Making the most of this learning opportunity

To prevent audio disruptions, all attendees will be muted. Questions can be posted in the Question area. If they are not addressed during the webinar, I will reply via email afterwards.

Questions may also be sent to stathelp@statease.com. Please provide your company name and, if you are using Design-Expert, the serial number (found under Help, About).

Note: The slides and a recording of this webinar will be posted on the Webinars page of the Stat-Ease website within a few days.
Stat-Ease Latest News

Just Released January 4!

“What’s New” webinar on February 17.

Live Web Process DOE Workshop

April 12-16

Agenda

Response Surface Analysis Steps

- Fit Summary
- ANOVA & Statistics
- Diagnostics
- Model Reduction
- Confirmation
- Wrap Up
Response Surface Method Case

Help, Tutorials: “Response Surface-Chemical Conversion”

This case study on a chemical process features two key responses:

- $y_1$ - Conversion (%)
- $y_2$ - Activity

There are three process factors:

- A - time (minutes)
- B - temperature (degrees C)
- C - catalyst (percent)

Central composite design runs were conducted in two blocks:

1. 8 factorial points, plus 4 center points (12 runs total)
2. 6 axial points, plus 2 center points (8 runs).

Central Composite Design

Model points

- Two-level factorial
  - Estimate linear effects and two-factor interactions.
- Center points
  - Estimate quadratic effects, replicated to estimate pure error and tie blocks together.
- Star (or axial) points
  - Estimate pure quadratic effects.
Response Surface Methods Case
Analysis Procedure

1. **Configure/Transform**: Start with no transformation.
2. **Fit Summary**: Comparative statistics on polynomial models. *Do not select an aliased model! There are not enough runs to estimate all the coefficients!*
4. **ANOVA**: Check model and lack of fit p-values, R-squares.
5. **Diagnostics**: Examine diagnostic graphs to validate model.
6. **Model Graphs**: If model adequately represents response, generate contour and 3D plots.
7. **Confirmation**: Verify the model predictions with confirmation runs.

**Keys to Analyzing an RSM Design**

---

Response Surface Methods Case
Fit Summary

<table>
<thead>
<tr>
<th>Source</th>
<th>Sequential p-value</th>
<th>Lack of Fit p-value</th>
<th>Adjusted R²</th>
<th>Predicted R²</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear</td>
<td>0.1640</td>
<td>0.0442</td>
<td>0.1374</td>
<td>-0.4682</td>
</tr>
<tr>
<td>2FI</td>
<td>0.0083</td>
<td>0.1442</td>
<td>0.5803</td>
<td>0.3691</td>
</tr>
<tr>
<td>Quadratic</td>
<td>0.0017</td>
<td>0.8574</td>
<td>0.8881</td>
<td>0.7891</td>
</tr>
<tr>
<td>Cubic</td>
<td>0.8538</td>
<td>0.4836</td>
<td>0.8396</td>
<td>-3.6399</td>
</tr>
</tbody>
</table>

**Guidelines**: p<0.05    p>0.10    higher + difference <0.2

*Do not select an aliased model! There are not enough runs to estimate all the coefficients for that model.*
Lack of Fit
Six Replicated Design Points

Linear model – significant lack of fit.

Quadratic model – insignificant lack of fit.

\[ F = \frac{MS_{\text{lack of fit}}}{MS_{\text{pure error}}} \]

Lack of fit compares the variation between the actual data and the predicted value, to the variation between the replicates. They should be similar in size. \textit{(Hint: No replicates = No lack of fit test)}

Response Surface Methods Case
Model Tab

\textit{Suggested model is the default – usually okay to start there.}
Agenda

Response Surface Analysis Steps

- Fit Summary
- ANOVA & Statistics
- Diagnostics
- Model Reduction
- Confirmation
- Wrap Up

Keys to Analyzing an RSM Design

Response Surface Methods Case

ANOVA for Quadratic Model

<table>
<thead>
<tr>
<th>Source</th>
<th>Sum of Squares</th>
<th>df</th>
<th>Mean Square</th>
<th>F-value</th>
<th>p-value</th>
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<td>Model</td>
<td>2561.82</td>
<td>9</td>
<td>284.65</td>
<td>16.87</td>
<td>&lt; 0.001</td>
</tr>
<tr>
<td>A-time</td>
<td>14.44</td>
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<td>14.44</td>
<td>0.8561</td>
<td>0.3790</td>
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<tr>
<td>B-temperature</td>
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<td>1</td>
<td>222.96</td>
<td>13.21</td>
<td>0.0054</td>
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<td>C-catalyst</td>
<td>525.64</td>
<td>1</td>
<td>525.64</td>
<td>31.15</td>
<td>0.0003</td>
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<td>36.13</td>
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<td>36.13</td>
<td>2.14</td>
<td>0.1774</td>
</tr>
<tr>
<td>AC</td>
<td>1035.12</td>
<td>1</td>
<td>1035.12</td>
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<td>&lt; 0.0001</td>
</tr>
<tr>
<td>BC</td>
<td>120.12</td>
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<tr>
<td>C²</td>
<td>397.61</td>
<td>1</td>
<td>397.61</td>
<td>23.57</td>
<td>0.0009</td>
</tr>
<tr>
<td>Residual</td>
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<td>9</td>
<td>16.87</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lack of Fit</td>
<td>46.60</td>
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<td>9.32</td>
<td>0.3542</td>
<td>0.8676</td>
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<td>105.25</td>
<td>4</td>
<td>26.31</td>
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</tr>
<tr>
<td>Cor Total</td>
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<td>19</td>
<td></td>
<td></td>
<td></td>
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</tbody>
</table>

Keys to Analyzing an RSM Design
Response Surface Methods Case
Post-ANOVA (Fit Statistics)

<table>
<thead>
<tr>
<th>Std. Dev.</th>
<th>R²</th>
<th>Adeq Precision</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.11</td>
<td>0.9440</td>
<td>16.2944</td>
</tr>
</tbody>
</table>

**Mean** 78.30  **Adjusted R²** 0.8881  **Predicted R²** 0.7891

**Standard Deviation**: the amount of random variation left in the process.

**Adjusted R²**: the amount of variation in the data, that is explained by the model. (higher is better)

**Predicted R²**: the amount of variation in predictions, that is explained by the model. (higher is better, and within .2 of adjusted R² to show that the model is not over-fit)

---

Response Surface Methods Case
Prediction Equations

### In Terms of Coded Factors:

<table>
<thead>
<tr>
<th>Conversion</th>
<th>=</th>
</tr>
</thead>
<tbody>
<tr>
<td>+81.60</td>
<td></td>
</tr>
<tr>
<td>+1.03</td>
<td>* A</td>
</tr>
<tr>
<td>+4.04</td>
<td>* B</td>
</tr>
<tr>
<td>+6.20</td>
<td>* C</td>
</tr>
<tr>
<td>+2.13</td>
<td>* AB</td>
</tr>
<tr>
<td>+11.37</td>
<td>* AC</td>
</tr>
<tr>
<td>-3.87</td>
<td>* BC</td>
</tr>
<tr>
<td>-1.90</td>
<td>* A²</td>
</tr>
<tr>
<td>+2.88</td>
<td>* B²</td>
</tr>
<tr>
<td>-5.25</td>
<td>* C²</td>
</tr>
</tbody>
</table>

### In Terms of Actual Factors:

<table>
<thead>
<tr>
<th>Conversion</th>
<th>=</th>
</tr>
</thead>
<tbody>
<tr>
<td>+1026.77403</td>
<td></td>
</tr>
<tr>
<td>-11.56883</td>
<td>* time</td>
</tr>
<tr>
<td>-18.70551</td>
<td>* temperature</td>
</tr>
<tr>
<td>+44.50242</td>
<td>* catalyst</td>
</tr>
<tr>
<td>+0.085000</td>
<td>* time * temperature</td>
</tr>
<tr>
<td>+4.55000</td>
<td>* time * catalyst</td>
</tr>
<tr>
<td>-1.55000</td>
<td>* temperature * catalyst</td>
</tr>
<tr>
<td>-0.075839</td>
<td>* time²</td>
</tr>
<tr>
<td>+0.11508</td>
<td>* temperature²</td>
</tr>
<tr>
<td>-21.01890</td>
<td>* catalyst²</td>
</tr>
</tbody>
</table>

Both equations useful for predictions. **Coded** is useful for interpretation (relative effects). **Actual** coefficients account for differences in factor ranges so not easy to interpret.
Response Surface Analysis Steps

- Fit Summary
- ANOVA & Statistics
- Diagnostics
- Model Reduction
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- Wrap Up

Response Surface Methods Case

Residual Analysis

Data

(Observed Values)

\( Y_i \)

Signal + Noise

Analysis

Filter Signal

Model

(Predicted Values)

\( \hat{Y}_i \)

Signal

Residuals

(Observed - Predicted)

\( e_i = Y_i - \hat{Y}_i \)

Noise

Independent \( N(0, s^2) \)
Response Surface Methods Case
Diagnostics – validate ANOVA

Fairly straight line 😊 No particular pattern 😐

Keys to Analyzing an RSM Design

Response Surface Methods Case
Influence – measures influence of each point

Change in model fit with/without point.
Change in predictions due to position in design space.
Change in predictions with/without point.
Change in each coefficient with/without point.

Keys to Analyzing an RSM Design

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Agenda

Response Surface Analysis Steps

- Fit Summary
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Keys to Analyzing an RSM Design

Response Surface Methods Case

Backing up: ANOVA – remove non-significant terms

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Keys to Analyzing an RSM Design
Algorithmic Model Reduction

Design-Expert software offers four Criteria and several Selection methods.

<table>
<thead>
<tr>
<th>Criterion</th>
<th>Selection method</th>
</tr>
</thead>
<tbody>
<tr>
<td>p-values (smaller better)</td>
<td>Forward, Backward, Stepwise</td>
</tr>
<tr>
<td>AICc (lower better)</td>
<td>Forward, Backward</td>
</tr>
<tr>
<td>BIC (lower better)</td>
<td>Forward, Backward</td>
</tr>
<tr>
<td>Adj R-squared (higher better)</td>
<td>All Hierarchical</td>
</tr>
</tbody>
</table>

For experiments with minimal collinearity all combinations of criterion and selection method work well. We recommend going with the default criterion of AICc, but change the selection method to backward. With high collinearity we also recommend a second pass using AICc with forward selection. Compare their respective models. If they agree, then you’re done. Otherwise try other methods before settling on a model.

All model reduction must be guided by the subject matter knowledge!

Algorithmic Model Reduction

Selection Methods

**Backward**: Start with all model terms. Eliminate the worst one and recalculate. Eliminate the next worst one and recalculate. Continue eliminating terms until the stopping condition is met.

**Forward**: Start with the linear term most correlated with the response. Add a term, calculate the statistical criterion, add another term and recalculate. Continue adding terms that add value to the model until the stopping condition is met.

**Stepwise** (p-value only): Start forward, recalculate and apply backward if needed, then forward, backward, etc until the stopping condition is met.
Algorithmic Model Reduction

For well designed experiments (having minimal collinearity problems) all methods yield reduced models that generate very similar surface renderings.

However, if you just collect historical data (e.g. from QC records on manufacturing) the factors will almost certainly be correlated. In such cases the terms kept in the reduced model will change depending on the criterion and method of reduction.

The solution: **Apply good DOE to avoid problems and help ensure getting a consistent model when reducing terms!**

---

Response Surface Methods Case
Model Graphs – find best settings
Agenda

Response Surface Analysis Steps

- Fit Summary
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Response Surface Methods Case

Last Step: Confirmation

The final stage of a designed experiment is to confirm that the model predictions are accurate in the original process.

Complete a few runs at the:

1. optimum, or
2. across the design space.

Enter data into the confirmation node and verify that the mean of the confirmation runs falls within the 95% prediction interval.
Response Surface Methods Case
Last Step: Confirmation

Enter the process conditions (location) for the runs.

Enter the run data.

Confirm that the Data Mean is within the 95% Prediction Interval.

(The Data Mean will be red if it is outside the interval.)
Response Surface Methods Case
Confirmation Failure??

What if the confirmation fails? Consider the following:

1. Was the analysis good – lack of fit, predicted $R^2$, diagnostics?
2. Did the process shift, is it stable?
3. Are there other process factors that may affect the system?

If confirmation fails, then you need to take an engineering/science look at the system and decide how you can get better data.

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**Keys to Analyzing an RSM Design**

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Final Remarks

All statistical analysis should be guided by subject matter knowledge.
- Does it make sense that the given terms are significant?
- Do the model graphs reflect the actual process?
- Do the confirmation runs verify the analysis?
Design-Expert 13 Exclusive Preview

Many new, user-requested features!
• Modify Design Space Wizard
• Round Factor Levels
• Poisson Regression
• Multiple Analyses
• Import Data Wizard
• Box Plot, Post-Build Edit Constraints, and more!

Continuing Education


**Cutting-Edge Tools Unveiled in Design-Expert Version 13 – February 17**

Learn about all the new DX13 features and how they will help you make the most of your experiments.

**Making the Most from Measuring Counts – March 11**

Discover how to use the new Poisson regression option for analyzing count data such as manufacturing defects, or other like data.
Stat-Ease Training: Sharpen Up Your DOE Skills

Modern DOE for Process Optimization (Apr 12-16)
Mixture Design for Optimal Formulations (Mar 22-25)

<table>
<thead>
<tr>
<th>Individuals</th>
<th>Teams (6+ people)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Improve your DOE skills</td>
<td>Choose your date &amp; time</td>
</tr>
<tr>
<td>Topics applicable to both novice and advanced practitioners</td>
<td>Add company case studies</td>
</tr>
</tbody>
</table>

Learn more: [www.statease.com](http://www.statease.com)
Contact: [workshops@statease.com](mailto:workshops@statease.com)

Resources*

<table>
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<td><img src="image3.png" alt="Formulation Simplified" /></td>
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</table>

* Taylor & Francis/CRC/ Productivity Press
New York, NY.
Thank you for listening!

Questions? Email shari@statease.com