6.780 SEMICOND. MANUF. — PROBLEM SET 5 SOLUTIONS — Spring 2003

Problem 1 Poly Etch Experiments

Part a 2-level, 5 factors $\Rightarrow 2^5 = 32$ runs (assuming no replicates)

Part b Variance in estimating a main effect?

- For each main effect (for each factor), we form a "contrast" or difference between the average at the high and low value for that factor; e.g. for factor A we have

$$\hat{E}_A = \bar{y}_{A+} - \bar{y}_{A-}$$

$$Var\{E_A\} = Var\{\underbrace{\bar{y}_{A+}}_{\text{average over 16 "high" runs for factor A}}\} + Var\{\underbrace{\bar{y}_{A-}}_{\text{average over 16 "low" settings for A}}\}$$

$$\hat{\sigma}^2_{E_A} = Var\{E_A\} = \frac{\sigma^2}{16} + \frac{\sigma^2}{16} = \frac{\sigma^2}{8}$$ //

Part c How form a 99% confidence interval on factor 1 (A)?

Given the variance above, this is just a standard interval estimate. Assuming σ^2 is known, then

$$E_A = (\bar{y}_{A+} - \bar{y}_{A-}) \pm z_{\alpha/2}\, \hat{\sigma}_{E_A}$$

Here $\alpha = 0.01 \Rightarrow z_{0.005} = 2.58$, so

$$E_A = (\bar{y}_{A+} - \bar{y}_{A-}) \pm 2.58\, \sigma/\sqrt{8}$$ // $= (\bar{y}_{A}^{+} - \bar{y}_{A-}) \pm 0.9126$

Part d Assume $\sigma = 200$ Å/min.
Want $\alpha = 0.01$ c.i. on main effects such that we are +/- 25 Å

→ How many replicates needed?

- First, just to parse the goal more clearly, we want

$$E_A = (\bar{y}_{A+} - \bar{y}_{A-}) \pm \underline{\underline{25 \text{ Å/min}}} \quad \text{at } \alpha = 0.01$$

and also a similar confidence interval on the interaction:

$$I_{AB} = \left(\frac{\bar{y}_{AB^+} - \bar{y}_{AB^-}}{2} \right) \quad \pm \; 25 \text{ Å/min} \quad \text{at } \alpha = 0.01$$

Note, for example, that without replications from the previous page we have

$$E_A = (\bar{y}_{A+} - \bar{y}_{A-}) \pm \underbrace{\overset{z_{\alpha/2}}{2.58}\,(\overset{\sigma}{200})\,/\overset{\text{due to how we form samples}}{\sqrt{8}}}$$

$\pm$ 182.4 Å/min, or not nearly tight enough.

- Next, let's generalize our result from the previous parts. With replicates, we have:

$$\hat{\sigma}_{E_A} = \text{Var}\{E_A\} = \frac{\sigma^2}{N/2} + \frac{\sigma^2}{N/2} = \frac{4\sigma^2}{N} \quad \text{where } N = \underset{\text{\# replicates}}{d} \cdot 2^{\overset{\text{\# factors}}{n}} = \text{\# runs}$$

- We can similarly estimate the variance in estimating an interaction effect:

$$\hat{I}_{AB} = \frac{\bar{y}_{AB^+} - \bar{y}_{AB^-}}{2} = \frac{E_{A(B^+)} - E_{A(B^-)}}{2}$$

that is, the interaction is the difference between effects one one factor when the second is high or low.

So
$$\text{Var}\{I_{AB}\} = \frac{1}{4}\text{Var}\{\underset{\substack{\text{formed from} \\ 1/2 \text{ data}}}{\bar{y}_{AB^+}}\} + \frac{1}{4}\text{Var}\{\underset{\substack{\text{are formed from other} \\ \text{half data}}}{\bar{y}_{AB^-}}\}$$

or
$$Var\{I_{AB}\} = \frac{1}{4}\left\{\frac{\sigma^2}{N/2}\right\} + \frac{1}{4}\left\{\frac{\sigma^2}{N/2}\right\} = \frac{\sigma^2}{N}$$

- Note that the same result applies for higher order interactions as well. In the case of third order interactions, one still forms a "contrast" by taking the difference in ave of two appropriately selected halves of the data (based on the "contrast pattern" for the design). Because the interaction is defined as ½ the difference in these two averages, we always find $\sigma^2_I = \sigma^2/N$ for the two-level factorial design. The factor of ¼ comes due to definition of ½ "effect".

- Now we can finally answer the question: we find that variance in estimating the main effect is always larger than that in estimating interactions:

$$Var\{E_A\} = 4\sigma^2/N$$
$$Var\{I\} = \sigma^2/N \qquad \text{where} \qquad N = d \cdot 32$$

replicates

So we need

$$z_{\alpha/2} \cdot 2\sigma/\sqrt{N} < 25 \text{ Å/min}$$

at $\alpha = 0.01$

$$\frac{(2.58)\,2\,(200 \text{ Å/min})}{\sqrt{N}} < 25 \text{ Å/min}$$

$$7.30 = \frac{2.58 \cdot 2 \cdot 200}{25\sqrt{32}} < \sqrt{d}\,\cancel{\sqrt{32}}$$

or $\quad d > 53.25 \quad \Rightarrow \quad \boxed{d = 54 \text{ replicates!}}$

Note that it takes a LOT of replicates to move our 99% confidence interval from ± 182.4 Å/min down to ± 25 Å/min.

Problem 2

Part a We'll begin with a basic MANOVA to examine the main effects in the 2^{4-1} half fraction design. In the MANOVA we are looking at Sum of Square and mean square values to test significance. In the factorial analysis (which we'll do in a moment) we calculate size of effects and confidence intervals on those effects. We assume that interactions are not significant.

Grand mean: $\bar{y} = 0.55$

NOTE: you should be able to do these sorts of simple analyses without a stats package, to be sure you understand the issues!

Main Effect contrasts:

$$\bar{y}_A^+ = \tfrac{1}{4}(.30+.68+.56+.93) = 0.6025$$
$$\bar{y}_A^- = \tfrac{1}{4}(.82+.17+.62+.38) = .4975$$
$$\bar{y}_B^+ = \tfrac{1}{4}(.82+.50+.38+.93) = .6575$$
$$\bar{y}_B^- = \tfrac{1}{4}(.17+.62+.30+.68) = .4425$$
$$\bar{y}_C^+ = \tfrac{1}{4}(.82+.17+.68+.50) = .5425$$
$$\bar{y}_C^- = \tfrac{1}{4}(.62+.30+.38+.93) = .5575$$
$$\bar{y}_D^+ = \tfrac{1}{4}(.82+.62+.68+.93) = .7625$$
$$\bar{y}_D^- = 1/4(.17+.30+.50+.38) = .3375$$

Sum of Squares:

$$SS_A = 4\cdot(\bar{y}_A^+ - \bar{y})^2 + 4(\bar{y}_A^- - \bar{y})^2 = 0.02205$$

$$SS_B = 0.09245$$
$$SS_C = 0.00045$$
$$SS_D = 0.36125$$

Residuals: We could use formulas to calculate $\hat{y}$ for each datapoint, and find $y-\hat{y}$, e.g.

$$\varepsilon_i = y_i - \hat{y}_i = y_i - \bar{y} - (y_A - \bar{y}) - (y_B - \bar{y}) - (y_C - \bar{y}) - (y_D - \bar{y})$$

where y_A is either y_A^+ or y_A^- depending on whether or not the i^{th} experimental point was at the + or − setting for factor A.

Much easier however, is to use $SS_{TOTAL} = SS_{AVE} + SS_A + \ldots + SS_D + SS_R$ and just fill SS_R in from table.

MANOVA TABLE

Source of Variation	Sum of Squares	d.o.f.	Mean Square	F_0	Pr(F)
Average	$SS_{AVE} = 2.42$	1	2.42		
Factor A	$SS_A = 0.02205$	1	0.02205	55.125	0.0051
B	$SS_B = 0.09245$	1	0.09245	231.125	0.0006
C	$SS_C = 0.00045$	1	0.00045	1.125	0.3667
D	$SS_D = 0.36125$	1	0.36125	903.125	< 0.0001
Residual	$SS_R = 0.0012$	3	0.0004		
Total	$SS_{TOT} = 2.8974$	8			

NOTES: $SS_{AVE} = n \cdot \bar{y}^2 = 8(0.55)^2 = 2.42$

$$SS_{TOT} = \sum y^2 = 2.8974$$

$$SS_R = SS_{TOT} - SS_{AVE} - (SS_A + SS_B + SS_C + SS_D) = 0.00120$$

Pr(F) calculated for Prob $\{F > F_0\}$, $F_0 = F_{1,3}$
This is hard to find in some tables; statistical packages usually calculate this. We can also use the fact that $F_{\alpha,1,3} = (t_{\alpha/2,3})^2$ or $\alpha/2$ on each side of t, and then use t tables to find significance for t_3

Another reasonable approach when using tables is to go forward rather than back out Pr(F). E.g. we could ask the question: "what F do we need to be 99% confident the factor is significant, i.e.

$$F_{0.01,1,3} = 34.12$$

$\therefore$ Factors A, B, & D have a significance of $\alpha = 0.01$ or better (Pr(F) < 0.01).

Part b We can do equivalent tests to check the significance of the size of effects.

- In essence, this is what we do with a "simple" (well, maybe not all that simple) factorial analysis.

Estimates of Effects:

$$\begin{aligned}
l_A &= \bar{y}_A^+ - \bar{y}_A^- = 0.105 \\
l_B &= \bar{y}_B^+ - \bar{y}_B^- = 0.215 \\
l_C &= \bar{y}_C^+ - \bar{y}_C^- = -0.015 \\
l_D &= \bar{y}_D^+ - \bar{y}_D^- = 0.425
\end{aligned}$$

Our estimate of variance is $SS_R/\nu_r = \frac{0.0012}{3} = .0004 = \hat{\sigma}^2$ or $\hat{\sigma} = 0.02$

- Thus, we can do a t-test to ask how likely it is to observe any particular effect if the process was acting "randomly" (that is, effect is not mean shifted), i.e.

$$\frac{l_A}{\text{std. err}\{l_A\}} \sim t_{\nu_r} = t_3$$

Note that std. err. $\{l_A\} = \sqrt{\text{Var}\{l_A\}}$. We're back to question of variance in our main effect (as in earlier PSET problem)

$$\begin{aligned}
\text{Var}\{l_A\} &= \text{Var}\{\bar{y}_A^+\} + \text{Var}\{\bar{y}_A^-\} \\
&= \frac{1}{16}\{4\sigma^2 + 4\sigma^2\} = \frac{\sigma^2}{2} = \frac{0.0004}{2}
\end{aligned}$$

Thus, we can do

$$t_0 = \frac{l_A}{\hat{\sigma}/\sqrt{2}} = \frac{0.105}{0.02/\sqrt{2}} = \frac{0.105}{0.01414} = 7.4246$$

Note that $t_0^2 = 7.4246^2 = 55.125$ = F_0 for Factor A in our MANOVA table!

$\text{Prob}(t_0 > t_3) = 0.0051$ or same level of significance as found in Manova table.

So A is significant to 99.49% confidence.

- With this factor effect analysis, however, we can <u>also</u> state things in terms of confidence intervals

$$l_A = 0.105 \pm t_{\alpha/2,3} \cdot \text{std. err.}\{l_A\}$$

e.g. For 99% confidence intervals, we know $t_{\alpha/2,3} = \underline{7.45}$

$$l_A = 0.105 \pm \underline{7.45} \cdot 0.01414$$

$$l_A = 0.105 \pm 0.105$$ ~ just <u>barely</u> significant at 99% level, consistent with the to earlier found.

We can again summarize significances from F TESTS:

	A	significant	at	99.49 % conf. ($\alpha = 0.0051$)
	B	significant	at	99.94 % conf. ($\alpha = 0.0006$)
i.e. not sign. ~	C	significant	at	63.37 % conf. ($\alpha = 0.3667$)
	D	significant	at	>99.99% conf. ($\alpha < 0.0001$)

(Part C) To recap the above differences:

- Factorial analysis gives estimates of <u>effect</u> magnitudes,

  MANOVA gives estimates of <u>significance</u> of effects.

- Factorial analysis also allows us to examine <u>interactions</u> and <u>confounding</u> patterns relatively easily, including estimates of magnitudes of interaction effects; MANOVA can also extend to look at interactions, but many packages get confused by confounding patterns.

Problem 3

We are given an existing central composite design with 5 center point replicates, for two factors x1 and x2, with output y. This gives a total of four full factorial points (which are not replicated), four axial points (also not replicated), and 5 replicated center points. We will analyze this design using linear regression in JMP.

Part a.

First, we construct a first order model with intercept and first order terms only:

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

We examine this in an ANOVA framework, as well as look at the values and significance of the coefficient estimates. Running JMP's "fit model" routines with y as the output, and *x1* and *x2* terms included, produces the following:

Summary of Fit

RSquare	0.358311
RSquare Adj	0.229973
Root Mean Square Error	2.584949
Mean of Response	1.838462
Observations (or Sum Wgts)	13

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	2	37.31115	18.6556	2.7919
Error	10	66.81962	6.6820	Prob > F
C. Total	12	104.13077		0.1088

Lack Of Fit

Source	DF	Sum of Squares	Mean Square	F Ratio
Lack Of Fit	6	66.467615	11.0779	125.8856
Pure Error	4	0.352000	0.0880	Prob > F
Total Error	10	66.819615		0.0002
				Max RSq
				0.9966

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	1.8384618	0.716936	2.56	0.0282
x1	0.9471221	0.913918	1.04	0.3245
x2	-1.94084	0.913918	-2.12	0.0597

Effect Tests

Source	Nparm	DF	Sum of Squares	F Ratio	Prob > F
x1	1	1	7.176315	1.0740	0.3245
x2	1	1	30.134839	4.5099	0.0597

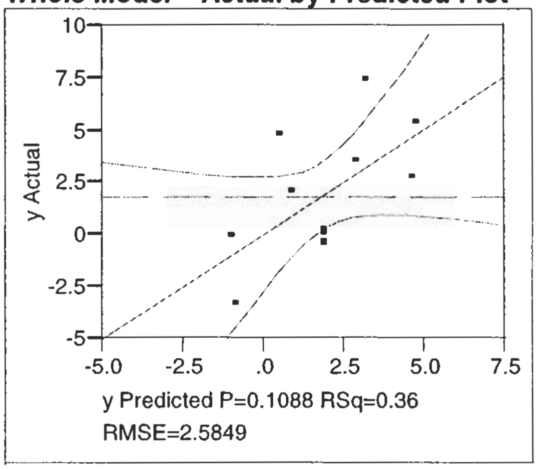
We see that the model is only marginally significant, with the probability of observing the F ratio of 2.7919 equal to 0.1088. Looking at the parameter estimates, we see that the intercept appears significant (Prob>|t| is 0.0282), and x2 looks significant. The factor *x1* does not appear to be significant, with t ratio probability of 0.3245. The overall R^2 for this fit is not very good: 0.358 (with adjusted R^2 of 0.23). This poor fit is begging for some further investigation, which we do in part b.

Part b.

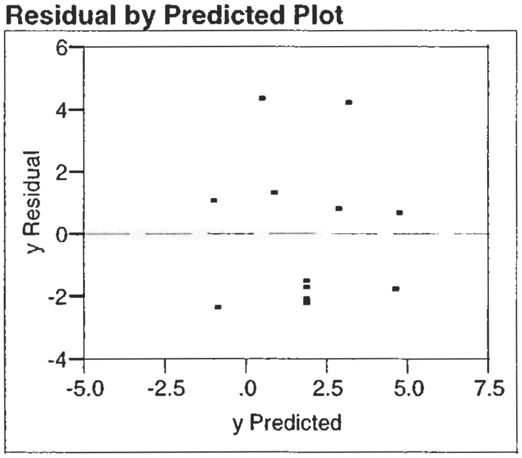
First, we look for any evidence of lack of fit. The JMP analysis nicely separates out the pure error (from the replicate information) from the total error, allowing us to see how much error we can attribute to lack of fit. In this case, it is quite large: the F ratio for evaluating the significance of the lack of fit mean square is huge 125.8856. The probability of observing this by chance is small: 0.0002. We can say with substantial confidence that our model suffers from a lack of fit.

The next step is to investigate the residuals. Plots of the whole model, followed by residuals versus the predicted value of *y* (this plot is generated in JMP during the model fit) show the following:

Whole Model – Actual by Predicted Plot

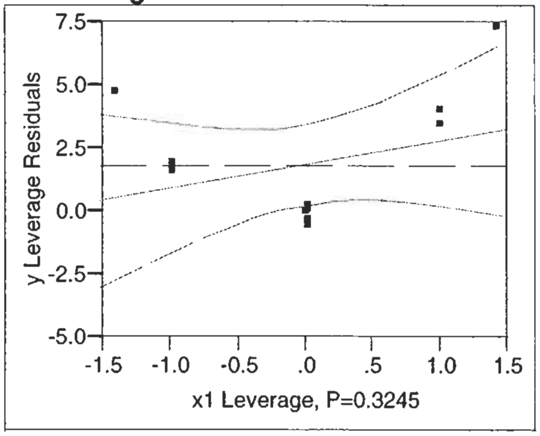


Residual by Predicted Plot

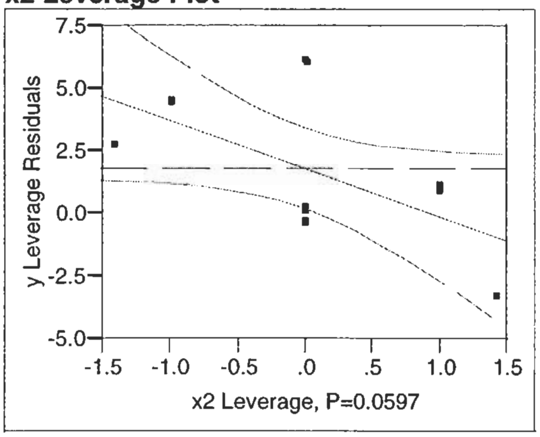


Here no clear dependency in the size or balance of the residual is seen. We also plot the residuals versus x1 and versus x2, to see if there is a factor dependency in the residuals:

x1 Leverage Plot



x2 Leverage Plot



In this case, we see a very clear quadratic dependence in the residuals of *x1*, and potentially in *x2*. This strongly suggests adding a second order (squared) term for *x1* and *x2*.

Part c.

Now we'll expand our RSM to include all second order terms (both interactions and quadratic terms):

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2$$

Our JMP package handles this nicely; we can simply add the interaction of *x1* with *x2*, and the "interaction" of *x1* with *x1*, and of *x2* with *x2* to get the quadratic terms to appear. The resulting model fit is shown below. Note that the earlier estimates do not change; we have a balanced design so the extra model terms are orthogonal and are just added to the model.

Summary of Fit

RSquare	0.992549
RSquare Adj	0.987226
Root Mean Square Error	0.332934
Mean of Response	1.838462
Observations (or Sum Wgts)	13

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	5	103.35485	20.6710	186.4851
Error	7	0.77592	0.1108	Prob > F
C. Total	12	104.13077		<.0001

Lack Of Fit

Source	DF	Sum of Squares	Mean Square	F Ratio
Lack Of Fit	3	0.42391603	0.141305	1.6057
Pure Error	4	0.35200000	0.088000	Prob > F
Total Error	7	0.77591603		0.3214
				Max RSq
				0.9966

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	0.0600005	0.148893	0.40	0.6990
x1&RS	0.9471158	0.11771	8.05	<.0001
x2&RS	-1.940839	0.11771	-16.49	<.0001
x1*x1	3.0325037	0.12623	24.02	<.0001
x2*x1	0.075	0.166467	0.45	0.6659
x2*x2	-0.142501	0.12623	-1.13	0.2961

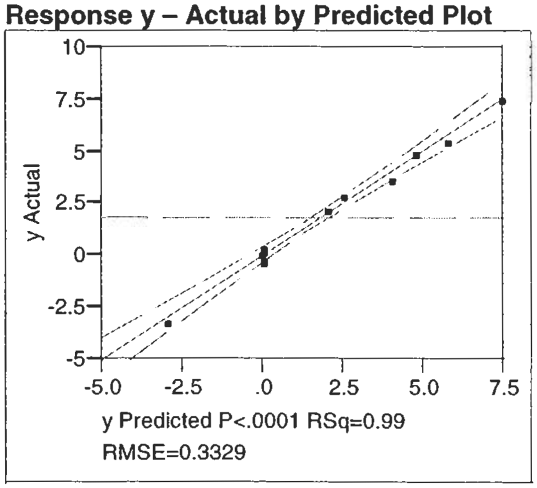
Effect Tests

Source	Nparm	DF	Sum of Squares	F Ratio	Prob > F
x1&RS	1	1	7.176219	64.7409	<.0001
x2&RS	1	1	30.134800	271.8640	<.0001
x1*x1	1	1	63.972517	577.1341	<.0001
x2*x1	1	1	0.022500	0.2030	0.6659
x2*x2	1	1	0.141262	1.2744	0.2961

Our model results are now dramatically improved. The parameter estimate are shown above, with the x_1, x_2, and x_1^2 terms all highly significant. Interestingly, the intercept term is no longer significant. The overall R^2 is now 0.995, an excellent fit. The lack of fit test is showing no evidence of remaining lack of fit. That is, the Prob > F of 0.32 indicates that 68% of the time, this ratio would be observed by chance alone.

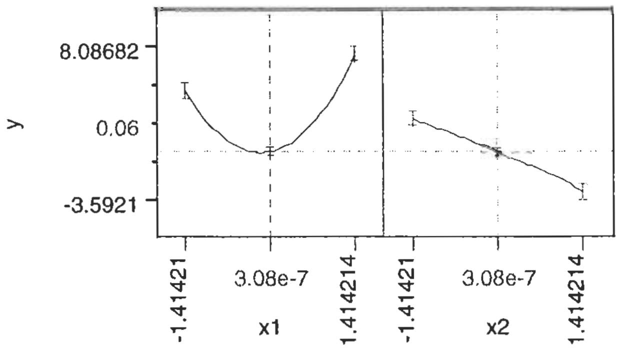
We also plot below the actual values of y versus the predicted values. Now we see very tight confidence bounds on the predictions.

Response y – Actual by Predicted Plot



JMP also produces a "prediction profiler" plot. This essentially shows the impact of each variable on the output. We see the strong quadratic dependence on *x1*, and a linear dependence on *x2*.

Prediction Profiler

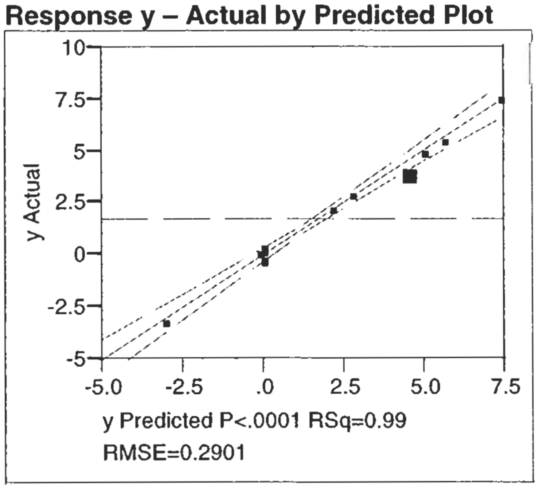


Part d.

In this part, we consider what happens if we were to lose one of our data points due to some kind of experimental problem. We will eliminate one of the corner factorial points, experimental run 1. We would expect this to be one of the more painful points to lose (certainly compared to the center replicates, and even compared to the axial runs), as it is one of the important indicators for interaction between the factors.

In JMP, we "exclude" row 1, and then rerun our fits. The model results are shown below; we observe that the parameter estimates change, but not hugely. The biggest change is in the estimate for x1, as might be expected.

Response y – Actual by Predicted Plot



Summary of Fit

RSquare	0.994969
RSquare Adj	0.990776
Root Mean Square Error	0.290119
Mean of Response	1.683333
Observations (or Sum Wgts)	12

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	5	99.87165	19.9743	237.3117
Error	6	0.50502	0.0842	Prob > F
C. Total	11	100.37667		<.0001

Lack Of Fit

Source	DF	Sum of Squares	Mean Square	F Ratio
Lack Of Fit	2	0.15301513	0.076508	0.8694
Pure Error	4	0.35200000	0.088000	Prob > F
Total Error	6	0.50501513		0.4858
				Max RSq
				0.9965

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>ltl
Intercept	0.0371961	0.130658	0.28	0.7855
x1&RS	1.3791009	0.113913	12.11	<.0001
x2&RS	-2.038021	0.113913	-17.89	<.0001
(x1-0.08333)*(x1-0.08333)	3.0856257	0.113913	27.09	<.0001
(x2-0.08333)*(x1-0.08333)	0.287486	0.187271	1.54	0.1757
(x2-0.08333)*(x2-0.08333)	-0.089379	0.113913	-0.78	0.4625

Effect Tests

Source	Nparm	DF	Sum of Squares	F Ratio	Prob > F
x1&RS	1	1	12.336758	146.5710	<.0001
x2&RS	1	1	26.941779	320.0908	<.0001
x1*x1	1	1	61.758114	733.7378	<.0001
x2*x1	1	1	0.198355	2.3566	0.1757
x2*x2	1	1	0.051817	0.6156	0.4625

Prediction Profiler