# Day 4 Homework Exercises

## Smarter Experimentation for Chemists

# Day 4 Homework Exercise 1

## Smarter Experimentation For Chemists

### Analyzing a Custom Central Composite Design

A response surface experiment using a central composite design was run to optimize Yield based on three variables: **Catalyst**, **Temperature**, and **Time**. The design and results are in the file **Custom CCD 3 Factors.jmp**.

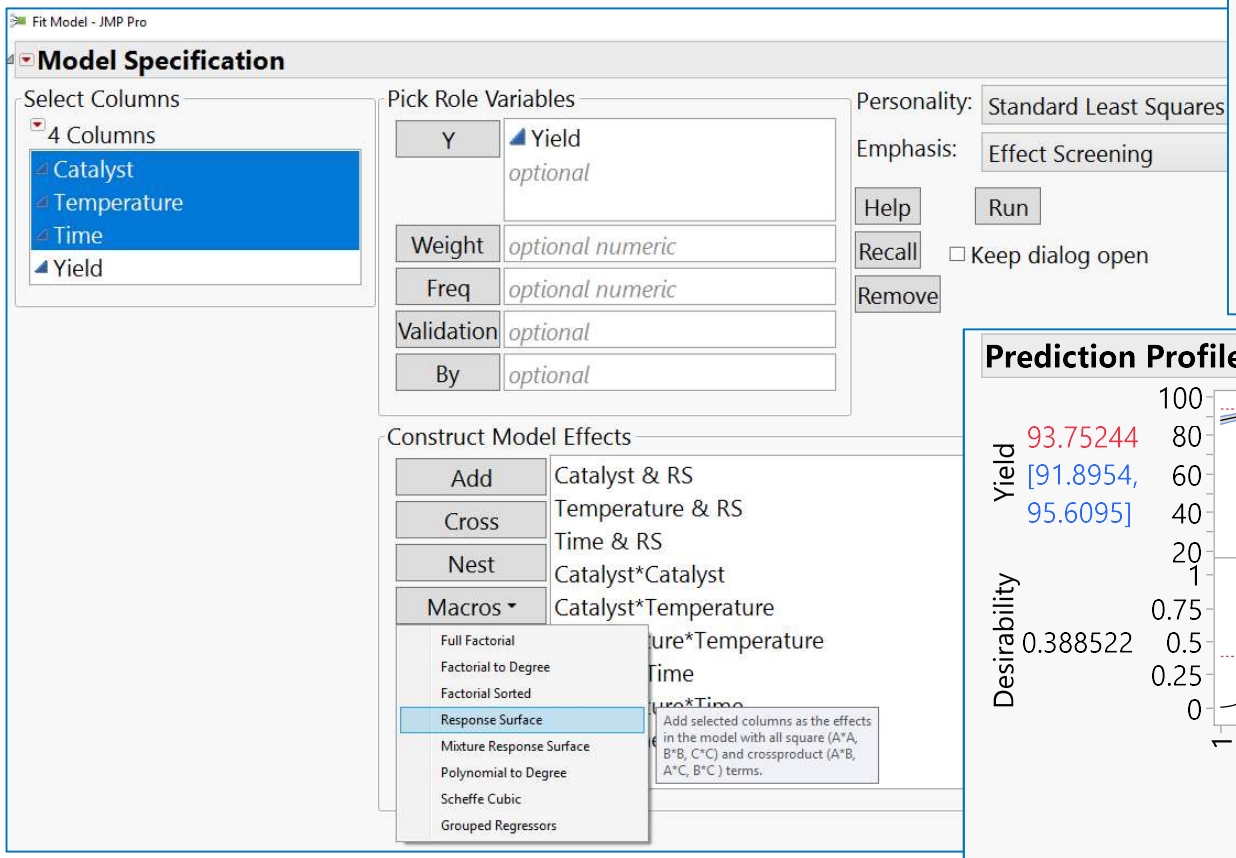
Open **Custom CCD 3 Factors.jmp** and fit a model for **Yield** using all main effects, two-way interactions, and quadratic effects. (Hint: In this file, the Model script has been removed. To fit the model, use **Analyze**, **Fit Model**. Then select **Yield** as the Y variable. To add the model effects, select all three factors, and then select **Macros**, **Response Surface**.)

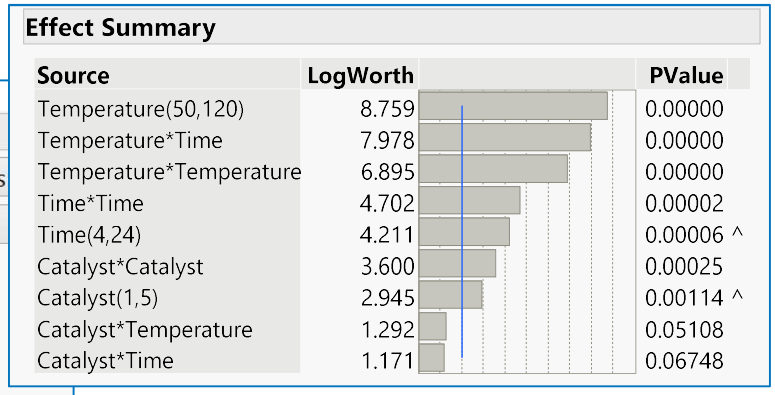
Questions:

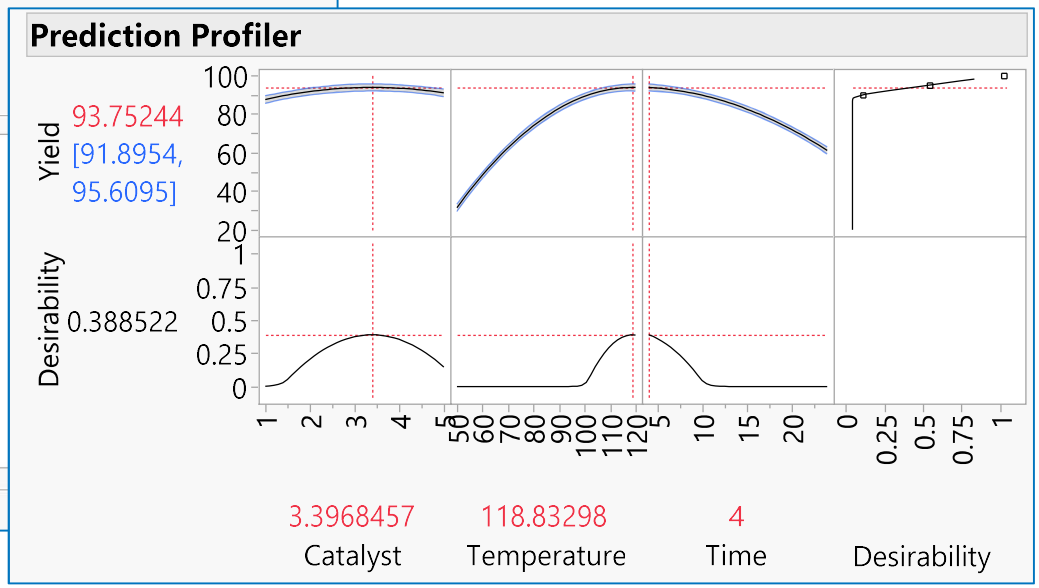
1. Which three effects are the most significant?
2. Using the Prediction Profiler, what are the optimal conditions to maximize Yield? What is the predicted yield at these settings?
3. Is there evidence of lack of fit? Interpret these results.
4. If you had conducted this study, what is a possible next step?

# Day 4 Homework Exercise 1

## Smarter Experimentation For Chemists



# Day 4 Homework Exercise 1

## Smarter Experimentation For Chemists

### Analyzing a Custom Central Composite Design

Solutions:

1. Which three effects are the most significant?

   The most significant effects are **Temperature**, the **Temperature*Time** interaction, and the quadratic effect for **Temperature**.

2. Using the Prediction Profiler, what are the optimal conditions to maximize Yield? What is the predicted yield at these settings?

   The optimal settings are **Catalyst** = 3.4, **Temperature** = 118.8, and **Time** = 4. At these settings, the predicted yield is 93.75. (Hint: Use the red triangle for the Prediction Profiler, and select **Optimization and Desirability, Maximize Desirability**.)

3. Is there evidence of lack of fit? Interpret these results.

   No, the p-value in the lack of fit table is 0.2001. There isn't evidence of lack of fit. The model we have fit adequately describes the relationship between the factors and the response. Hint: It helps to look at the Actual by Predicted plot. (This is an option under the top red triangle, **Row Diagnostics**, **Plot Actual by Predicted**.) If you see points that fall far from the predicted response value, you might have lack of fit.

4. If you had conducted this study, what is a possible next step?

   You might run a confirmation trial at the optimal setting.

# Day 4 Homework Exercise 2

## Smarter Experimentation For Chemists

### Optimizing the Heck Reaction

In this practice, you analyze the five-factor, 22-run custom response surface design to identify settings that optimize yield.

The data are in the file **Custom 5 Response Surface.jmp**.

Run the analysis, and slowly reduce the model. (Remove terms with PValue > 0.05, interactions first.) Then maximize desirability to identify settings that maximize yield.

Questions:

1. Which terms are in the reduced model?
2. Look at the following plots (available from the top red triangle under Row Diagnostics): Residual by Predicted, Actual by Predicted, and Studentized Residuals. Do you see any unusual patterns or outliers? Interpret what you see. Does the model explain the relationship between the factors and the response?
3. What are the optimal settings? What is the predicted yield at these settings?

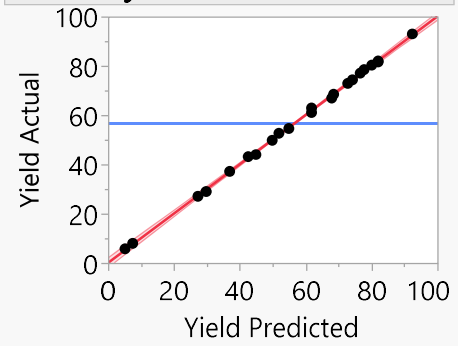
# Day 4 Homework Exercise 2

## Smarter Experimentation For Chemists

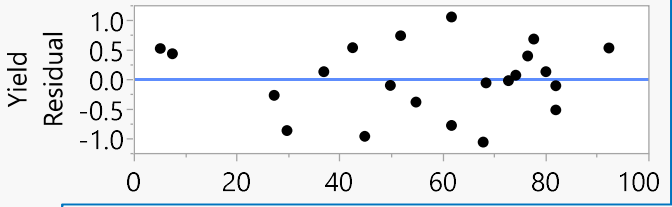
**Effect Summary**

| Source | LogWorth | PValue |
|---|---|---|
| Temperature(50,120) | 17.147 | 0.00000 |
| Temperature*Time | 14.958 | 0.00000 |
| Temperature*Temperature | 14.031 | 0.00000 |
| Volume(1.5,10) | 13.748 | 0.00000 |
| Volume*Volume | 11.928 | 0.00000 |
| Time*Time | 9.129 | 0.00000 |
| Time(4,24) | 7.765 | 0.00000 ^ |
| Catalyst*Catalyst | 5.505 | 0.00000 |
| Catalyst(1,5) | 3.842 | 0.00014 ^ |

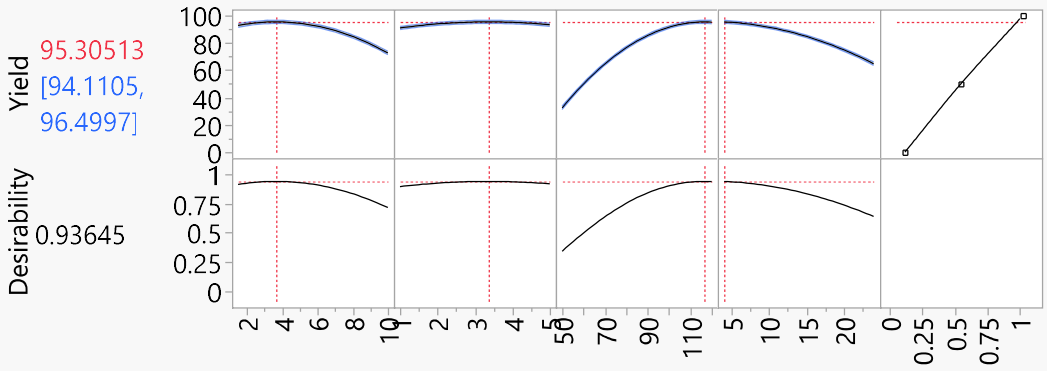
**Actual by Predicted Plot**



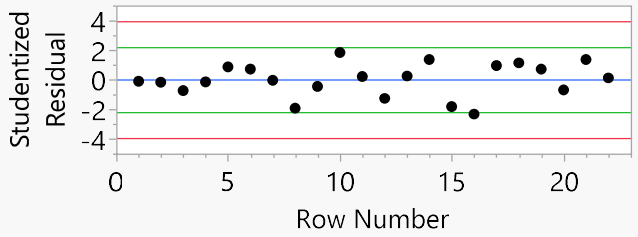

**Residual by Predicted Plot**




**Prediction Profiler**




**Studentized Residuals**




Externally studentized residuals with 95% simultaneous limits (Bonferroni) in red, individual limits in green.

# Day 4 Homework Exercise 2

## Smarter Experimentation For Chemists

### Optimizing the Heck Reaction

Solutions:

1. Which terms are in the reduced model?

   See **Effect Summary** plot on previous page.

2. Look at the following plots (available from the top red triangle under Row Diagnostics): Residual by Predicted, Actual by Predicted, and Studentized Residuals. Do you see any unusual patterns or outliers? Interpret what you see. Does the model explain the relationship between the factors and the response?

   There aren't any unusual patterns or outliers. The model seems to do a good job of explaining the relationship between the factors and the response.

3. What are the optimal settings? What is the predicted yield at these settings?

   See **Prediction Profiler** plot on previous page.