Design of Engineering Experiments Part 5 – The 2^k Factorial Design

- Text reference, Chapter 6
- **Special case** of the general factorial design; *k* factors, all at two levels
- The two levels are usually called **low** and **high** (they could be either quantitative or qualitative)
- Very widely used in industrial experimentation
- Form a basic "building block" for other very useful experimental designs (DNA)
- Special (short-cut) methods for analysis
- We will make use of Design-Expert

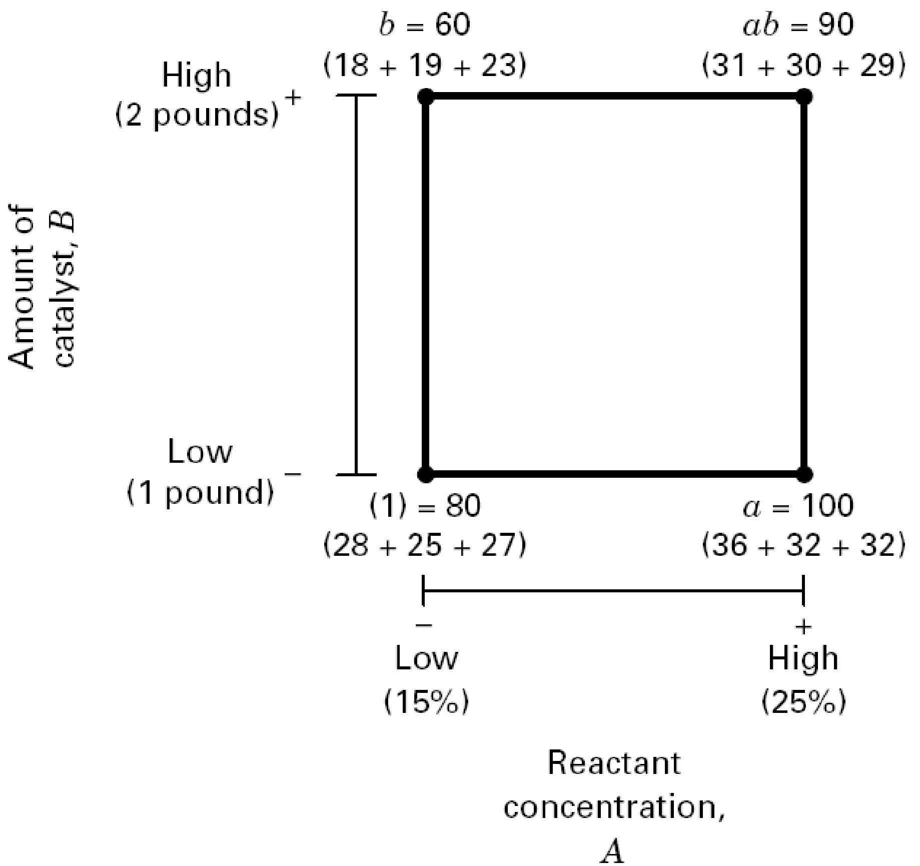
CHAPTER 6

Two-Level Factorial Designs

CHAPTER OUTLINE

The supplemental material is on the textbook website www.wiley.com/go/global/montgomery.

The Simplest Case: The 2^2



■ **FIGURE 6.1 Treatment combinations in the 2^2 design**

"-" and "+" denote the low and high levels of a factor, respectively

- Low and high are arbitrary terms
- Geometrically, the four runs form the corners of a square
- Factors can be quantitative or qualitative, although their treatment in the final model will be different

Chemical Process Example

Factor		Treatment	Replicate			
A	*B*	Combination	I	II	III	Total
−	−	*A* low, *B* low	28	25	27	80
+	−	*A* high, *B* low	36	32	32	100
−	+	*A* low, *B* high	18	19	23	60
+	+	*A* high, *B* high	31	30	29	90

A = reactant concentration, *B* = catalyst amount,
y = recovery

Analysis Procedure for a Factorial Design

- Estimate factor **effects**
- **Formulate** model
  - With replication, use full model
  - With an unreplicated design, use normal probability plots
- Statistical **testing** (ANOVA)
- **Refine** the model
- Analyze **residuals** (graphical)
- **Interpret** results

Estimation of Factor Effects

$$A = \bar{y}_{A^+} - \bar{y}_{A^-}$$
$$= \frac{ab+a}{2n} - \frac{b+(1)}{2n}$$
$$= \tfrac{1}{2n}[ab + a - b - (1)]$$
$$B = \bar{y}_{B^+} - \bar{y}_{B^-}$$
$$= \frac{ab+b}{2n} - \frac{a+(1)}{2n}$$
$$= \tfrac{1}{2n}[ab + b - a - (1)]$$
$$AB = \frac{ab+(1)}{2n} - \frac{a+b}{2n}$$
$$= \tfrac{1}{2n}[ab + (1) - a - b]$$

See textbook, pg. 235-236 for **manual** calculations

The effect estimates are: *A* = 8.33, *B* = -5.00, *AB* = 1.67

Practical interpretation?

Design-Expert analysis

$$\text{Contrast}_{ABC\ldots Z} = (a \pm 1)(b \pm 1)(c \pm 1)\ldots\ldots\ldots(z \pm 1)$$

$$ABC\ldots Z = \frac{2(\text{Contrast}_{ABC\ldots Z})}{n2^K}$$

$$SS_{ABC\ldots Z} = \frac{(\text{Contrast}_{ABC\ldots Z})^2}{n2^K}$$

$$SS_T = \Sigma\Sigma\Sigma\Sigma\ldots \Sigma Y^2_{ij\ldots k} - Y^2_{\ldots\ldots} / ab\ldots n$$

Statistical Testing - ANOVA

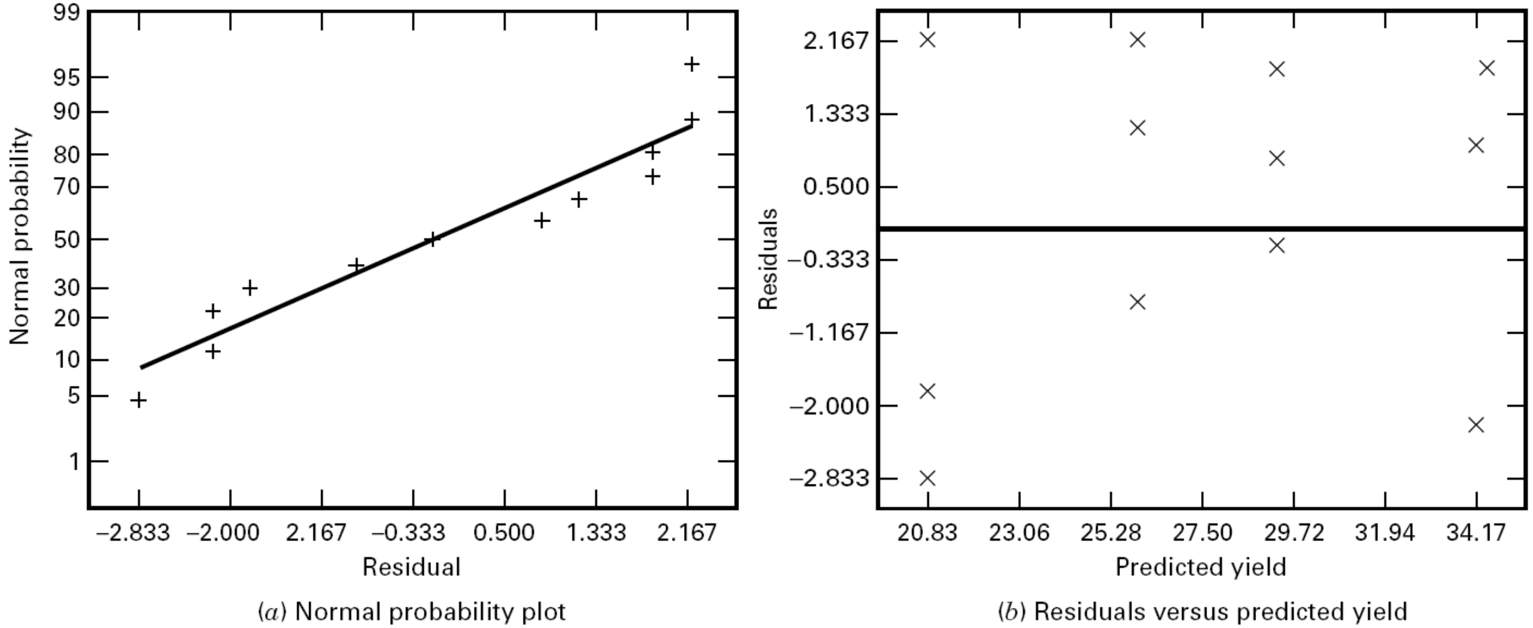
■ **TABLE 6.1**

Analysis of Variance for the Experiment in Figure 6.1

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_q	*P*-Value
A	208.33	1	208.33	53.15	0.0001
B	75.00	1	75.00	19.13	0.0024
AB	8.33	1	8.33	2.13	0.1826
Error	31.34	8	3.92		
Total	323.00	11			

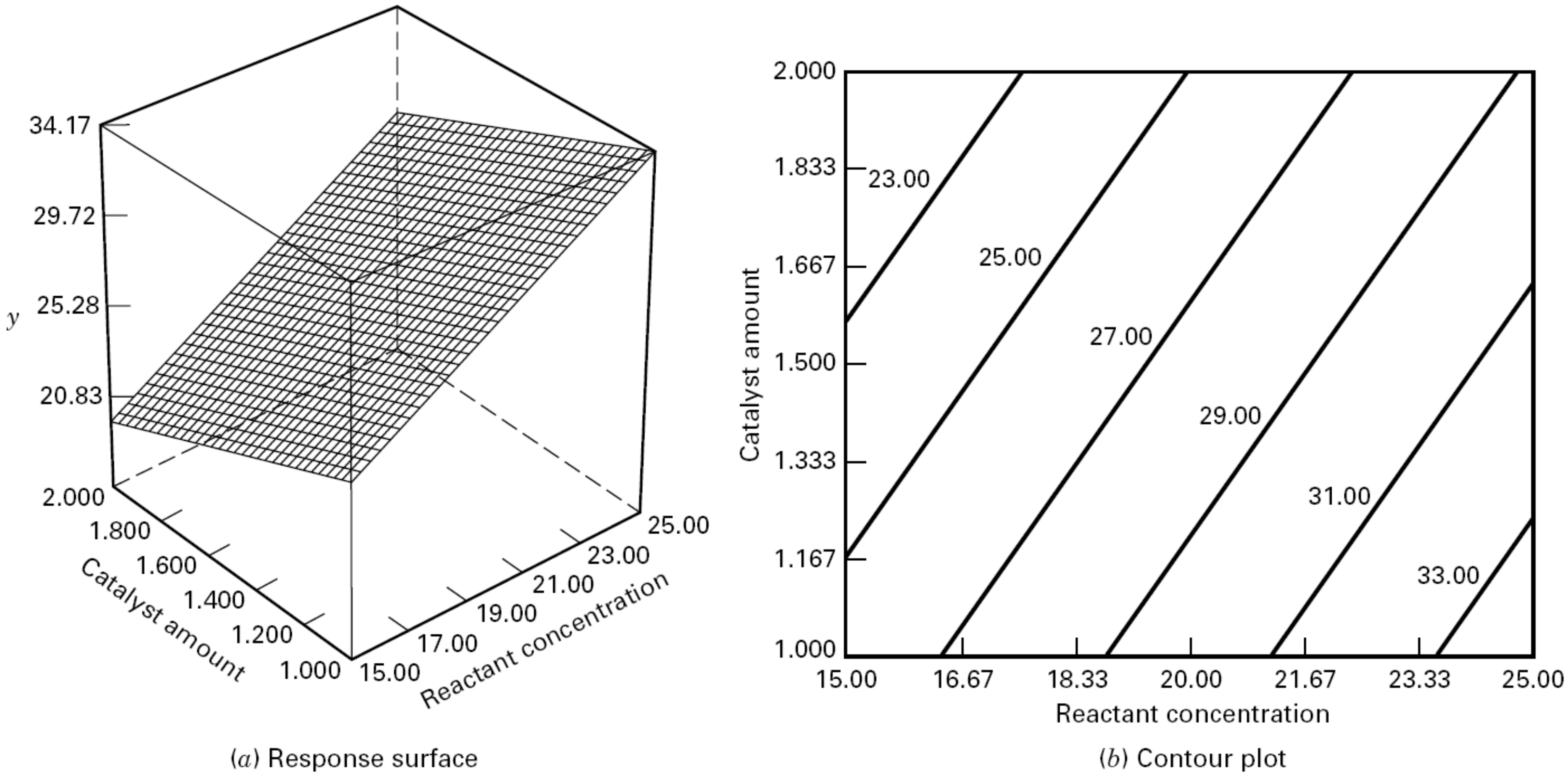
The *F*-test for the "model" source is testing the significance of the overall model; that is, is either *A*, *B*, or *AB* or some combination of these effects important?

Residuals and Diagnostic Checking



■ **FIGURE 6.2** **Residual plots for the chemical process experiment**

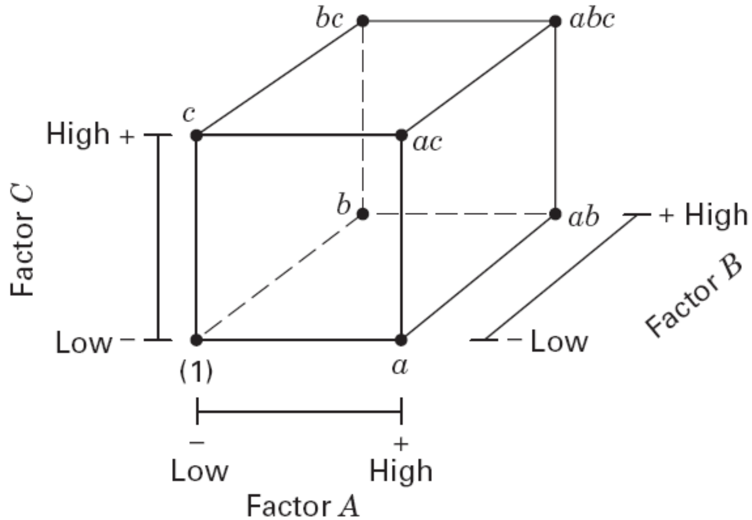
The Response Surface



■ **FIGURE 6.3** **Response surface plot and contour plot of yield from the chemical process experiment**

The 2^3 Factorial Design

■ **FIGURE 6.4**
The 2^3 factorial design



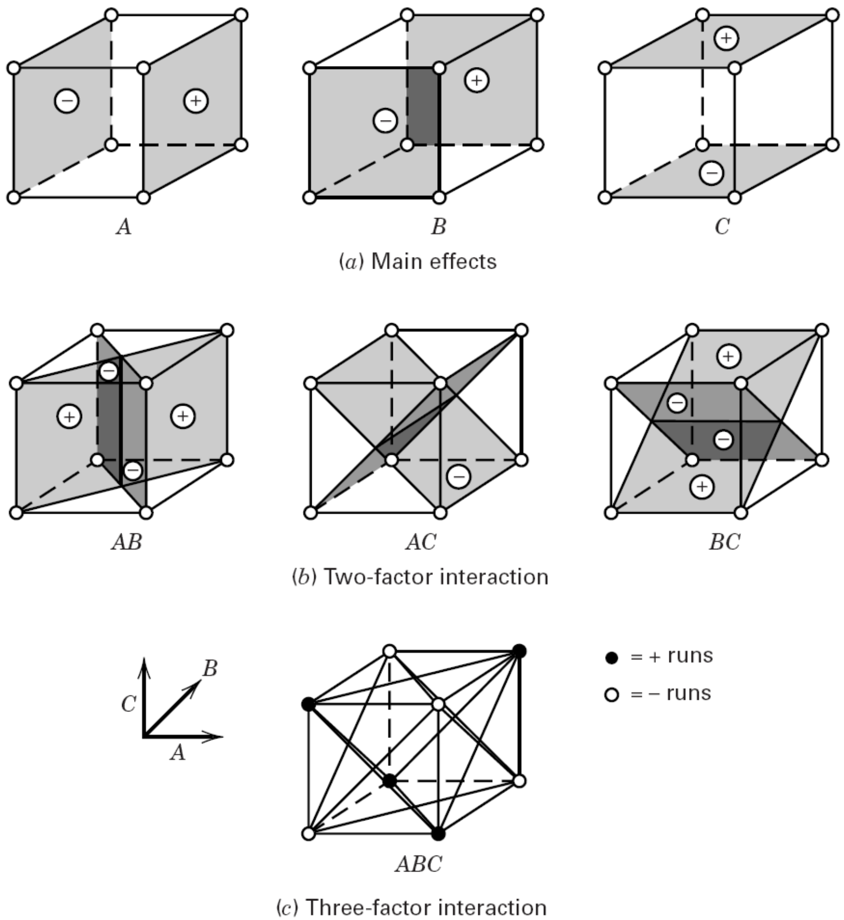
(a) Geometric view

Run	Factor A	B	C
1	−	−	−
2	+	−	−
3	−	+	−
4	+	+	−
5	−	−	+
6	+	−	+
7	−	+	+
8	+	+	+

(b) Design matrix

Effects in The 2^3 Factorial Design

■ **FIGURE 6.5**
Geometric presentation of contrasts corresponding to the main effects and interactions in the 2^3 design



$$A = \bar{y}_{A^+} - \bar{y}_{A^-}$$

$$B = \bar{y}_{B^+} - \bar{y}_{B^-}$$

$$C = \bar{y}_{C^+} - \bar{y}_{C^-}$$

etc, etc, ...

Analysis done via computer

An Example of a 2^3 Factorial Design

■ **TABLE 6.4**
The Plasma Etch Experiment, Example 6.1

Run	Coded Factors A	B	C	Etch Rate Replicate 1	Replicate 2	Total	Factor Levels	Low (−1)	High (+1)
1	−1	−1	−1	550	604	(1) = 1154	*A* (Gap, cm)	0.80	1.20
2	1	−1	−1	669	650	*a* = 1319	*B* (C_2F_6 flow, SCCM)	125	200
3	−1	1	−1	633	601	*b* = 1234	*C* (Power, W)	275	325
4	1	1	−1	642	635	*ab* = 1277			
5	−1	−1	1	1037	1052	*c* = 2089			
6	1	−1	1	749	868	*ac* = 1617			
7	−1	1	1	1075	1063	*bc* = 2138			
8	1	1	1	729	860	*abc* = 1589			

A = gap, *B* = Flow, *C* = Power, *y* = Etch Rate

Table of – and + Signs for the 2^3 Factorial Design (pg. 218)

■ **TABLE 6.3**

Algebraic Signs for Calculating Effects in the 2^3 Design

Treatment Combination	Factorial Effect							
	I	*A*	*B*	*AB*	*C*	*AC*	*BC*	*ABC*
(1)	+	−	−	+	−	+	+	−
a	+	+	−	−	−	−	+	+
b	+	−	+	−	−	+	−	+
ab	+	+	+	+	−	−	−	−
c	+	−	−	+	+	−	−	+
ac	+	+	−	−	+	+	−	−
bc	+	−	+	−	+	−	+	−
abc	+	+	+	+	+	+	+	+

Properties of the Table

- Except for column *I*, every column has an equal number of + and – signs
- The sum of the product of signs in any two columns is zero
- Multiplying any column by *I* leaves that column unchanged (identity element)
- The product of any two columns yields a column in the table:

$$A \times B = AB$$

$$AB \times BC = AB^2C = AC$$

- **Orthogonal** design
- Orthogonality is an important property shared by all factorial designs

Estimation of Factor Effects

■ **TABLE 6.5**

Effect Estimate Summary for Example 6.1

Factor	Effect Estimate	Sum of Squares	Percent Contribution
A	−101.625	41,310.5625	7.7736
B	7.375	217.5625	0.0409
C	306.125	374,850.0625	70.5373
AB	−24.875	2475.0625	0.4657
AC	−153.625	94,402.5625	17.7642
BC	−2.125	18.0625	0.0034
ABC	5.625	126.5625	0.0238

ANOVA Summary – Full Model

■ **TABLE 6.6**
Analysis of Variance for the Plasma Etching Experiment

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	*P*-Value
Gap (*A*)	41,310.5625	1	41,310.5625	18.34	0.0027
Gas flow (*B*)	217.5625	1	217.5625	0.10	0.7639
Power (*C*)	374,850.0625	1	374,850.0625	166.41	0.0001
AB	2475.0625	1	2475.0625	1.10	0.3252
AC	94,402.5625	1	94,402.5625	41.91	0.0002
BC	18.0625	1	18.0625	0.01	0.9308
ABC	126.5625	1	126.5625	0.06	0.8186
Error	18,020.5000	8	2252.5625		
Total	531,420.9375	15			

Model Coefficients – Full Model

Factor	Coefficient Estimated	DF	Standard Error	95% CI Low	95% CI High	VIF
Intercept	776.06	1	11.87	748.70	803.42	
A-Gap	−50.81	1	11.87	−78.17	−23.45	1.00
B-Gas flow	3.69	1	11.87	−23.67	31.05	1.00
C-Power	153.06	1	11.87	125.70	180.42	1.00
AB	−12.44	1	11.87	−39.80	14.92	1.00
AC	−76.81	1	11.87	−104.17	−49.45	1.00
BC	−1.06	1	11.87	−28.42	26.30	1.00
ABC	2.81	1	11.87	−24.55	30.17	1.00

Refine Model – Remove Nonsignificant Factors

■ **TABLE 6.7** (*Continued*)

Response: Etch rate
ANOVA for Selected Factorial Model
Analysis of variance table [Partial sum of squares]

Source	Sum of Squares	DF	Mean Square	*F* Value	Prob > *F*
Model	5.106E+005	3	1.702E+005	97.91	<0.0001
A	*41310.56*	*1*	*41310.56*	*23.77*	*0.0004*
C	*3.749E+005*	*1*	*3.749E+005*	*215.66*	*<0.0001*
AC	*94402.56*	*1*	*94402.56*	*54.31*	*<0.0001*
Residual	20857.75	12	1738.15		
Lack of Fit	*2837.25*	*4*	*709.31*	*0.31*	*0.8604*
Pure Error	*18020.50*	*8*	*2252.56*		
Cor Total	5.314E+005	15			

Std. Dev.	41.69	R-Squared	0.9608
Mean	776.06	Adj R-Squared	0.9509
C.V.	5.37	Pred R-Squared	0.9302
PRESS	37080.44	Adeq Precision	22.055

Factor	Coefficient Estimate	DF	Standard Error	95% CI Low	95% CI High	VIF
Intercept	776.06	1	10.42	753.35	798.77	
A-Gap	−50.81	1	10.42	−73.52	28.10	1.00
C-Power	153.06	1	10.42	130.35	175.77	1.00
AC	−76.81	1	10.42	−99.52	−54.10	1.00

Final Equation in Terms of Coded Factors:

Etch rate	=
+776.06	
−50.81	* *A*
+153.06	* *C*
−76.81	* *A* * *C*

Final Equation in Terms of Actual Factors:

Etch rate	=
−5415.37500	
+4354.68750	* Gap
+21.48500	* Power
−15.36250	* Gap * Power

Model Coefficients – Reduced Model

Factor	Coefficient Estimate	DF	Standard Error	95% CI Low	95% CI High	VIF
Intercept	776.06	1	10.42	753.35	798.77	
A-Gap	−50.81	1	10.42	−73.52	28.10	1.00
C-Power	153.06	1	10.42	130.35	175.77	1.00
AC	−76.81	1	10.42	−99.52	−54.10	1.00

Model Summary Statistics for Reduced Model

- R^2 and adjusted R^2

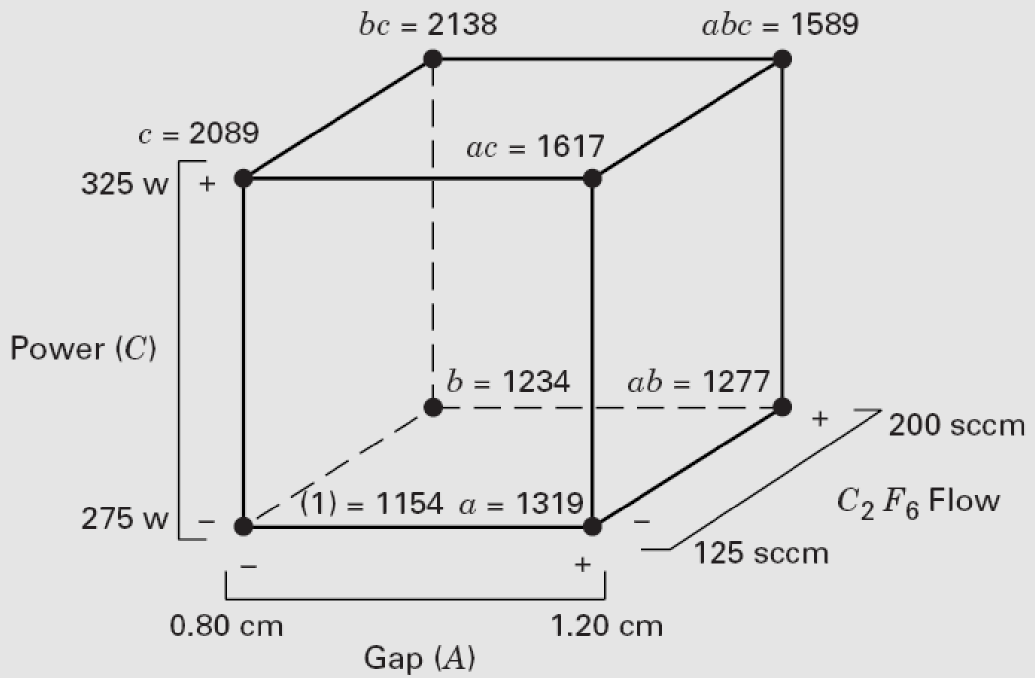
$$R^2 = \frac{SS_{Model}}{SS_T} = \frac{5.106 \times 10^5}{5.314 \times 10^5} = 0.9608$$

$$R^2_{Adj} = 1 - \frac{SS_E / df_E}{SS_T / df_T} = 1 - \frac{20857.75/12}{5.314 \times 10^5 / 15} = 0.9509$$

- R^2 for prediction (based on PRESS)

$$R^2_{\text{Pred}} = 1 - \frac{PRESS}{SS_T} = 1 - \frac{37080.44}{5.314 \times 10^5} = 0.9302$$

Model Interpretation



■ **FIGURE 6.6** **The 2^3 design for the plasma etch experiment for Example 6.1**

Cube plots are often useful visual displays of experimental results

The General 2^k Factorial Design

- Section 6-4, pg. 253, Table 6-9, pg. 25
- There will be k main effects, and

$$\binom{k}{2} \text{ two-factor interactions}$$

$$\binom{k}{3} \text{ three-factor interactions}$$

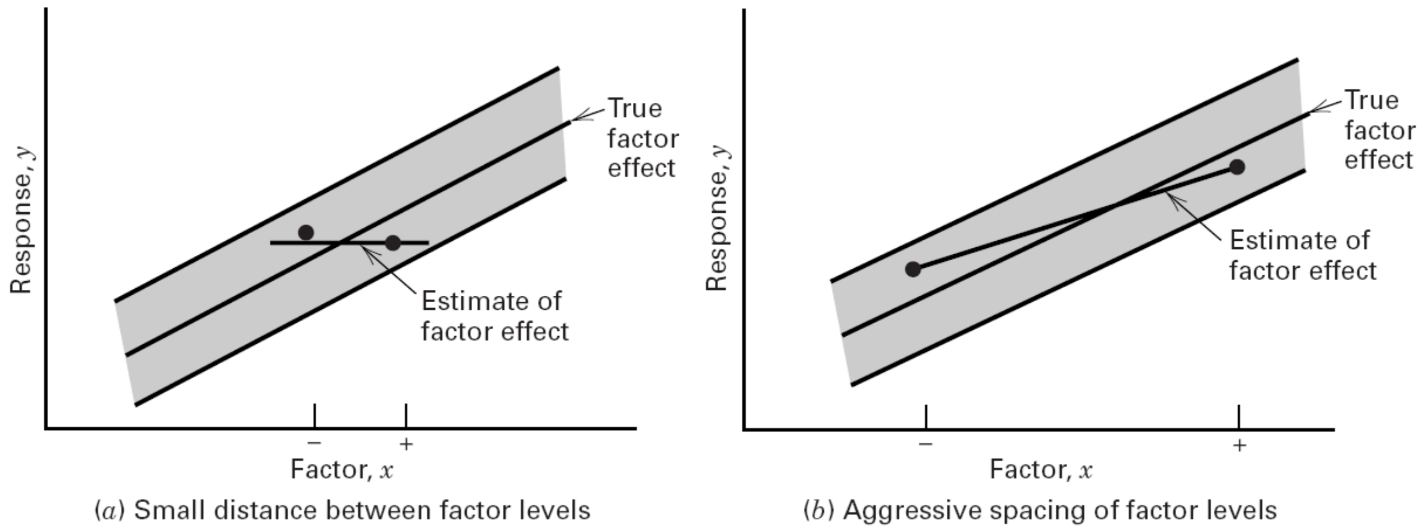
$$\vdots$$

$$1\ k - \text{factor interaction}$$

6.5 Unreplicated 2^k Factorial Designs

- These are 2^k factorial designs with **one observation** at each corner of the "cube"
- An unreplicated 2^k factorial design is also sometimes called a "**single replicate**" of the 2^k
- These designs are very widely used
- Risks…if there is only one observation at each corner, is there a chance of unusual response observations spoiling the results?
- Modeling "noise"?

Spacing of Factor Levels in the Unreplicated 2^k Factorial Designs



■ **FIGURE 6.9** **The impact of the choice of factor levels in an unreplicated design**

If the factors are spaced too closely, it increases the chances that the noise will overwhelm the signal in the data

More aggressive spacing is usually best

Unreplicated 2^k Factorial Designs

- Lack of replication causes potential **problems** in statistical testing
  - Replication admits an estimate of "pure error" (a better phrase is an **internal estimate** of error)
  - With no replication, fitting the full model results in zero degrees of freedom for error
- Potential **solutions** to this problem
  - Pooling high-order interactions to estimate error
  - **Normal probability plotting** of effects (Daniels, 1959)
  - Other methods…see text

Example of an Unreplicated 2^k Design

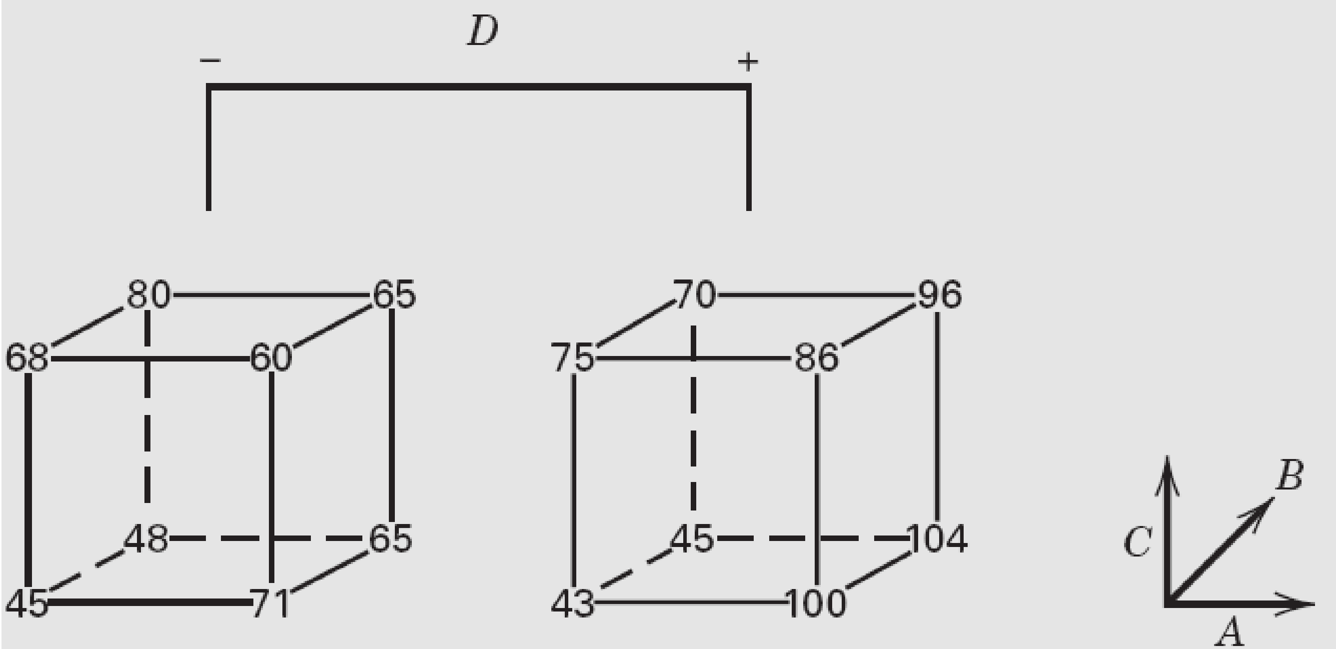
- A 2^4 factorial was used to investigate the effects of four factors on the filtration rate of a resin
- The factors are A = temperature, B = pressure, C = mole ratio, D= stirring rate
- Experiment was performed in a pilot plant

The Resin Plant Experiment

■ **TABLE 6.10**
Pilot Plant Filtration Rate Experiment

Run Number	Factor *A*	*B*	*C*	*D*	Run Label	Filtration Rate (gal/h)
1	−	−	−	−	(1)	45
2	+	−	−	−	*a*	71
3	−	+	−	−	*b*	48
4	+	+	−	−	*ab*	65
5	−	−	+	−	*c*	68
6	+	−	+	−	*ac*	60
7	−	+	+	−	*bc*	80
8	+	+	+	−	*abc*	65
9	−	−	−	+	*d*	43
10	+	−	−	+	*ad*	100
11	−	+	−	+	*bd*	45
12	+	+	−	+	*abd*	104
13	−	−	+	+	*cd*	75
14	+	−	+	+	*acd*	86
15	−	+	+	+	*bcd*	70
16	+	+	+	+	*abcd*	96

The Resin Plant Experiment



■ **FIGURE 6.10** **Data from the pilot plant filtration rate experiment for Example 6.2**

■ **TABLE 6.11**

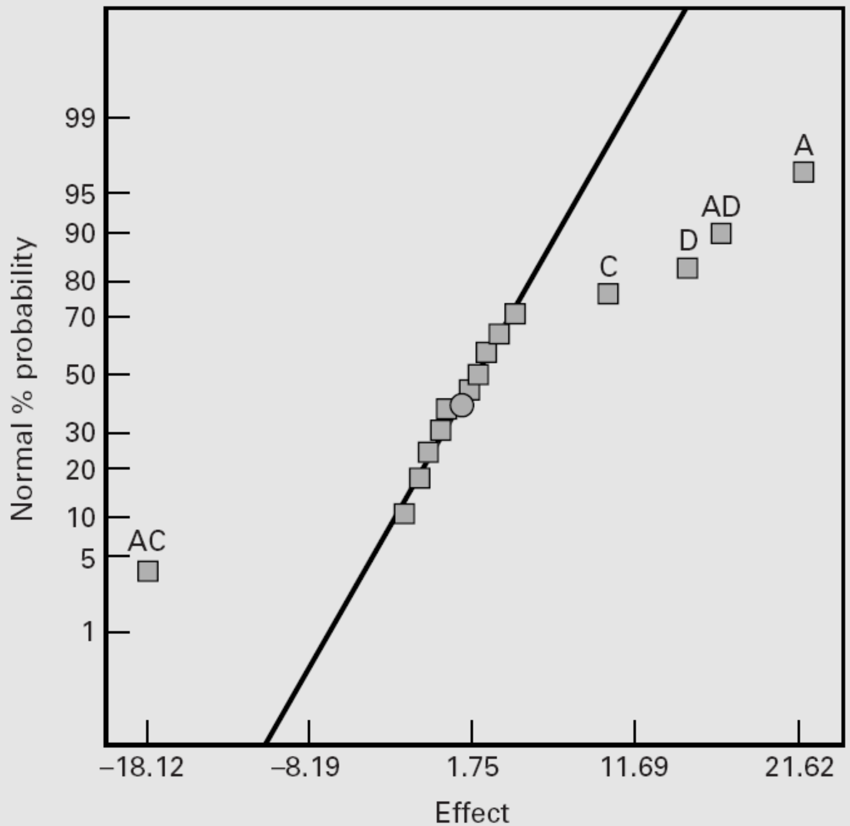
Contrast Constants for the 2^4 Design

	A	*B*	*AB*	*C*	*AC*	*BC*	*ABC*	*D*	*AD*	*BD*	*ABD*	*CD*	*ACD*	*BCD*	*ABCD*
(1)	−	−	+	−	+	+	−	−	+	+	−	+	−	−	+
a	+	−	−	−	−	+	+	−	−	+	+	+	+	−	−
b	−	+	−	−	+	−	+	−	+	−	+	+	−	+	−
ab	+	+	+	−	−	−	−	−	−	−	−	+	+	+	+
c	−	−	+	+	−	−	+	−	+	+	−	−	+	+	−
ac	+	−	−	+	+	−	−	−	−	+	+	−	−	+	+
bc	−	+	−	+	−	+	−	−	+	−	+	−	+	−	+
abc	+	+	+	+	+	+	+	−	−	−	−	−	−	−	−
d	−	−	+	−	+	+	−	+	−	−	+	−	+	+	−
ad	+	−	−	−	−	+	+	+	+	−	−	−	−	+	+
bd	−	+	−	−	+	−	+	+	−	+	−	−	+	−	+
abd	+	+	+	−	−	−	−	+	+	+	+	−	−	−	−
cd	−	−	+	+	−	−	+	+	−	−	+	+	−	−	+
acd	+	−	−	+	+	−	−	+	+	−	−	+	+	−	−
bcd	−	+	−	+	−	+	−	+	−	+	−	+	−	+	−
abcd	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+

Estimates of the Effects

■ **TABLE 6.12**
Factor Effect Estimates and Sums of Squares for the 2^4 Factorial in Example 6.2

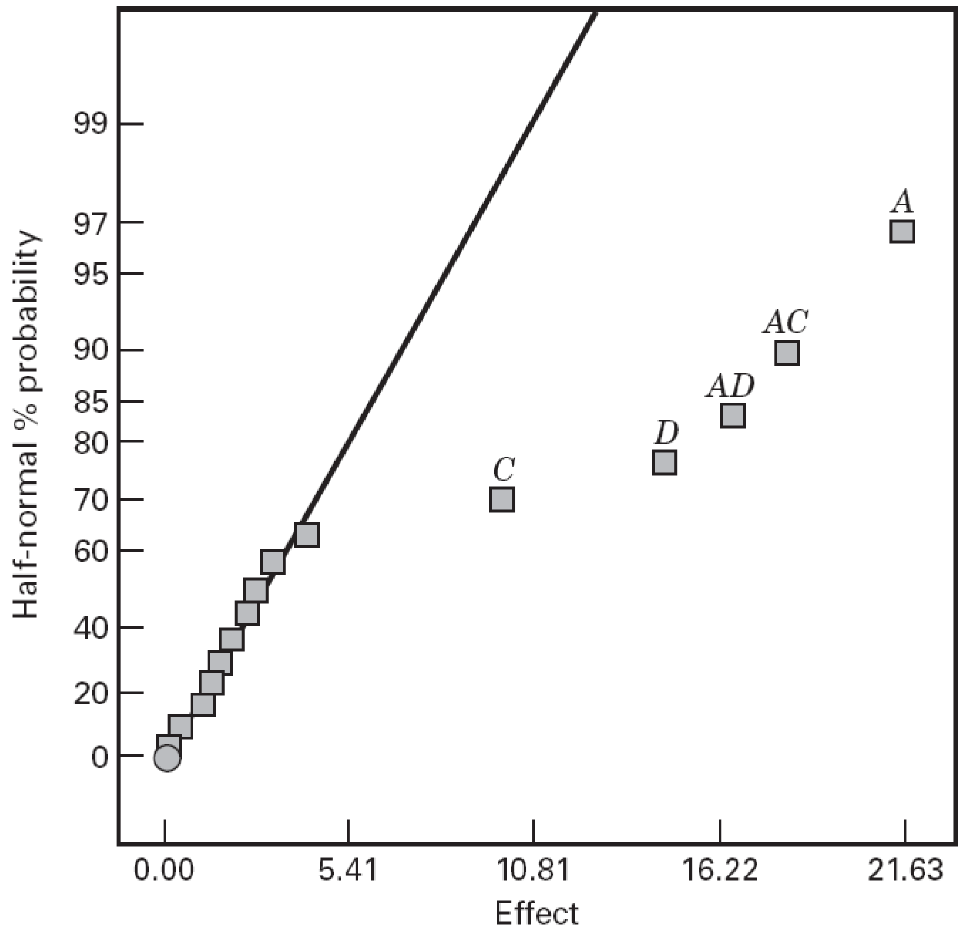
Model Term	Effect Estimate	Sum of Squares	Percent Contribution
A	21.625	1870.56	32.6397
B	3.125	39.0625	0.681608
C	9.875	390.062	6.80626
D	14.625	855.563	14.9288
AB	0.125	0.0625	0.00109057
AC	−18.125	1314.06	22.9293
AD	16.625	1105.56	19.2911
BC	2.375	22.5625	0.393696
BD	−0.375	0.5625	0.00981515
CD	−1.125	5.0625	0.0883363
ABC	1.875	14.0625	0.245379
ABD	4.125	68.0625	1.18763
ACD	−1.625	10.5625	0.184307
BCD	−2.625	27.5625	0.480942
ABCD	1.375	7.5625	0.131959



■ **FIGURE 6.11** **Normal probability plot of the effects for the 2^4 factorial in Example 6.2**

The Half-Normal Probability Plot of Effects

■ **FIGURE 6.15**
Half-normal plot of the factor effects from Example 6.2



Design Projection: ANOVA Summary for the Model as a 2^3 in Factors A, C, and D

■ **TABLE 6.13**

Analysis of Variance for the Pilot Plant Filtration Rate Experiment in *A*, *C*, and *D*

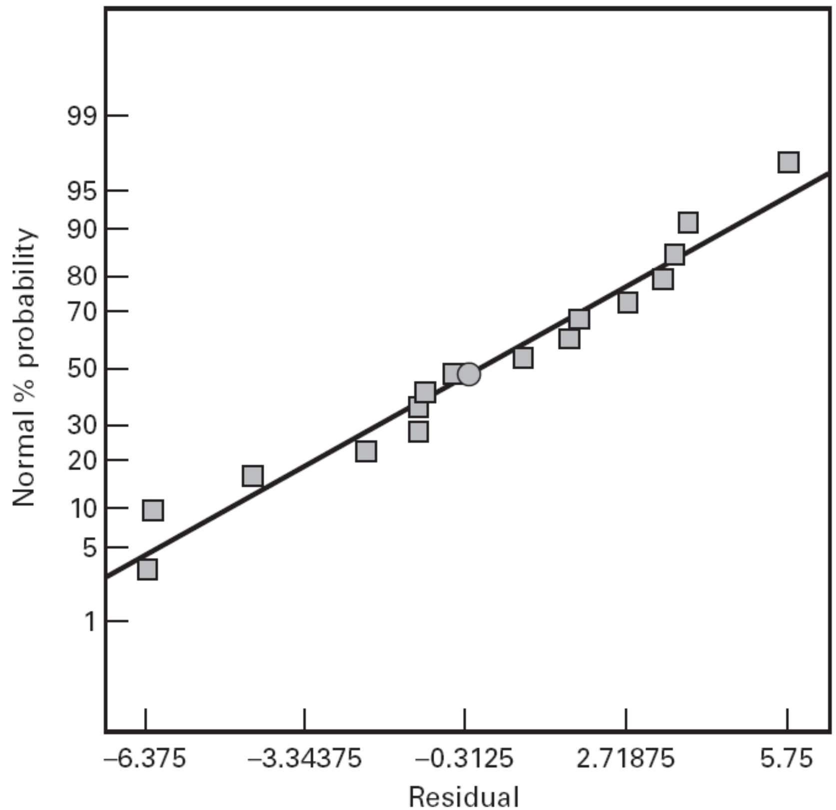
Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	*P*-Value
A	1870.56	1	1870.56	83.36	<0.0001
C	390.06	1	390.06	17.38	<0.0001
D	855.56	1	855.56	38.13	<0.0001
AC	1314.06	1	1314.06	58.56	<0.0001
AD	1105.56	1	1105.56	49.27	<0.0001
CD	5.06	1	5.06	<1	
ACD	10.56	1	10.56	<1	
Error	179.52	8	22.44		
Total	5730.94	15			

The Regression Model

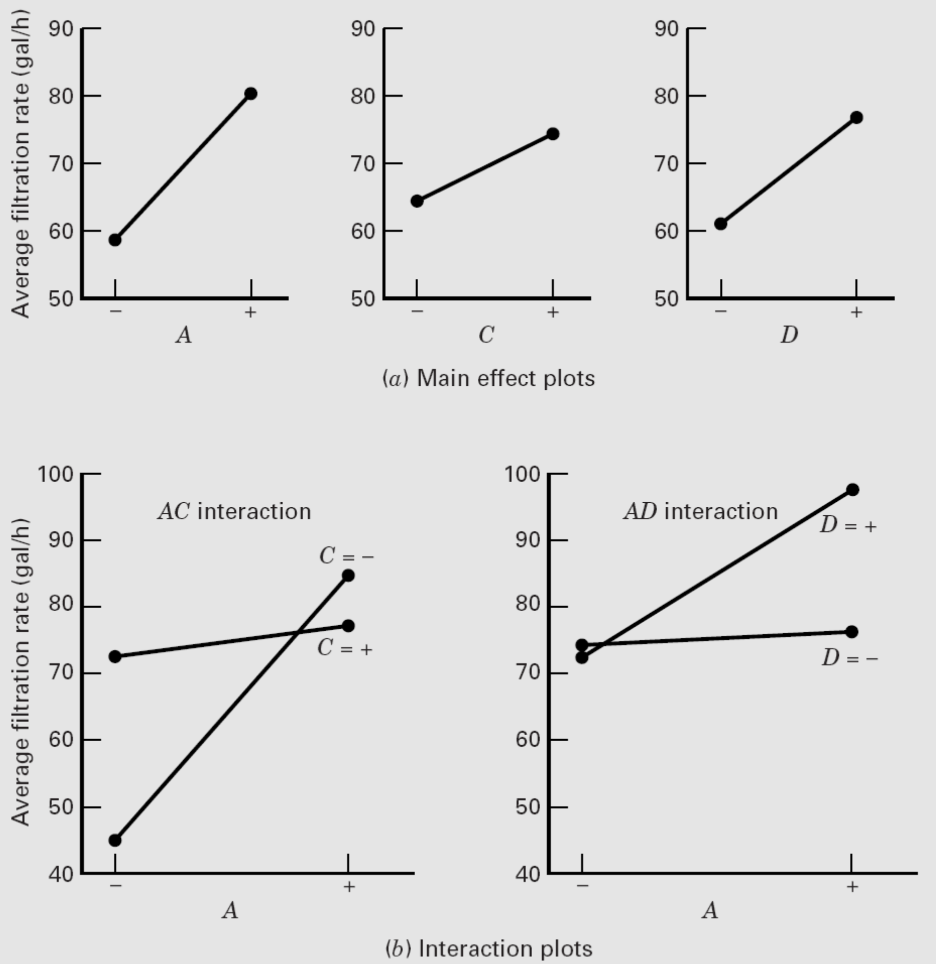
$$\hat{y} = 70.06 + \left(\frac{21.625}{2}\right)x_1 + \left(\frac{9.875}{2}\right)x_3 + \left(\frac{14.625}{2}\right)x_4 - \left(\frac{18.125}{2}\right)x_1x_3 + \left(\frac{16.625}{2}\right)x_1x_4$$

Model Residuals are Satisfactory

■ **FIGURE 6.13**
Normal probability plot of residuals for Example 6.2

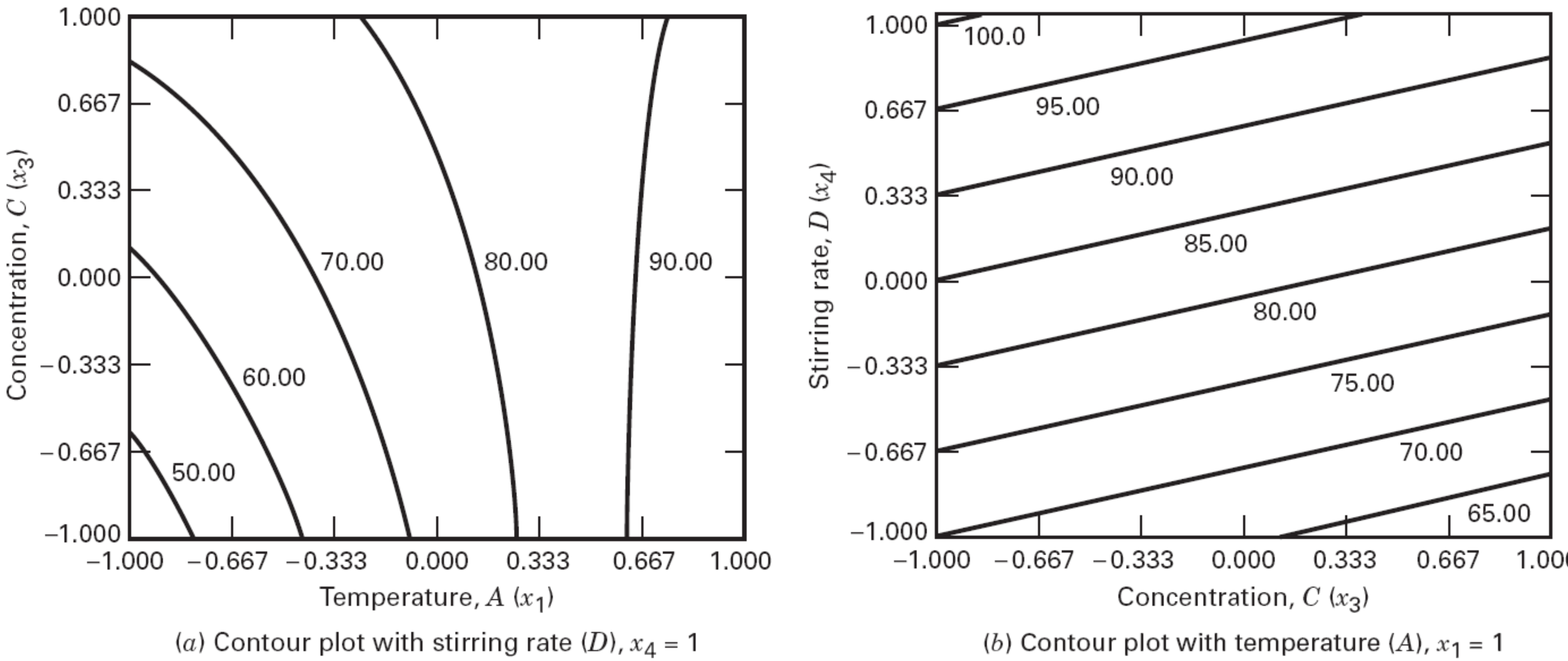


Model Interpretation – Main Effects and Interactions



■ **FIGURE 6.12** **Main effect and interaction plots for Example 6.2**

Model Interpretation – Response Surface Plots



■ **FIGURE 6.14 Contour plots of filtration rate, Example 6.2**

With concentration at either the low or high level, high temperature and high stirring rate results in high filtration rates

■ TABLE 6.14

JMP Screening Platform Output for Example 6.2

Response Y

Summary of Fit

RSquare	1
RSquare Adj	-
Root Mean Square Error	-
Mean of Response	70.0625
Observations (or Sum Wgts)	16

Sorted Parameter Estimates

Term	Estimate	Relative Std Error	Pseudo t-Ratio	Pseudo t-Ratio	Pseudo p-Value
Temp	10.8125	0.25	8.24		0.0004*
Temp*Conc	−9.0625	0.25	−6.90		0.0010*
Temp*StirR	8.3125	0.25	6.33		0.0014*
StirR	7.3125	0.25	5.57		0.0026*
Conc	4.9375	0.25	3.76		0.0131*
Temp*Pressure*StirR	2.0625	0.25	1.57		0.1769
Pressure	1.5625	0.25	1.19		0.2873
Pressure*Conc*StirR	−1.3125	0.25	−1.00		0.3632
Pressure*Conc	1.1875	0.25	0.90		0.4071
Temp*Pressure*Conc	0.9375	0.25	0.71		0.5070
Temp*Conc*StirR	−0.8125	0.25	−0.62		0.5630
Temp*Pressure*Conc*StirR	0.6875	0.25	0.52		0.6228
Conc*StirR	−0.5625	0.25	−0.43		0.6861
Pressure*StirR	−0.1875	0.25	−0.14		0.8920
Temp*Pressure	0.0625	0.25	0.05		0.9639

No error degrees of freedom, so ordinary tests uncomputable. Relative Std Error corresponds to residual standard error of 1. Pseudo t-Ratio and p-Value calculated using Lenth PSE = 1.3125 and DFE = 5

Effect Screening

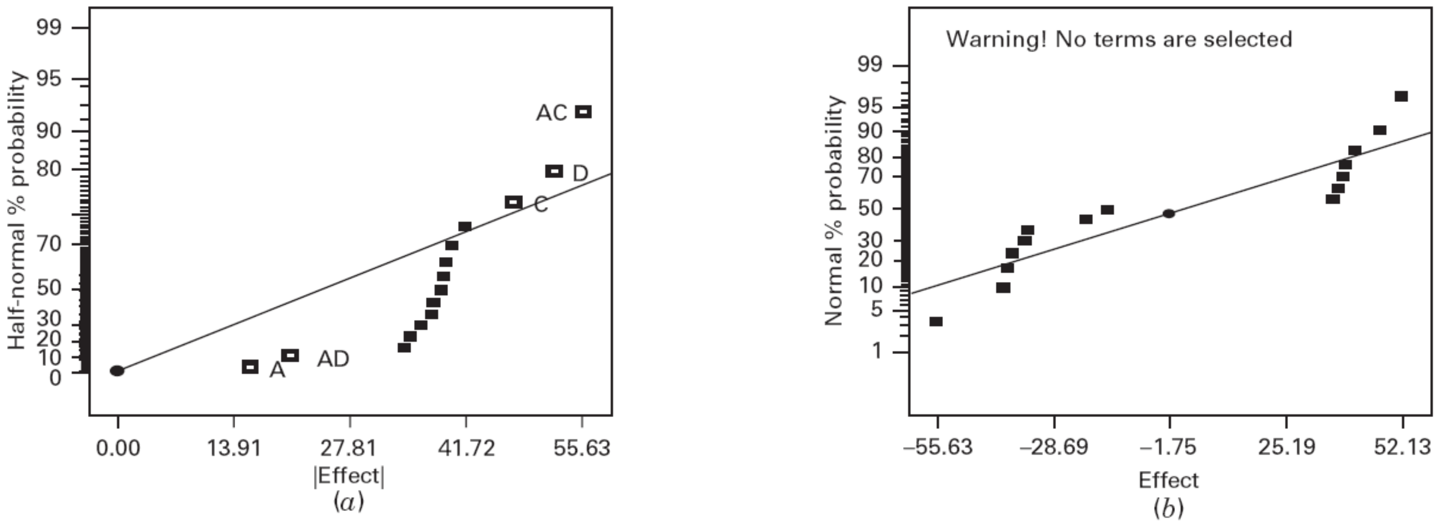
The parameter estimates have equal variances.
The parameter estimates are not correlated.

Lenth PSE

1.3125

Orthog t Test used Pseudo Standard Error

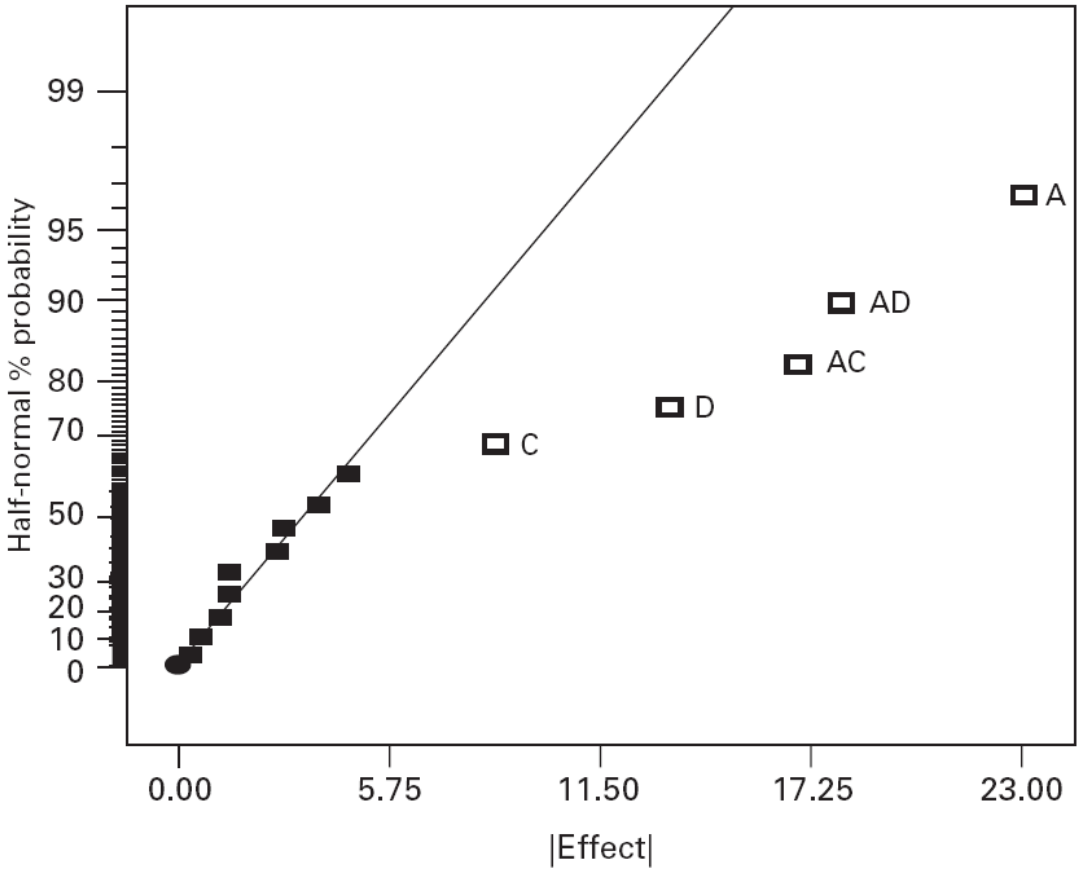
Outliers: suppose that *cd* = 375 (instead of 75)



■ **FIGURE 6.17** **The effect of outliers. (*a*) Half-normal probability plot. (*b*) Normal probability plot**

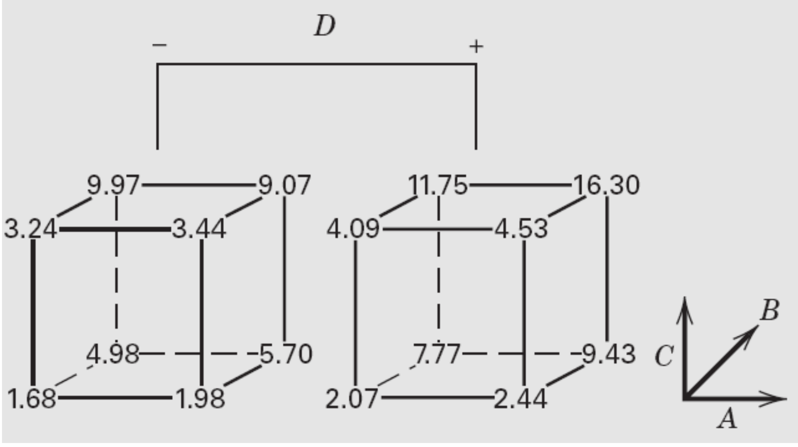
Dealing with Outliers

- Replace with an estimate
- Make the highest-order interaction zero
- In this case, estimate *cd* such that $ABCD = 0$
- Analyze only the data you have
- Now the design isn't orthogonal
- Consequences?



■ **FIGURE 6.18**
Analysis of Example 6.2 with an outlier removed

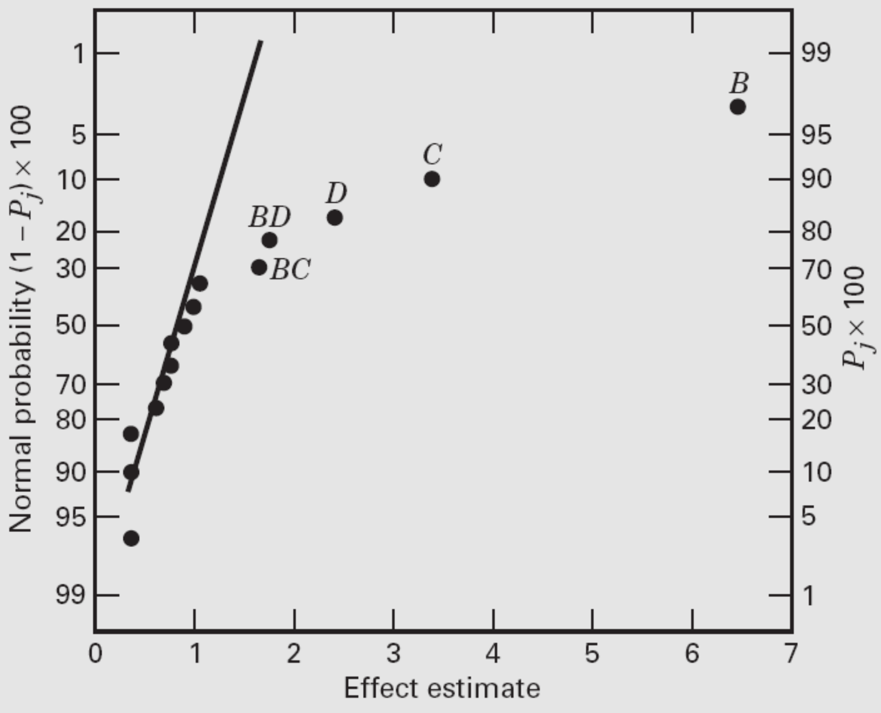
The Drilling Experiment Example 6.3



■ FIGURE 6.19 Data from the drilling experiment of Example 6.3

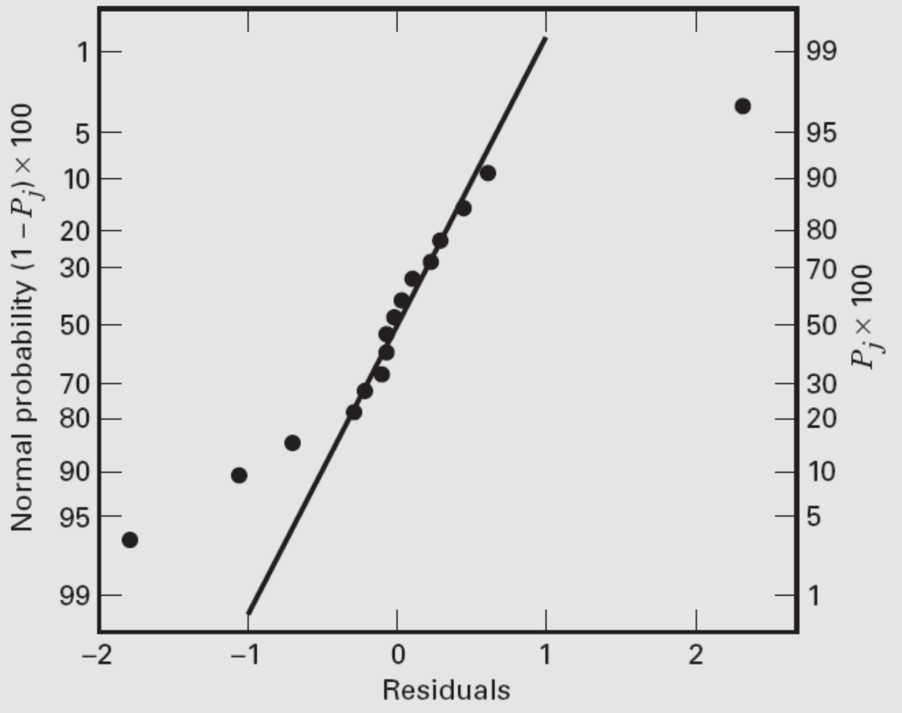
A = drill load, *B* = flow, *C* = speed, *D* = type of mud, *y* = advance rate of the drill

Normal Probability Plot of Effects – The Drilling Experiment

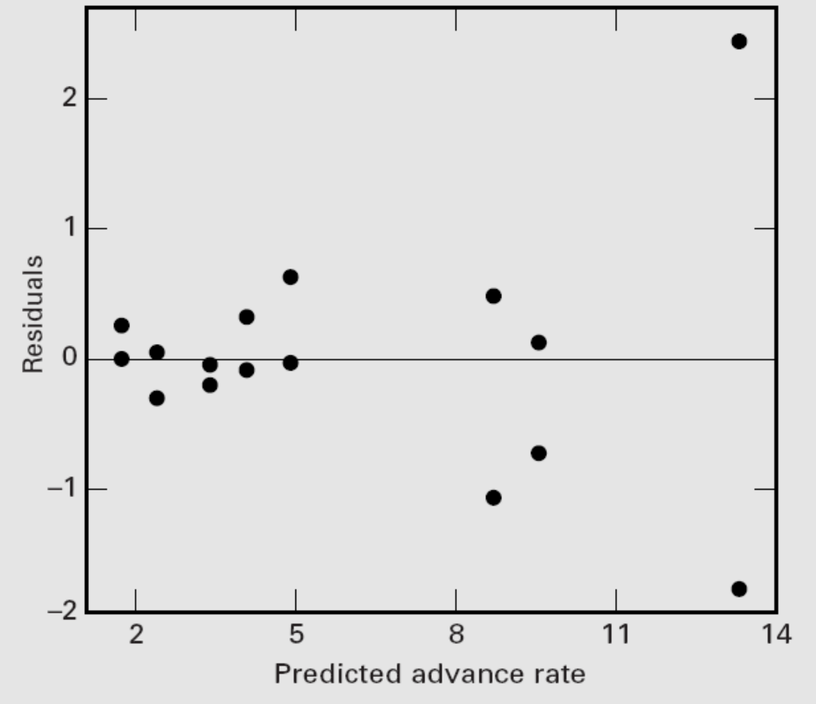


■ **FIGURE 6.20** **Normal probability plot of effects for Example 6.3**

Residual Plots



■ **FIGURE 6.21** **Normal probability plot of residuals for Example 6.3**



■ **FIGURE 6.22** **Plot of residuals versus predicted advance rate for Example 6.3**

Residual Plots

- The residual plots indicate that there are problems with the **equality of variance** assumption
- The usual approach to this problem is to employ a **transformation** on the response
- **Power family** transformations are widely used

$$y^* = y^\lambda$$

- Transformations are typically performed to
  - Stabilize variance
  - Induce at least approximate normality
  - Simplify the model

Selecting a Transformation

- **Empirical** selection of lambda
- Prior (theoretical) knowledge or experience can often suggest the form of a transformation
- **Analytical** selection of lambda…the Box-Cox (1964) method (simultaneously estimates the model parameters and the transformation parameter lambda)
- Box-Cox method implemented in Design-Expert

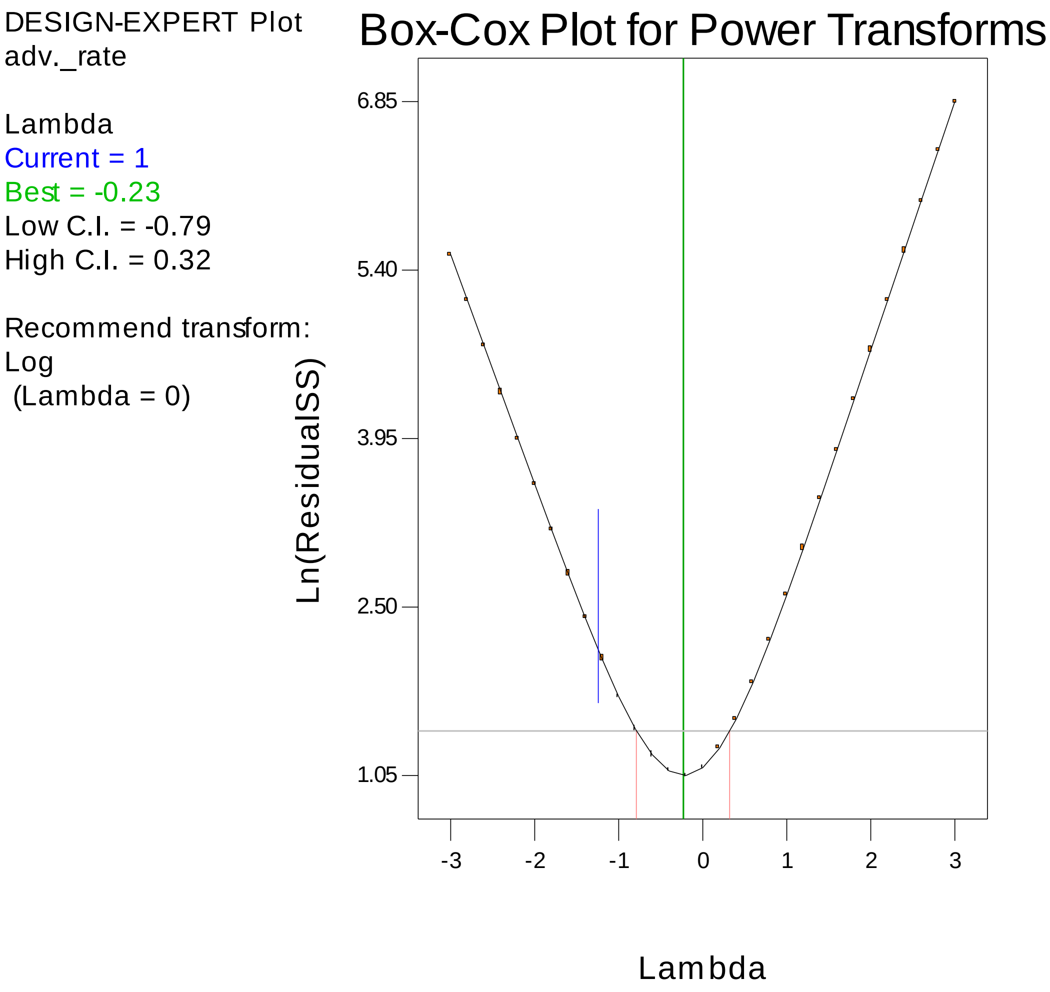
We have noted that the **power family** of transformations $y^* = y^\lambda$ is very useful, where λ is the parameter of the transformation to be determined (e.g., $\lambda = \frac{1}{2}$ means use the square root of the original response). Box and Cox (1964) have shown how the transformation parameter λ may be estimated simultaneously with the other model parameters (overall mean and treatment effects). The theory underlying their method uses the method of maximum likelihood. The actual computational procedure consists of performing, for various values of λ, a standard analysis of variance on

$$y^{(\lambda)} = \begin{cases} \dfrac{y^\lambda - 1}{\lambda \dot{y}^{\lambda-1}} & \lambda \neq 0 \\ \dot{y} \ln \ y & \lambda = 0 \end{cases} \tag{15.1}$$

where $\dot{y} = \ln^{-1}[(1/n) \sum \ln y]$ is the geometric mean of the observations. The maximum likelihood estimate of λ is the value for which the error sum of squares, say $SS_E(\lambda)$, is a minimum. This value of λ is usually found by plotting a graph of $SS_E(\lambda)$ versus λ and then reading the value of λ that minimizes $SS_E(\lambda)$ from the graph. Usually, between 10 and 20 values of λ are sufficient for estimating the optimum value. A second iteration using a finer mesh of values can be performed if a more accurate estimate of λ is necessary.

Notice that we *cannot* select the value of λ by *directly* comparing the error sums of squares from analyses of variance on y^λ because for each value of λ the error sum of squares is measured on a different scale. Furthermore, a problem arises in y when $\lambda = 0$, namely, as λ approaches zero, y^λ approaches unity. That is, when $\lambda = 0$, all the response values are a constant. The component $(y^\lambda - 1)/\lambda$ of Equation 15-1 alleviates this problem because as λ tends to zero, $(y^\lambda - 1)/\lambda$ goes to a limit of $\ln y$. The divisor component $\dot{y}^{\lambda-1}$ in Equation 15-1 rescales the responses so that the error sums of squares are directly comparable.

The Box-Cox Method

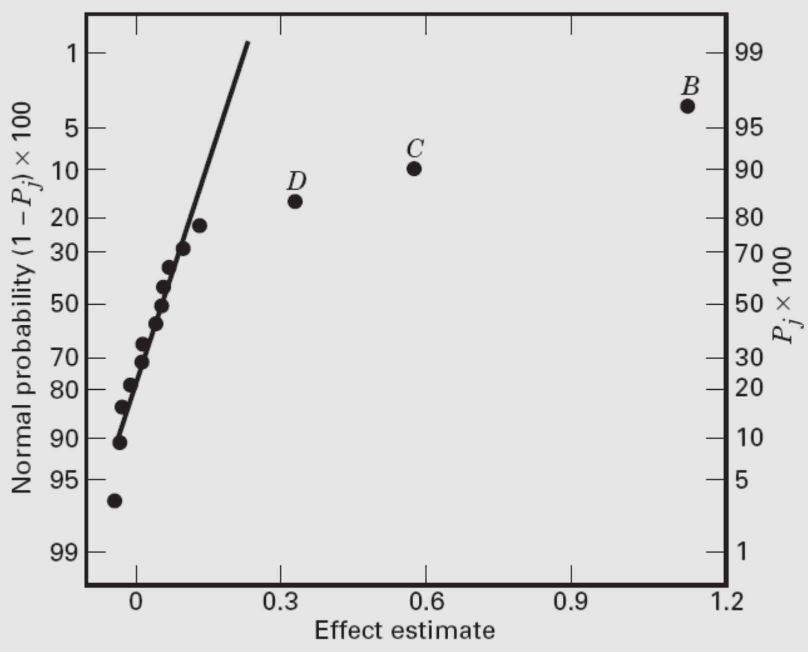


A **log** transformation is recommended

The procedure provides a **confidence interval** on the transformation parameter lambda

If unity is included in the confidence interval, no transformation would be needed

Effect Estimates Following the Log Transformation



■ **FIGURE 6.23** Normal probability plot of effects for Example 6.3 following log transformation

Three main effects are large

No indication of large interaction effects

What happened to the interactions?

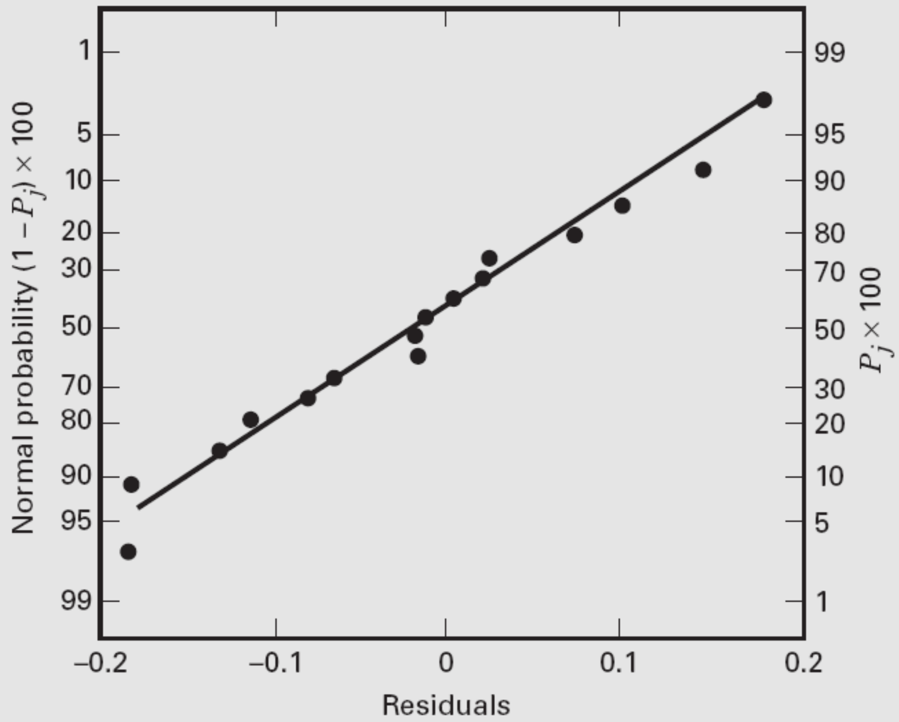
ANOVA Following the Log Transformation

■ **TABLE 6.16**

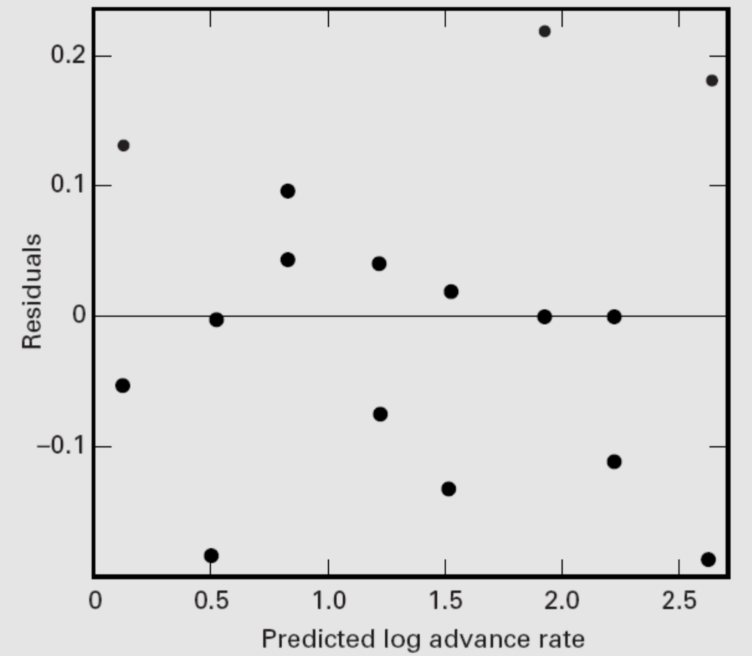
Analysis of Variance for Example 6.3 following the Log Transformation

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	*P*-Value
B (Flow)	5.345	1	5.345	381.79	<0.0001
C (Speed)	1.339	1	1.339	95.64	<0.0001
D (Mud)	0.431	1	0.431	30.79	<0.0001
Error	0.173	12	0.014		
Total	7.288	15			

Following the Log Transformation



■ **FIGURE 6.24** **Normal probability plot of residuals for Example 6.3 following log transformation**



■ **FIGURE 6.25** **Plot of residuals versus predicted advance rate for Example 6.3 following log transformation**

The Log Advance Rate Model

- Is the log model "better"?
- We would generally prefer a **simpler model** in a transformed scale to a more complicated model in the original metric
- What happened to the interactions?
- Sometimes transformations provide insight into the underlying **mechanism**

Other Examples of Unreplicated 2^k Designs

- The sidewall panel experiment (Example 6.4, pg. 274)
  - Two factors affect the mean number of defects
  - A third factor affects variability
  - Residual plots were useful in identifying the dispersion effect
- The oxidation furnace experiment (Example 6.5, pg. 245)
  - Replicates versus repeat (or duplicate) observations?
  - Modeling within-run variability

- Example 6.6, Credit Card Marketing, page 278
  - Using DOX in marketing and marketing research, a growing application
  - Analysis is with the JMP screening platform

Other Analysis Methods for Unreplicated 2^k Designs

- Lenth's method (see text, pg. 262)
  - Analytical method for testing effects, uses an estimate of error formed by pooling small contrasts
  - Some adjustment to the critical values in the original method can be helpful
  - Probably most useful as a supplement to the normal probability plot
- Conditional inference charts (pg. 264)

Overview of Lenth's method

Suppose that we have m contrasts of interest, say $c_1, c_2, \ldots, c_m$. If the design is an unreplicated 2^k factorial design, these contrasts correspond to the $m = 2^k - 1$ factor effect estimates. The basis of Lenth's method is to estimate the variance of a contrast from the smallest (in absolute value) contrast estimates. Let

$$s_0 = 1.5 \times \text{median}(|c_j|)$$

and

$$PSE = 1.5 \times \text{median}(|c_j| : |c_j| < 2.5 s_0)$$

PSE is called the "pseudo standard error," and Lenth shows that it is a reasonable estimator of the contrast variance when there are not many active (significant) effects.

For an individual contrast, compare to the margin of error

$$ME = t_{0.025,d} \times PSE$$

where the degrees of freedom are defined as $d = m/3$. For inference on a group of contrasts Lenth suggests using the **simultaneous margin of error**

$$SME = t_{\gamma,d} \times PSE$$

where the percentage point of the t distribution used is $\gamma = 1 - (1 + 0.95^{1/m})/2$.

To illustrate Lenth's method, consider the 2^4 experiment in Example 6.2. The calculations result in $s_0 = 1.5 \times |-2.625| = 3.9375$ and $2.5 \times 3.9375 = 9.84375$, so

$$PSE = 1.5 \times |1.75| = 2.625$$

$$ME = 2.571 \times 2.625 = 6.75$$

$$SME = 5.219 \times 2.625 = 13.70$$

Now consider the effect estimates in Table 6.12. The *SME* criterion would indicate that the four largest effects (in magnitude) are significant because their effect estimates exceed *SME*. The main effect of *C* is significant according to the *ME* criterion, but not with respect to *SME*. However, because the *AC* interaction is clearly important, we would probably include *C* in the list of significant effects. Notice that in this example, Lenth's method has produced the same answer that we obtained previously from examination of the normal probability plot of effects.

Adjusted multipliers for Lenth's method

Suggested because the original method makes too many type I errors, especially for small designs (few contrasts)

Number of Contrasts	7	15	31
Original *ME*	3.764	2.571	2.218
Adjusted *ME*	2.295	2.140	2.082
Original *SME*	9.008	5.219	4.218
Adjusted *SME*	4.891	4.163	4.030

Simulation was used to find these adjusted multipliers

Lenth's method is a nice supplement to the normal probability plot of effects

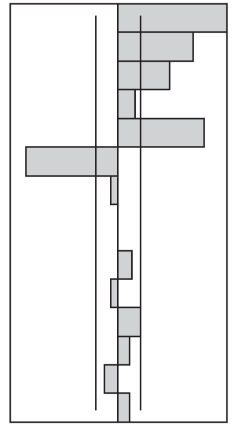
JMP has an excellent implementation of Lenth's method in the screening platform

■ **TABLE 6.14**

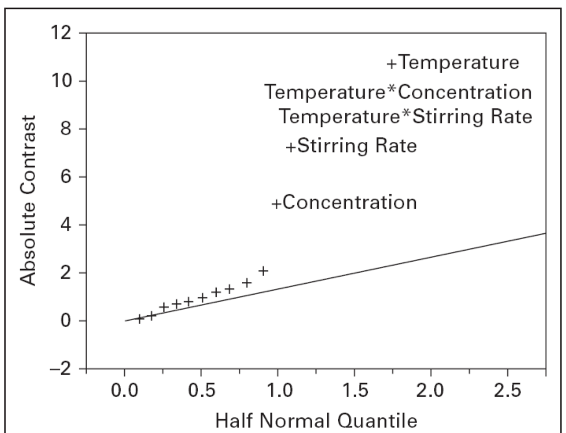
JMP Screening Platform Output for Example 6.2

Screening for Filtration Rate Contrasts

Term	Contrast	Lenth *t*-Ratio	Individual *p*-value	Simultaneous *p*-value
Temperature	10.8125	8.24	0.0006*	0.0037*
Stirring Rate	7.3125	5.57	0.0029*	0.0168*
Concentration	4.9375	3.76	0.0096*	0.0755
Pressure	1.5625	1.19	0.2280	0.9611
Temperature *Stirring Rate	8.3125	6.33	0.0014*	0.0102*
Temperature *Concentration	−9.0625	−6.90	0.0011*	0.0072*
Stirring Rate *Concentration	−0.5625	−0.43	0.7032	1.0000
Temperature *Pressure	0.0625	0.05	0.9671	1.0000
Stirring Rate *Pressure	−0.1875	−0.14	0.8995	1.0000
Concentration *Pressure	1.1875	0.90	0.3471	0.9990
Temperature *Stirring Rate *Concentration	−0.8125	−0.62	0.5820	1.0000
Temperature *Stirring Rate* Pressure	2.0625	1.57	0.1272	0.7666
Temperature *Concentration *Pressure	0.9375	0.71	0.4580	1.0000
Stirring Rate *Concentration *Pressure	−1.3125	−1.00	0.3055	0.9945
Temperature *Stirring Rate *Concentration *Pressure	0.6875	0.52	0.6435	1.0000



Half Normal Plot



Lenth PSE = 1.3125

P-Values derived from a simulation of 10000 Lenth *t* ratios

The 2^k design and design optimality

The model parameter estimates in a 2^k design (and the effect estimates) are least squares estimates. For example, for a 2^2 design the model is

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \varepsilon$$

$$\begin{aligned}
(1) &= \beta_0 + \beta_1(-1) + \beta_2(-1) + \beta_{12}(-1)(-1) + \varepsilon_1 \\
a &= \beta_0 + \beta_1(1) + \beta_2(-1) + \beta_{12}(1)(-1) + \varepsilon_2 \\
b &= \beta_0 + \beta_1(-1) + \beta_2(1) + \beta_{12}(-1)(1) + \varepsilon_3 \\
ab &= \beta_0 + \beta_1(1) + \beta_2(1) + \beta_{12}(1)(1) + \varepsilon_4
\end{aligned}$$

← The four observations from a 2^2 design

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon},\ \mathbf{y} = \begin{bmatrix} (1) \\ a \\ b \\ ab \end{bmatrix}, \mathbf{X} = \begin{bmatrix} 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 \end{bmatrix}, \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_{12} \end{bmatrix}, \boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \end{bmatrix}$$

The least squares estimate of β is

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$$

$$= \begin{bmatrix} 4 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 4 \end{bmatrix}^{-1} \begin{bmatrix} (1)+a+b+ab \\ a+ab-b-(1) \\ b+ab-a-(1) \\ (1)-a-b+ab \end{bmatrix}$$

The "usual" contrasts

The $\mathbf{X}'\mathbf{X}$ matrix is diagonal – consequences of an orthogonal design

$$\begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \hat{\beta}_2 \\ \hat{\beta}_{12} \end{bmatrix} = \frac{1}{4}\mathbf{I}_4 \begin{bmatrix} (1)+a+b+ab \\ a+ab-b-(1) \\ b+ab-a-(1) \\ (1)-a-b+ab \end{bmatrix} = \begin{bmatrix} \frac{(1)+a+b+ab}{4} \\ \frac{a+ab-b-(1)}{4} \\ \frac{b+ab-a-(1)}{4} \\ \frac{(1)-a-b+ab}{4} \end{bmatrix}$$

The regression coefficient estimates are exactly half of the 'usual" effect estimates

The matrix $\mathbf{X}'\mathbf{X}$ has interesting and useful properties:

$$V(\hat{\beta}) = \sigma^2 (\text{diagonal element of } (\mathbf{X}'\mathbf{X})^{-1})$$

$$= \frac{\sigma^2}{4}$$

← Minimum possible value for a four-run design

$$|(\mathbf{X}'\mathbf{X})| = 256$$

← Maximum possible value for a four-run design

Notice that these results depend on both the design that you have chosen and the model

What about predicting the response?

$$V[\hat{y}(x_1, x_2)] = \sigma^2 \mathbf{x}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}$$

$$\mathbf{x}' = [1, x_1, x_2, x_1 x_2]$$

$$V[\hat{y}(x_1, x_2)] = \frac{\sigma^2}{4}(1 + x_1^2 + x_2^2 + x_1^2 x_2^2)$$

The maximum prediction variance occurs when $x_1 = \pm 1, x_2 = \pm 1$

$$V[\hat{y}(x_1, x_2)] = \sigma^2$$

The prediction variance when $x_1 = x_2 = 0$ is

$$V[\hat{y}(x_1, x_2)] = \frac{\sigma^2}{4}$$

What about **average** prediction variance over the design space?

Average prediction variance

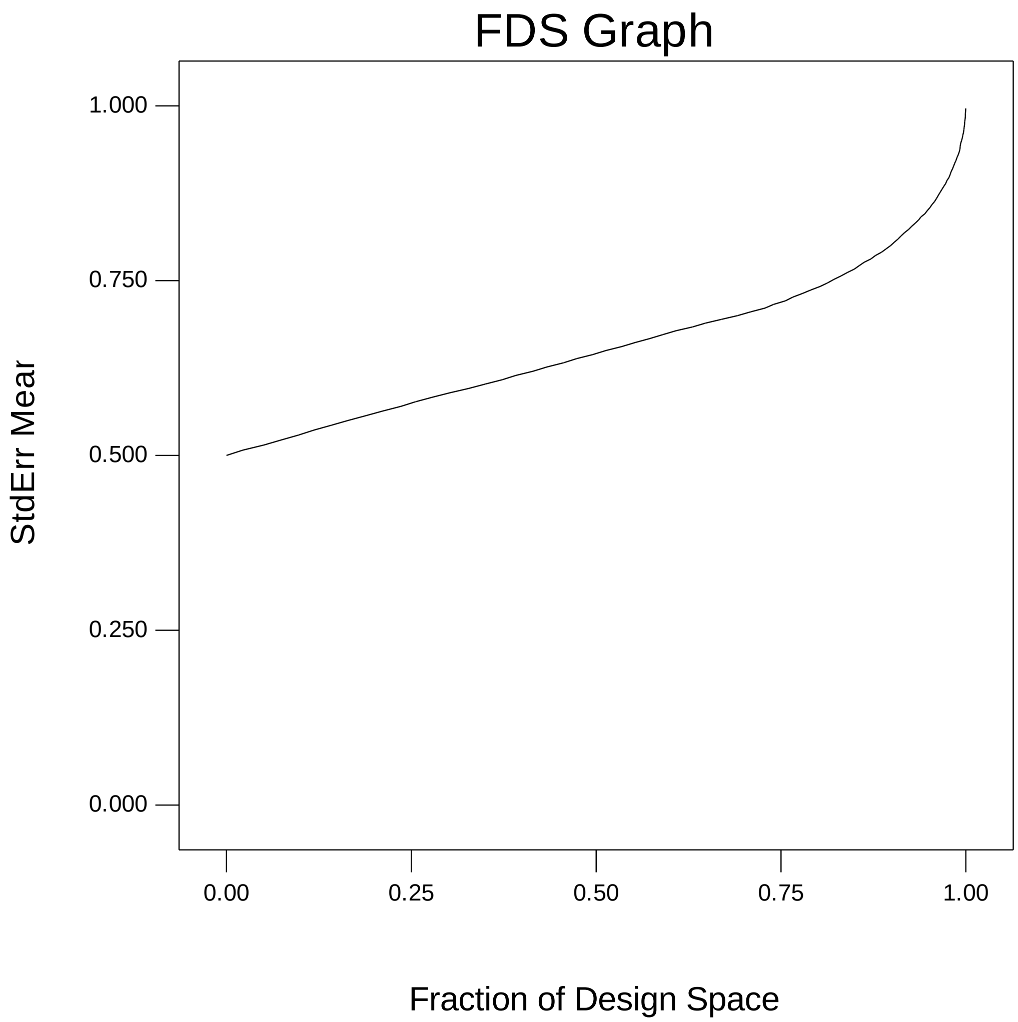
$$I = \frac{1}{A}\int_{-1}^{1}\int_{-1}^{1} V[\hat{y}(x_1, x_2) dx_1 dx_2 \qquad A = \text{area of design space} = 2^2 = 4$$

$$= \frac{1}{4}\int_{-1}^{1}\int_{-1}^{1} \sigma^2 \frac{1}{4}(1 + x_1^2 + x_2^2 + x_1^2 x_2^2) dx_1 dx_2$$

$$= \frac{4\sigma^2}{9}$$

Design-Expert® Software

Min StdErr Mean: 0.500
Max StdErr Mean: 1.000
Cuboidal
radius = 1
Points = 10000



For the 2^2 and in general the 2^k

- The design produces regression model coefficients that have the **smallest** variances (*D*-optimal design)
- The design results in **minimizing** the **maximum** variance of the predicted response over the design space (*G*-optimal design)
- The design results in **minimizing** the **average** variance of the predicted response over the design space (*I*-optimal design)

Optimal Designs

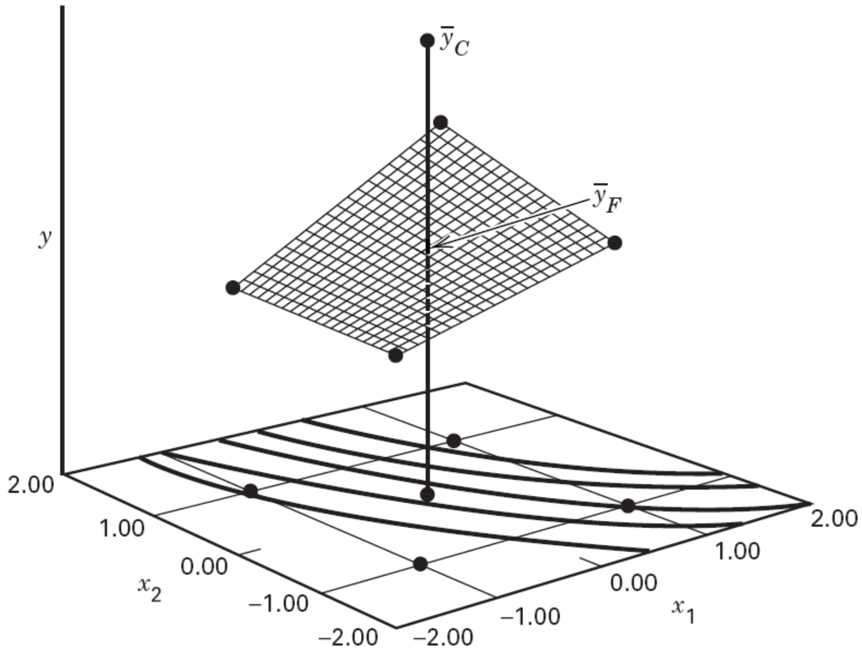
- These results give us some assurance that these designs are “good” designs in some general ways
- Factorial designs typically share some (most) of these properties
- There are excellent computer routines for finding optimal designs (JMP is outstanding)

Addition of Center Points to a 2^k Designs

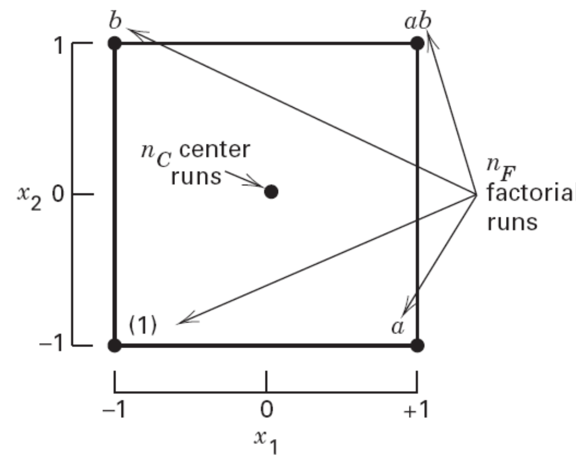
- Based on the idea of replicating **some** of the runs in a factorial design
- Runs at the center provide an estimate of error and allow the experimenter to distinguish between two possible models:

First-order model (interaction) $y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \sum_{j>i}^{k} \beta_{ij} x_i x_j + \varepsilon$

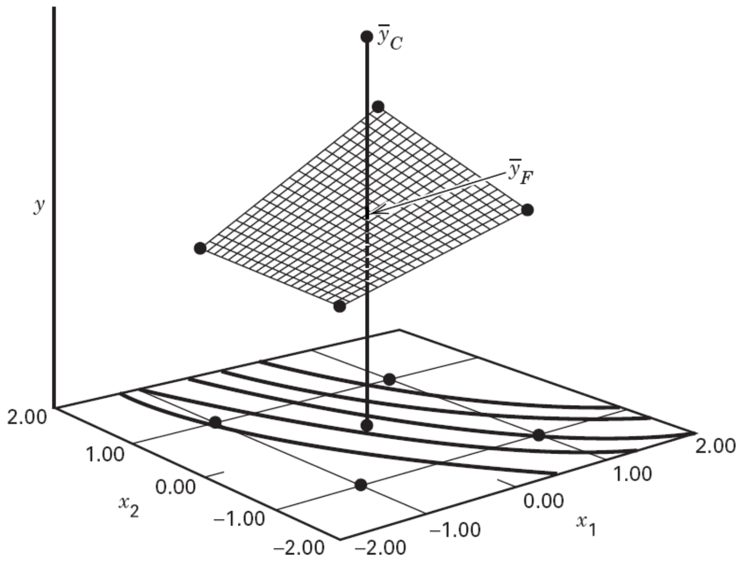
Second-order model $y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \sum_{j>i}^{k} \beta_{ij} x_i x_j + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \varepsilon$



■ FIGURE 6.37 A 2^2 design with center points



■ FIGURE 6.38 A 2^2 design with center points



■ **FIGURE 6.37** A 2^2 design with center points

$$\bar{y}_F = \bar{y}_C \Rightarrow \text{ no "curvature"}$$

The hypotheses are:

$$H_0 : \sum_{i=1}^{k} \beta_{ii} = 0$$

$$H_1 : \sum_{i=1}^{k} \beta_{ii} \neq 0$$

$$SS_{\text{Pure Quad}} = \frac{n_F n_C (\bar{y}_F - \bar{y}_C)^2}{n_F + n_C}$$

This sum of squares has a single degree of freedom

Example 6.7, Pg. 286

Refer to the original experiment shown in Table 6.10. Suppose that four center points are added to this experiment, and at the points $x1=x2=x3=x4=0$ the four observed filtration rates were 73, 75, 66, and 69. The average of these four center points is 70.75, and the average of the 16 factorial runs is 70.06. Since are very similar, we suspect that there is no strong curvature present.

$$n_C = 4$$

Usually between 3 and 6 center points will work well

Design-Expert provides the analysis, including the *F*-test for pure quadratic curvature

Table 6.22 summarizes the analysis of variance for this experiment. In the upper portion of the table, we have fit the full model. The mean square for pure error is calculated from the center points as follows:

$$MS_E = \frac{SS_E}{n_C - 1} = \frac{\sum_{\text{Center points}} (y_i - \overline{y}_c)^2}{n_C - 1} \quad \textbf{(6.29)}$$

Thus, in Table 6.22,

$$MS_E = \frac{\sum_{i=1}^{4} (y_i - 70.75)^2}{4 - 1} = \frac{48.75}{3} = 16.25$$

The difference $\overline{y}_F - \overline{y}_C = 70.06 - 70.75 = -0.69$ is used to compute the pure quadratic (curvature) sum of squares in the ANOVA table from Equation 6.30 as follows:

$$SS_{\text{Pure quadratic}} = \frac{n_F n_C (\overline{y}_F - \overline{y}_C)^2}{n_F + n_C}$$

$$= \frac{(16)(4)(-0.69)^2}{16 + 4} = 1.51$$

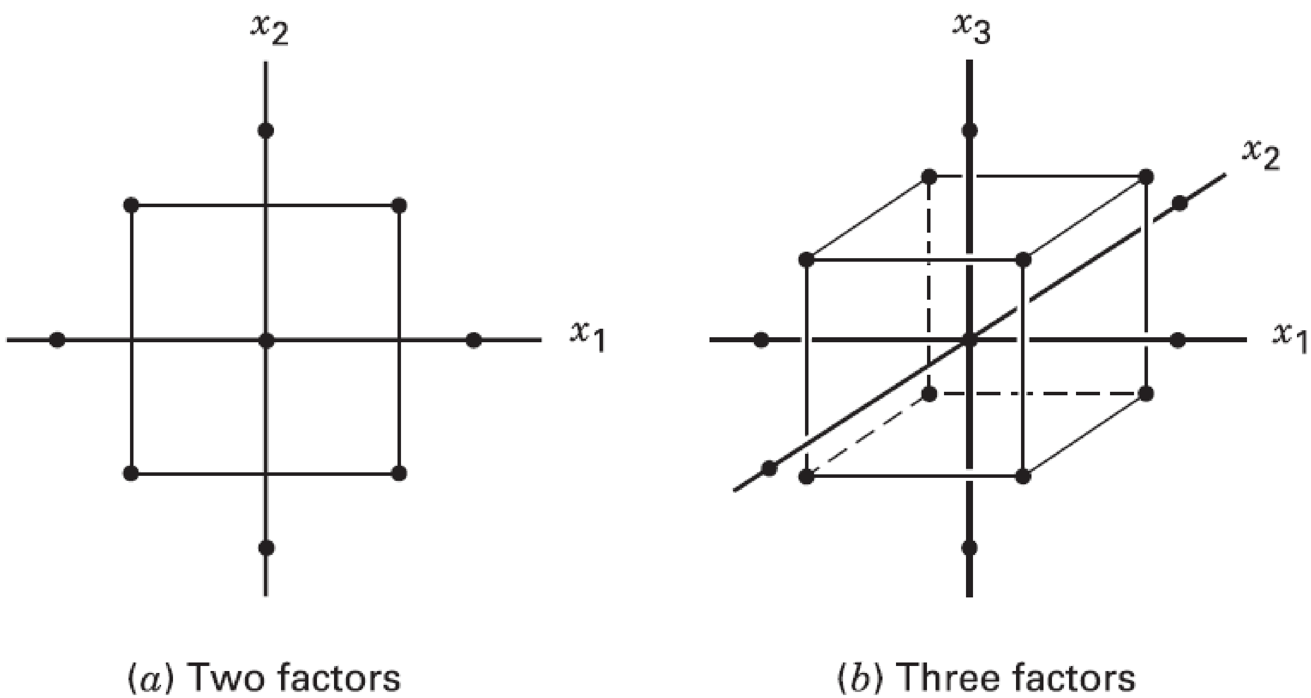
ANOVA for Example 6.7

■ **TABLE 6.24** *(Continued)*

ANOVA for the Reduced Model

Source of Variation	Sum of Squares	DF	Mean Square	F	Prob > F
Model	5535.81	5	1107.16	59.02	< 0.000
A	*1870.56*	*1*	*1870.56*	*99.71*	*< 0.000*
C	*390.06*	*1*	*390.06*	*20.79*	*0.0005*
D	*855.56*	*1*	*855.56*	*45.61*	*< 0.000*
AC	*1314.06*	*1*	*1314.06*	*70.05*	*< 0.000*
AD	*1105.56*	*1*	*1105.56*	*58.93*	*< 0.000*
Pure quadratic curvature	1.51	1	1.51	0.081	0.7809
Residual	243.87	13	18.76		
Lack of fit	*195.12*	*10*	*19.51*	*1.20*	*0.4942*
Pure error	*48.75*	*3*	*16.25*		
Cor total	5781.20	19			

If curvature is significant, augment the design with axial runs to create a central composite design. The CCD is a very effective design for fitting a second-order response surface model

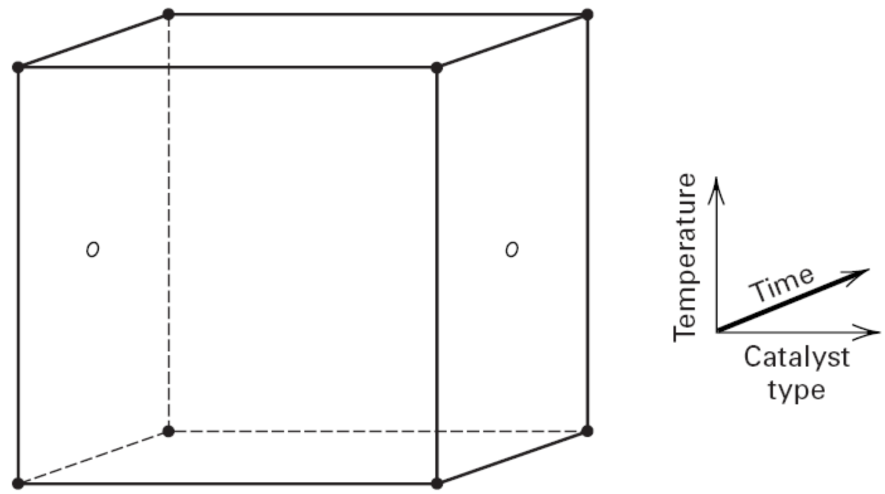


■ **FIGURE 6.39** Central composite designs

Practical Use of Center Points (pg. 289)

- Use **current operating conditions** as the center point
- Check for **“abnormal” conditions** during the time the experiment was conducted
- Check for **time trends**
- Use center points as the first few runs when there is little or no information available about the magnitude of **error**
- Center points and **qualitative** factors?

Center Points and Qualitative Factors



■ FIGURE 6.40 A 2^3 factorial design with one qualitative factor and center points