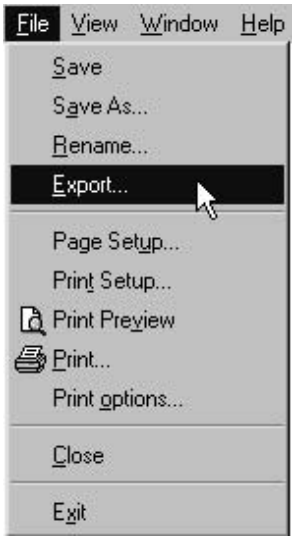
Covered in This Section

- Exporting data and metadata
- Importing data
  - Designs
  - Responses

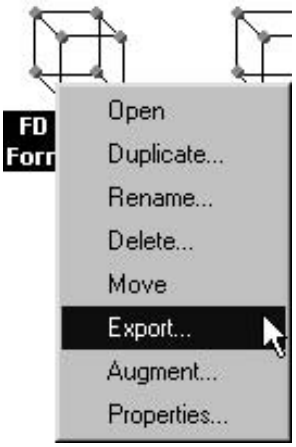
Exporting Information

In this example, you export the Tablet Formulation design. To invoke the wizard, do one of the following:

- Open the Tablet Formulation design, and select **File** → **Export**.

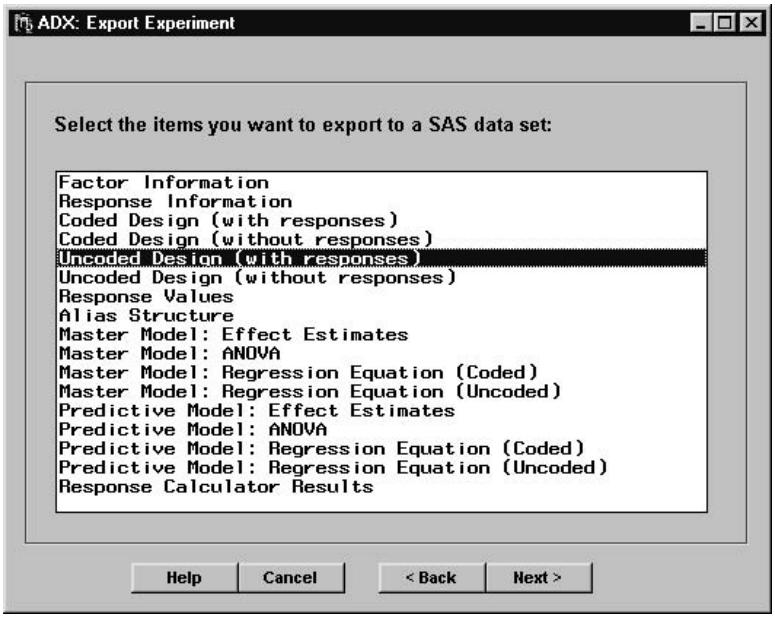


- Or, from the ADX desktop, click and then right-click on the FD Tablet Formulation design, and select **Export**.



To export information with the Export Experiment wizard, do the following:

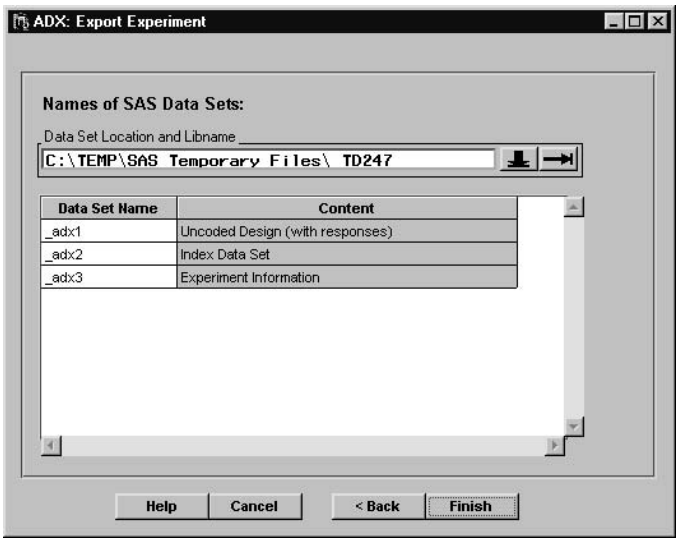
1. Choose the format in which you want to save the exported information. In this case, a SAS data set (the default) is the desired format, so leave this window as is.
2. Click **Next**. This window lists the types of information that ADX can export. Select **Uncoded Design (with responses)**. (Hold down the CTRL key and click to export more than one type.)



3. Click **Next**. This window shows you the default names of the SAS data sets that will contain the uncoded design, an index, and design summary information. These last two data sets are always saved, and the index data set contains the

names of the other data sets. For example, you can use the index data set to build a star schema representation of the design in a data warehouse.

By default, the SAS data sets will be stored in the temporary WORK library, with the filenames shown in this window. You can later relocate and rename these files with a SAS program. Alternatively, you can click the down arrow to choose a permanent library in which to store the data sets.



4. When you are done, click **Finish**. ADX will create the SAS data sets.

Note: Exporting data to an external format, such as Microsoft Excel, requires that SAS/ACCESS be installed.

You can now use the SAS Explorer or a SAS program to verify that the file was exported and to further process the information.

Importing Data

ADX can import data from a SAS data set. If SAS/ACCESS software is installed, ADX can also import data from a Microsoft Excel spreadsheet, a dBase database, a delimited text file, and files with other common formats.

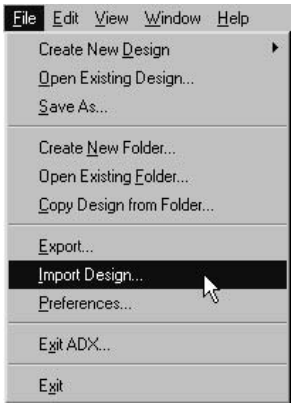
You can import a complete design or just the responses.

Importing a Complete Design

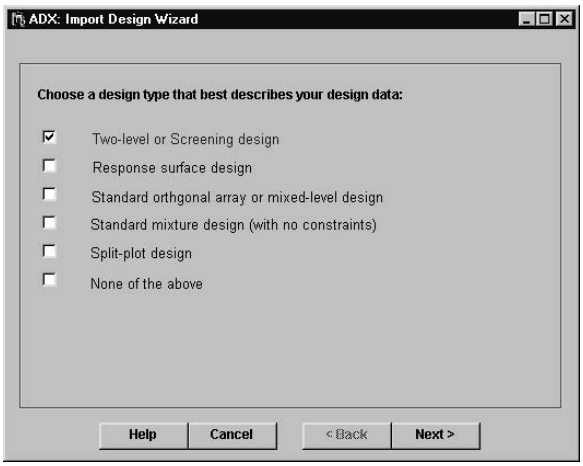
In this section you import the data set you created in the section "Exporting Information" on page 209. To import a design from the SAS data set, follow these steps:

1. Close all designs to return to the ADX desktop. If you want to import the design into another folder, follow the steps outlined in the section "Changing the Current Folder" on page 205.

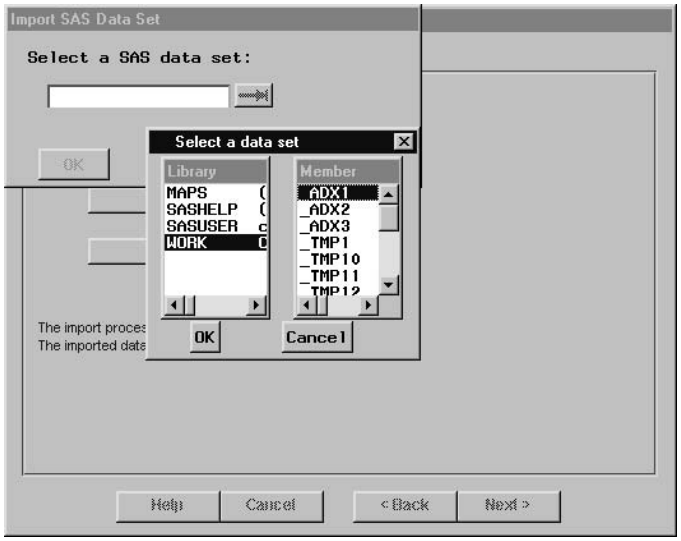
2. Select **File** → **Import Design**.



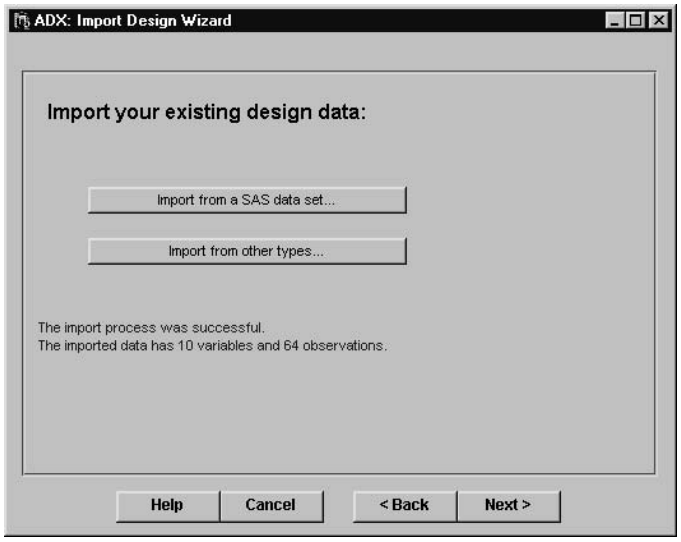
3. Select the design type that most closely fits the purpose of the design you want to import. In this case, you will simply create another two-level design with the data set.



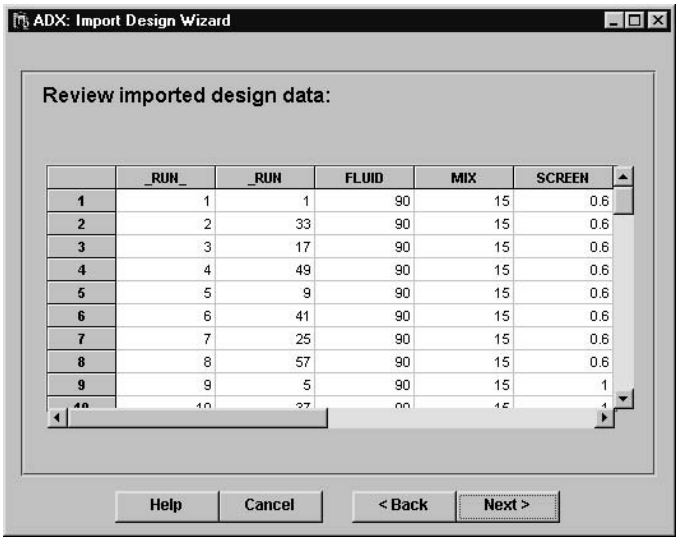
4. Click **Next**. This window directs you to select the source of your data: either a SAS data set or (if SAS/ACCESS is installed) an external data source. Select **SAS data set**.
5. Navigate to the data set you created in the section "Exporting Information" on page 209, which might differ somewhat from the illustration. Click **OK**.



6. ADX indicates whether the import was successful. If not, check the data source and try again.

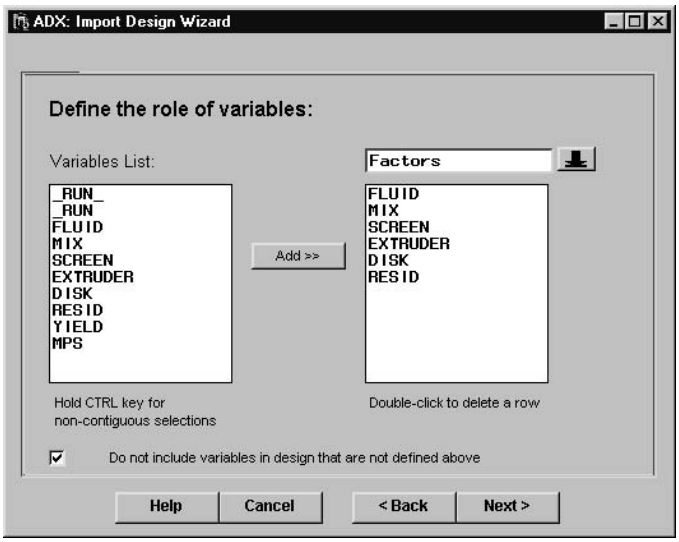


7. Click **Next**. This window shows you the data that were imported. Here you can verify whether you selected the file you wanted. If not, click **Back** and select another file.

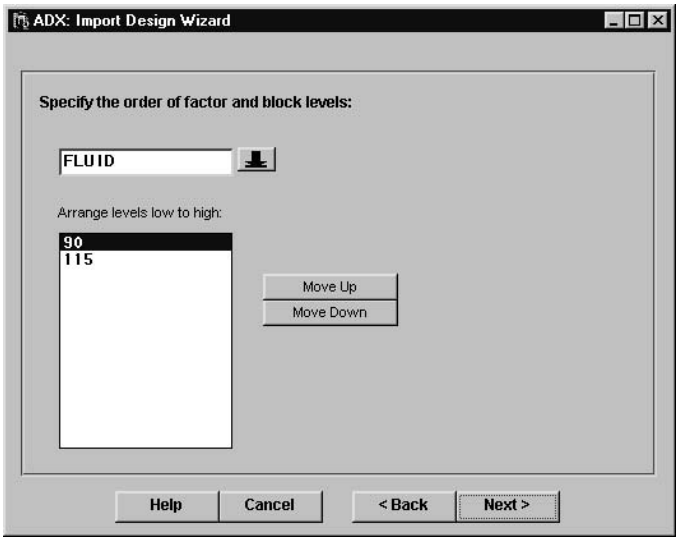


	RUN	_RUN	FLUID	MIX	SCREEN
1	1	1	90	15	0.6
2	2	33	90	15	0.6
3	3	17	90	15	0.6
4	4	49	90	15	0.6
5	5	9	90	15	0.6
6	6	41	90	15	0.6
7	7	25	90	15	0.6
8	8	57	90	15	0.6
9	9	5	90	15	1

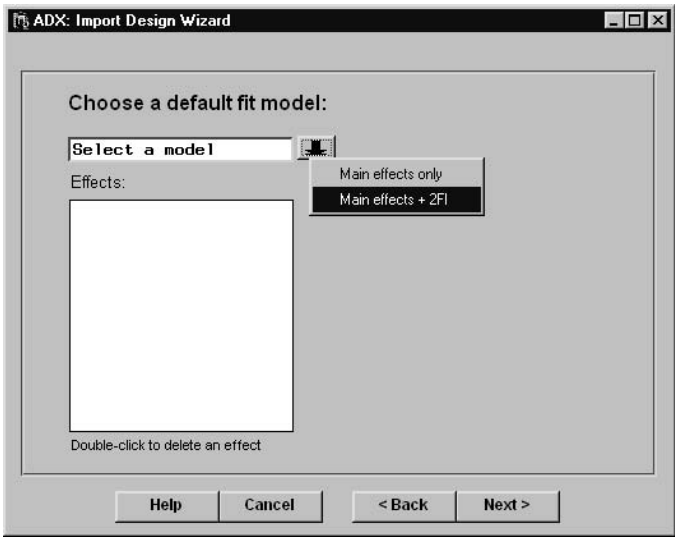
8. Click **Next**. You can use this window to assign roles to columns. The down arrow enables you to select the role: factor, response, or block. Click the column name and click **Add** to assign a column to that role.
9. Repeat the previous step for **Responses**, and, if applicable, **Blocks**. (There is no block variable in this case.)
10. If you want to exclude columns from the design, select the check box labeled **Do not include variables in design that are not defined above**.



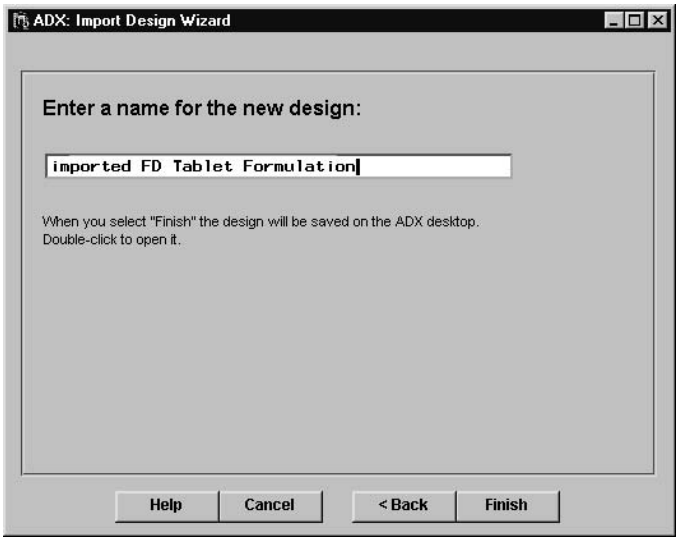
11. Click **Next**. Order the levels for each factor if necessary. ADX does this automatically, but you might want to reorder the levels of categorical factors.



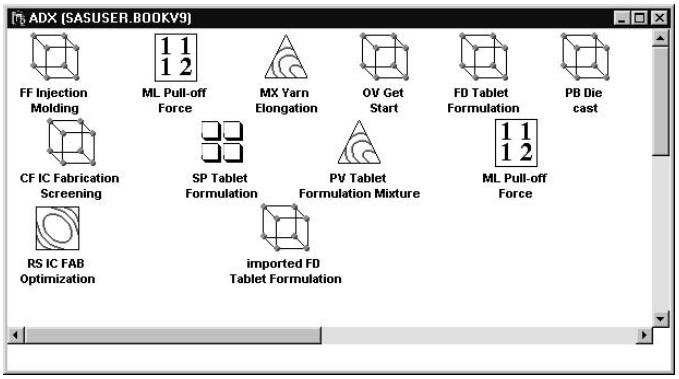
12. Click **Next**. Specify a default master model. You can choose a main-effects model or one that also includes two-factor interactions. Double-click any effects you want to delete (for example, to induce nesting). (**Note:** Be sure to select a model in which all effects are estimable.)



13. Click **Next**. Enter the name of the design and click **Finish**.



14. The new design is saved in the current folder on the ADX desktop. You can now treat this design as if it were created in ADX.



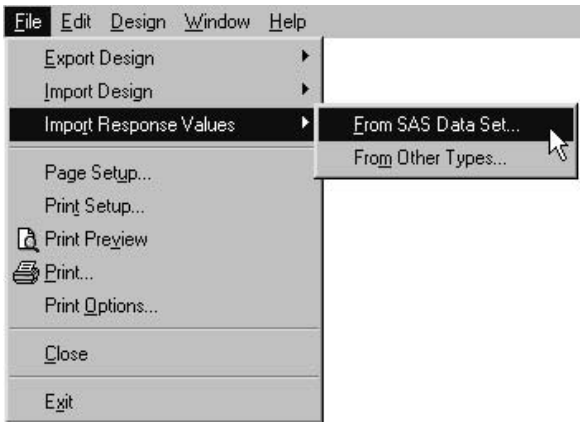
Importing Responses into a Design

In some experimental situations the response values for a design are recorded in an external data source, such as a spreadsheet. Assuming that the design was initially created in ADX, you can use the import facility in ADX to merge the response values with the design. (Of course, this assumes that the response values have the same order as the design runs.)

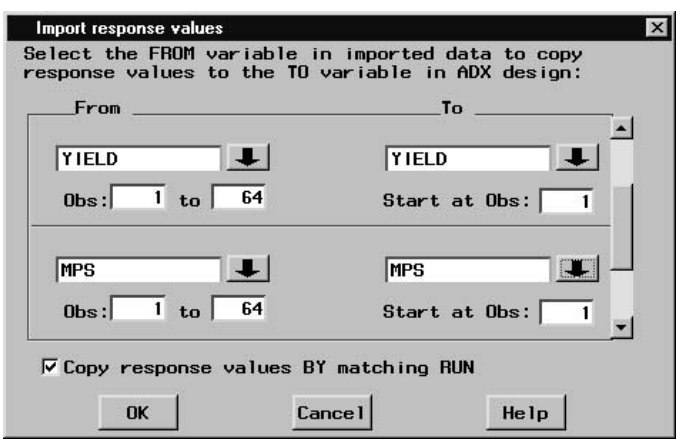
To merge response values with a design, do the following:

1. Open the design.
2. Click **Edit Responses**.

3. Select **File** → **Import Response Values** → **From SAS Data Set**. (Note that if SAS/ACCESS is installed, you can choose an external source by selecting **From Other Types**.)



4. Navigate to the location of the data set.
5. In the Import Response Values window, there are two columns, labeled **From** and **To**, and a row for each response variable in the design. Use the down arrows and the pop-up menus in the **From** column to select the variable to import for each response in the **To** column.



6. Click **OK** to import the response values.

The values will be copied from the data set in the order in which they are encountered. If the runs are ordered differently, then create a column called RUN in the data set. When you import the response values, the check box **Copy response values BY matching RUN** will be selected, and the run order specified by RUN will be used.

Copying and Pasting Response Values

You can copy response values from a spreadsheet and paste them into a design. Follow these steps:

1. In the spreadsheet, select the values to copy by dragging the mouse pointer, and select **Edit** → **Copy**.
2. In ADX, open the design and click **Edit Responses**. Right-click in the first row of the response column and select **Paste** from the menu.
3. Press **Enter**.

Points to Remember

- ADX can export design information, including the factor and response data.
- ADX can export summary data for each design, such as factor and response names.
- You can create a new design from another data source, or you can merge response values.
- If SAS/ACCESS is installed, you can export and import data from spreadsheets.
- You can copy response values from a spreadsheet and paste them into a design in ADX.

Appendix A
Glossary of ADX Terms

Alias Structure of a Design

In a fractional factorial design, it is impossible to completely distinguish the influences that all the effects have on the response. The aliasing structure of the design shows which effects are indistinguishable. Each row of the alias structure corresponds to a measurable effect on the response; any or all of the effects in a given row could be responsible for the measured effect. ADX provides a tab for examining the alias structure in the Design Details window.

See also **Resolution**. For details, refer to Montgomery (1997) or other standard references on design of experiments.

Analysis of Variance

Performing an analysis of variance (ANOVA) on a linear model enables you to assess the model effects on the variation in the response. The overall ANOVA analyzes the significance of the entire model.

Bayes Effect Plot

A Bayes effect plot displays the probability that each effect is active according to the Bayesian analysis of Box and Meyer (1986). This analysis is especially useful in saturated or near-saturated fractional factorial designs, when there are not enough degrees of freedom left to estimate error and perform F tests on the effects. In this case, the principle of effect sparsity suggests that most of the effects in the design (about 80%) will be inactive.

With 0.20 as a prior probability for effect activity, posterior probabilities can be computed using standard Bayesian theory. Roughly speaking, this analysis gives the probability that each effect is active. The posterior probabilities can be quite sensitive to the prior. For this reason, you should examine the posteriors over a range of priors. If an effect has a high probability of activity over most of the range, this can be taken as good evidence that it indeed has a significant effect on the response.

Blocking Factor

A blocking factor is an experimental factor that might contribute to response variability but that is otherwise not of interest. Typically, a blocking factor can be controlled in laboratory conditions but not in field settings.

A blocking scheme is used in a factorial design to account for variability in the response that might otherwise be attributed incorrectly to other factors or to experimental error.

Box-Behnken Design

A Box-Behnken design is a fraction of a 3^N design used to estimate a full quadratic model in N factors. It consists of all 2^k possible combinations of high and low levels for different subsets of the factors of size k, with all other factors at their central levels. The subsets are chosen according to a balanced incomplete block design for N treatments in blocks of size k. A number of center points with all factors at their central levels can also be added.

Since each factor takes no more than three different values, and since only k factors are not at their central levels in any one run, these designs can be easier to implement than comparable central composite designs. However, unlike central composite designs, they are not conducive to sequential experimentation.

Box Plot

A box plot displays differences in the distributions of the selected response when categorized by factor levels. Like a main-effects plot, a box plot can demonstrate potentially significant effects. However, box plots can also bring to light the heteroscedasticity of the response (a significant effect of a factor on the variance of the response). ADX provides box plots with summary statistics such as the median and the interquartile range.

ADX can categorize the responses by using more than one factor; in this case the factors are stratified. This enables you to see the interaction of two effects on the mean and variance of the response, if enough data are present.

Center Point

Often the low and high values of a factor in a fractional factorial design are chosen around a central, nominal value—perhaps the current operating conditions. Center points are included in a design to add extra prediction precision in this region or to allow testing for lack of fit. You can add as many center points to the design as you want, although they are allowed only when at least one of the factors is numeric.

Central Composite Design

A central composite design for N factors is a full or fractional replication of the complete 2^N design, augmented by 2^N axial points and a given number of center points. There is one axial point for either extreme of each factor, with all other factors at their central values. A center point has every factor at its central value. All terms in the second-order model can be estimated, and the center points enable you to test for a lack of fit.

Confounding Rules

The confounding rules for a fractional factorial design are the equations that specify how it is constructed. In general, for two-level factors, the confounding rules assign the values of certain factors to be the product of values of other factors. ADX chooses confounding rules that generate a maximum resolution design with minimum aberration.

Constrained Mixture Design

In a mixture design, when the mixture factors are subject to additional constraints (besides summing to one), there are two different possibilities for design generation:

- If the constraints are lower bounds, then a regular simplex-centroid design can be transformed into a design for the constrained factors.
- If there are both upper and lower bounds on the factors, then the feasible region no longer has a regular shape. However, the vertices and generalized face centroids of the feasible region provide good potential design points. ADX chooses an optimal design from these points when generating a constrained mixture design. Refer to Snee (1975) and Cornell (1990) for details.

Constraint

Sometimes the nature of an experiment does not allow you to set factor levels freely. These constraints are modeled through linear inequalities, such as

$$X1 + X2 + X3 \leq 0.8$$

Constraints on the factors usually do not admit classical fractional factorial designs or response surface designs. ADX automatically uses an optimal design in these cases.

Mixture designs involving constraints often arise in practice. ADX uses a Scheffé analysis for these designs. See **Constrained Mixture Design** for more details.

Contour Optimizer

Resembling the contour plot in many ways, the contour optimizer in ADX gives a two-dimensional representation of a response surface. This tool is used to locate optimum factor settings for a desired response. The display can be annotated and included in a report. See **Contour Plots** for more details.

Contour Plot A contour plot is a two-dimensional representation of a three-dimensional response surface, where curves of equal predicted response are plotted. If no more than two factors in the design appear to affect the response, the contour plot can be a good way to summarize the response surface. Otherwise, ADX provides a matrix of contour plots created by fixing levels of nondisplayed variables.

The contours of the standard error of prediction are printed along with those of the predicted response. This indicates how well the fitted response surface predicts the true response.

Cube Plot A cube plot is a three-dimensional representation of the observed response surface, with the average responses indicated at the cube vertices. It is especially useful for fractional factorial designs when few factors and interactions are significant.

Design Augmentation

Sometimes a researcher needs more information from an experiment than is provided by an initial design. Through the addition of carefully chosen runs, the estimation and prediction capability can be enhanced. This process is called design augmentation.

ADX currently supports four types of design augmentation:

- **Augment a two-level design to a response surface design**. This enables you to estimate quadratic effects. Center points and axial runs are added to the original design to make it a central composite design.
- **Fold over a two-level design**. This involves adding complementary runs to a two-level fractional factorial design with Resolution 3. This increases the resolution to four but doubles the number of runs.
- **Break alias strings of certain effects by adding optimal runs**. This technique, like folding over, allows the estimation of more effects but typically does not require the addition of as many runs. ADX uses the Optimal Design interface to generate these runs.
- **Deleting inactive factors and projecting into a higher-resolution design**. This involves dropping the inactive factors permanently from an experiment and projecting the design in the subset of the remaining factors.

Design Type

ADX provides the following design types:

- Two-Level Designs
- Response Surface Designs
- Mixture Designs
- Mixed-Level Designs
- Optimal Designs
- Split-Plot Designs

Desirability When an experiment involves multiple responses, the overall response outcome depends on all or some of the individual responses. For example, you might want to minimize the first response, maximize the second response, or keep the third response close to a target value. You can use the desirability feature available in the Prediction Profiler plot in the Optimize window to define a desirability function for each individual response. The overall desirability of the product would be the geometric mean of the desirability of individual responses. For more information, refer to Derringer and Suich (1980).

Factor Also referred to as an independent or predictor variable, a factor is a variable included in a model to account for variation in a response. Factors are the variables whose values (levels) you set to study their relationship to a response. You often experiment with many potentially influential factors at the same time. However, the more factors there are in the experiment, the more runs will be required. Weigh the number of factors against the size and resolution of corresponding designs in order to determine which designs are appropriate for your situation.

Factorial Plot A factorial plot shows a tree plot displaying the response for combinations of levels of the main effects. Each node represents the response for the associated combination of factor levels. Refer to Beckman (1996) for details.

Fractional Factorial Design

A fractional factorial design is a factorial design in which not all combinations of factor levels are run. These designs are useful when runs are costly and higher-order interactions are not significant.

Half-Normal Plot

A half-normal plot is a plot of the absolute values of the responses against the expected order statistics from a folded normal distribution. Outliers, which deviate from the standard deviation line, indicate possibly active effects.

Hybrid Design

Roquemore (1976) developed a set of saturated or near-saturated second-order designs called hybrid designs. A hybrid design is very efficient. Unlike the small composite designs, hybrid designs are quite competitive with central composite designs when design size is taken into account.

Influential Observation

An influential observation is an observation that has a large impact on the results. Note that these are different from outliers, which are observations not explained by the model. Influential observations should be analyzed with care.

Interaction Effect An interaction effect measures the extent to which the effect of one factor on the response changes for different values of one or more other factors.

The presence of a factor in a significant interaction does not necessarily mean that its main effect is also significant. However, if an interaction is deemed to be significant and is therefore retained in the predictive model, it is good practice to include the constituent main effects.

Interaction Plot

An interaction plot displays the effect of a pair of factors on the response. For each value of one of the factors, a line connecting the mean responses at the low and high levels of the other factor is shown. An interaction effect is indicated when the lines have unequal slopes.

Lenth Plot A Lenth plot is a bar chart used to determine possible significant effects. The plot is created using a method, proposed by Lenth (1989), that computes a simultaneous margin of error (SME) around zero. Effect sizes that exceed the SME are flagged as possibly significant.

Lenth uses a pseudostandard error (PSE) to construct the SME. A preliminary estimate of the standard error is computed as 1.5 times the median of the absolute value of the estimated effects. Then the PSE is computed based on a trimmed median of the effects. Only the effects within 2.5 times the preliminary estimate are included in the trimmed median in an attempt to include only the inactive effects in the estimate.

Levels of a Factor

Levels are the values or settings of the factors in an experiment.

Main Effect An effect measures the extent to which the response depends on the factors involved in the effect. A main effect is the change in the response due to a single factor. For two-level factors, the main effect is the difference between the mean response at the high level of a factor and the mean response at its low level.

Main-Effects Plot

A main-effects plot displays the effect of a single factor on the response by plotting a line from the mean response at the low level of the factor to the mean response at the high level. Confidence intervals are plotted around the means. A nearly horizontal main-effect line generally indicates that the factor has little effect on the response.

A main-effects plot can be an effective way of presenting the effect of a single factor but yields little information about the whole model.

Master Model

A master model includes the effects that are initially considered for the experiment. ADX assigns a master model to each response by default. The master model is the model that is fit when you first click **Fit**. You can modify the master model at any time.

Minimum Aberration Design

A minimum aberration design (Fries and Hunter 1980) is designed to alias as few lower-order interactions as possible. The aberration criterion distinguishes fractional factorial designs with the same number of runs, the same number of factors, and the same resolution. Usually, you want a design with the highest resolution and the lowest aberration. All the standard fractional factorial designs in ADX are minimum aberration.

Mixed-Level Design

A mixed-level design is a relatively small design for two- and three-level factors, often used in the Taguchi (1978) approach to quality engineering. Most mixed-level designs included in the ADX Interface are orthogonal arrays. These designs usually have Resolution 3 and are ineffective for exploring interactions.

Mixture Design

The factors in a mixture design correspond to the proportion of components in a blend. They cannot be negative and must sum to one.

Refer to Cornell (1990) for details on mixture designs.

Model

The observed value for a response variable is assumed to be the sum of the effects of experimental factors, their interactions, and random error. A model is the collection of these effects together with the error structure.

In a typical study, an experiment with a model involving main effects and two-factor interactions is first run to identify significant factors. Then an experiment with a model involving the main, quadratic, and interaction effects of these significant factors is run to optimize the responses.

Normal Plot

A normal plot is constructed by plotting the sorted values of the responses (empirical quantiles) versus the theoretical quantiles from a normal distribution.

The normal plot is used to determine active (significant) effects. Inactive effects correspond to points that lie on or near a line whose slope is the standard deviation of the error, while active effects correspond to points that depart from the line.

Optimal Design

Standard designs have assured degrees of precision and orthogonality that are important for the exploratory nature of experimentation. However, when standard designs are inappropriate you can use optimal designs. You can use optimal designs under the following conditions:

- when not all combinations of the factor levels are feasible
- when the region of experimentation is irregularly shaped
- when resource limitations restrict the number of experiments that can be performed
- when there is a nonstandard model

For any of these situations you can generate an efficient experimental design by specifying a set of candidate design points and a model. ADX uses PROC OPTEX to determine points so that the terms in the model can be estimated as efficiently as possible. Refer to the *SAS/QC User's Guide* for details.

Orthogonal Array

The orthogonal arrays included in the ADX Interface are relatively small designs for two- and three-level factors. These are often used in the Taguchi (1978) approach to quality engineering. They are also called mixed-level designs.

Orthogonal arrays can be used for studying quantitative factors, but the requirement of orthogonality between factors usually makes the designs large, while providing insufficient information about interactions. In studying quantitative factors, it is usually more appropriate to use two-level designs, followed by response surface designs.

Outer Array

In Taguchi (1978) applications, the response observed for each combination of factors is a function, called the signal-to-noise ratio, computed over several observations (the outer array). The outer array represents a range of uncontrollable operating conditions (noise), and the intent is to estimate the effect of these conditions on the response.

Outlier

An outlier is a data point that differs from the general trend of the data by more than is expected by chance alone. An outlier might be an erroneous data point or one not explained by the same model as the rest of the data.

Pareto Plot

A Pareto plot is a bar chart of scaled absolute effect estimates. By default, the estimates are scaled by the sum of the absolute effect estimates. The plot can also display the square of the estimates scaled by the sum of squares of the estimates. In both cases, the bars are sorted in descending order.

In a typical Pareto plot, there are a few tall bars and many short bars. This illustrates the Pareto principle: in a typical experiment, relatively few effects will be significant.

Plackett-Burman Design

A Plackett-Burman design is a minimum-run, orthogonal design for estimating main effects. In ADX, Plackett-Burman designs are available for 2 to 47 factors. The number of runs in a Plackett-Burman design is the smallest multiple of 4 greater than the number of factors.

These designs estimate only main effects, and these effects are confounded with a linear combination of two-factor interaction effects. Thus, they are considered Resolution 3 designs. If analysis suggests that interaction effects are active, these designs can be augmented.

Plackett-Burman designs are primarily useful for screening a large number of factors, and should be used with caution.

Randomization

In a properly designed experiment, it is essential to randomize the order of the runs. This is done to neutralize the effect of any systematic biases that might be involved in the experiment and to validate the assumptions underlying the analysis. The ADX Interface makes it easy to randomize a design.

Regression

A regression is a function that describes the relationship between an expected response and one or more effects. The most common regression is linear regression, where the method of least squares is used to estimate the coefficients in a linear function of effects (main effects or interactions).

ADX uses regression techniques to fit a predictive model to a response.

Regression Coefficients

A linear regression model has the form

$$\mathbf{E}(Y) = b_0 + b_1 x_1 + b_2 x_2 + \cdots + b_p x_p$$

where $x_1, \ldots, x_p$ are the independent variables of the model. The $b_0, b_1, \ldots, b_p$ terms are the regression coefficients; they show the direction and magnitude of the dependence of the expected response on the associated independent variables.

Regular Fractional Factorial Design

In regular fractional factorial designs, any two effects are either orthogonal or completely aliased. That is, for every pair of effects, either every level of one occurs with every level of the other, or every level of one occurs within exactly one level of the other. In general, a small fractional factorial design will admit fewer estimable effects, and it will involve more aliased effects than a large one. In ADX, fractional factorial designs are available for as many as 50 factors and as many as 128 runs, and in blocks with as few as two runs. Design and block sizes are always powers of 2.

Residual Plot An important assumption in regression analysis is that the residual errors, the deviations of the observed values of the response from their expectations, are independent and identically distributed with a mean of zero. You can verify this assumption by viewing a residual plot.

Resolution The resolution of a design gives an indication of which effects can be estimated. If a design has Resolution R, then all interactions up to order E are estimable and are not aliased with each other, where E is the integer part of $(R-1)/2$. Furthermore, if R is even, these interactions are not aliased with any $(E+1)$-order interactions.

In particular:

- In a design of Resolution 3, the main effects are not aliased with each other, but they are confounded with two-factor interactions.
- In a design of Resolution 4, the main effects are not aliased with each other or with any two-factor interactions, but some two-factor interactions are aliased with each other.
- In a design of Resolution 5 or more, all main effects and two-factor interactions are estimable free of each other.

Note: Roman numerals are often used to denote resolution.

Response Designed experiments study the dependence of the response on the factors of the design. Often this involves identifying the significant factors and then optimizing the response. The experimental design consists of the specific combinations of levels of the design factors that are chosen for observation of the response.

Response Surface Design

A response surface design is often used to model both the linear and the quadratic behavior of the response over the design region. Typically, a preliminary two-level design has already been run to determine the significant factors, and now you want to study the relationship between the response and these significant factors in more detail.

Run

A run is the basic experimental unit, with one setting for each of the factors of the experiment and for which a single value will be observed for each response. In industrial applications, this might correspond to a single run of the process, with certain settings for the various process variables. Choose the number of runs in the experimental design by balancing all other design parameters—number of factors, resolution, and block size—against your experimental budget. As a general rule, you should spend about 25% of your experimental budget on a preliminary, exploratory study such as a screening experiment.

Saturated Design

In a saturated design (also called a screening experiment or an orthogonal array) there are as many observations as there are parameters to estimate in the model. Thus, there are no degrees of freedom left over to provide an independent estimate of the error variance. A saturated design allows many factors to be studied with relatively few runs, but because it gives no information about the underlying variation, it should be used cautiously.

Scatter Plot

A scatter plot is a two- or three-dimensional plot showing the joint variation of two (or three) variables from a group of observations. The coordinates of each point in the plot correspond to the data values for a single observation.

Signal-to-Noise Ratio

A signal-to-noise ratio is one of a variety of measures of response performance, relating the mean response (or "signal") to the variation in the response (or "noise"). The use of signal-to-noise ratios is associated with the Taguchi (1978) approach to quality engineering. You might want to estimate the effect of factors on the value of the response or on its variability or perhaps on both simultaneously. Alternatively, you might want a performance measure that increases as the response decreases.

Signal-to-noise ratios are calculated for groups of experimental runs, so multiple response values are required. Usually these are observed over an outer array.

Simplex-Centroid Design

A simplex-centroid design of degree m is composed of mixtures consisting of the following types of blends:

- only one component present
- all pairs of two components present in equal amounts
- all triples of three components present in equal amounts
- and so on, up to all combinations of $m - 1$ components present in equal amounts
- all components present in equal amounts (the centroid)

With such a design it is possible to fit a mixture model up to degree m.

A q-component simplex-centroid design consists of $2q - 1$ distinct design points. Because they are relatively efficient designs for fitting the special cubic model, simplex-centroid designs are often used when the experimenter believes that some cubic terms might be missing in the final model. The simplex-centroid design is also used to provide experimental coverage of the response surface in the center of planes and hyperplanes.

Simplex-Lattice Design

A simplex lattice is a uniformly spaced set of points (or "lattice") on a simplex. When a simplex-lattice design is used in mixture experiments, the responses are measured at the simplex-lattice composition points.

Small Composite Design

For a small composite design, the fractional portion is neither a complete 2^k nor a Resolution 5 fraction, but rather a special Resolution 3 fraction in which no four-letter word occurs among the defining relations. As a result, the total run size is reduced from that of a central composite design. Small composite designs are less efficient for estimating linear and interaction coefficients than central composite designs.

Split-Plot Design

A split-plot design modifies the classical fractional factorial design structure to accommodate differences in the precision to which different effects can be estimated. The split-plot structure was originally designed to analyze agricultural experiments in which a large area of land used for the experiment was divided into large plots, called whole plots. These whole plots were subdivided into smaller plots, called subplots, and treatments were assigned to units within the subplots. The assumption was that the subplots were more homogeneous than the whole plots and therefore analysis of effects between the subplots required a different analysis from the effects between the whole plots.

Today, the split-plot construction is used to accommodate randomization issues such as hard-to-change factors and environmental nuisance factors. ADX uses the mixed-model approach to analyzing split plots.

Surface Plot A surface plot is a graph of one response against two factors. ADX enables you to rotate the surface for maximum utility.

Two-Level Design

In a two-level design, each factor occurs at only two levels, usually a high value and a low value. A two-level screening design is usually used at the initial stages of experimentation to identify factors that significantly affect the response.

Appendix B
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Index

T

U

V

Z

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