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**!
Preview at the end of this webinar.

Live Web Process DOE Workshop
**February 8-12**

**Modern DOE for Process Optimization**
Optimize your processes by mastering factorial and response surface designs in this 1-week (5 half-day sessions) instructor-led online course. 9:00am - 12:30pm (USA Central Time)

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**Agenda**

- **Fundamentals of an RSM design**
- Central Composite design
- Box-Behnken design
- Optimal design
- Wrap Up & Peek at DX13
DOE Umbrella
Where do Response Surface (RSM) designs fit?

Key Properties for an RSM Design

1. Fit desired polynomial – model points are selected to estimate the polynomial chosen by the experimenter.
2. Lack of fit test – additional information to test model adequacy.
   ✓ Include 4-5 more unique design points than coefficients in the model.
   ✓ Include 4-5 replicates to provide an estimate of “pure” error.
3. Low prediction error - generate useful predictions throughout the region of interest.
4. Reasonable number of runs – just enough runs to get necessary information.
1. Polynomial Models

Most response surface designs fit a full quadratic model:
\[ \hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 \]

Shape parameters *(pictures on following slide)*:
- Intercept – a horizontal plane.
- Linear terms – slopes (gradients) of the plane.
- Two-Factor interactions – twists in the plane.
- Squared terms – symmetric curvature.
- Cubic terms – asymmetry (inflection).

1. Polynomial Models

Coefficients define shape of response surface

<table>
<thead>
<tr>
<th>Intercept</th>
<th>Linear terms</th>
<th>Two-Factor Interaction</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1" alt="Intercept" /></td>
<td><img src="image2" alt="Linear terms" /></td>
<td><img src="image3" alt="Two-Factor Interaction" /></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Quadratic</th>
<th>Cubic</th>
<th>Cubic</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image4" alt="Quadratic" /></td>
<td><img src="image5" alt="Cubic" /></td>
<td><img src="image6" alt="Cubic" /></td>
</tr>
</tbody>
</table>

Keys to RSM Design

7

8
2. Selecting Design Points
Model, Lack of Fit, Replicates

- Model points
- Lack of Fit points
- Replicates

3. Prediction Error

Design point locations should keep the standard error of predictions in the middle of the design relatively low.
Top Three Response Surface Designs

Central Composite

Optimal

Box-Behnken

*All of these designs are statistically sound, and likely more efficient than what an experimenter would create by hand.*

Keys to RSM Design

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Keys to RSM Design
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.

Central Composite Design
Template for 3 Factors

<table>
<thead>
<tr>
<th>Factorial points:</th>
<th>A</th>
<th>B</th>
<th>C</th>
</tr>
</thead>
<tbody>
<tr>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Axial (star) points:</th>
<th>-α</th>
<th>0</th>
<th>0</th>
</tr>
</thead>
<tbody>
<tr>
<td>α</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>-α</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>α</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>-α</td>
<td>0</td>
</tr>
</tbody>
</table>

| Center points: | 0  | 0  | 0  |
|               | 0  | 0  | 0  |
|               | 0  | 0  | 0  |
|               | 0  | 0  | 0  |
|               | 0  | 0  | 0  |

α (alpha) is the coded distance from the center to the axial (star) points.
Central Composite Design
Example 3 Factor design – Tutorials “Conversion”

Customize the axial runs by rounding or modifying.

Choices for Alpha
Watch Out for Axial Points Going Too Far Out

CCD Options (highlights):

- **Rotatable** *(default k< 6)*
  Ideal statistically but increases quickly as the number of factors (k) goes up.

- **Practical** *(default k > 5)*
  Alpha = k⁴ (4th root) pushes axials outside the box, but not too far.

- **Face centered** *(not advised for k>8)*
  Alpha = 1 makes CCDS only 3 level, but variance inflation factors (VIFs) increase with more factors.

*keeps prediction error equal at points equidistant from the center*
Central Composite Design
Keys for usage

- **Axial points**: watch the experimental values of the axial points
  - Use practical alpha if needed
  - Manually adjust the factor setting if a point is too far out (i.e., goes negative)

- **Center point replicates**: use default replicates of the center point – keeps the prediction error in the middle of the design low

- **Blocking**: use statistical blocking if the design needs to be run over multiple days, or to remove another potential source of noise (details beyond this webinar)

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Box-Behnken Design
Point Layout (3-factor example)

The geometry of the 3-factor design involves 12 points lying on a sphere about the center (in this case at v2) with 5 replicates of the center point.

Box-Behnken Design
Design Matrix (3-factor example)

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>C</th>
</tr>
</thead>
<tbody>
<tr>
<td>−1</td>
<td>−1</td>
<td>0</td>
</tr>
<tr>
<td>+1</td>
<td>−1</td>
<td>0</td>
</tr>
<tr>
<td>−1</td>
<td>+1</td>
<td>0</td>
</tr>
<tr>
<td>+1</td>
<td>+1</td>
<td>0</td>
</tr>
<tr>
<td>−1</td>
<td>0</td>
<td>−1</td>
</tr>
<tr>
<td>+1</td>
<td>0</td>
<td>−1</td>
</tr>
<tr>
<td>−1</td>
<td>0</td>
<td>+1</td>
</tr>
<tr>
<td>+1</td>
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<td>+1</td>
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<td>0</td>
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<td>0</td>
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<td>+1</td>
</tr>
<tr>
<td>*0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

*We suggest 5 center points

No runs where all factors are set to the extremes.
Box-Behnken Design

**Description:**
- Efficient three-level design for fitting second-order response surfaces for up to 21 factors.

**Advantages:**
- Only 3 levels (vs 5 for CCD)
- Can be blocked orthogonally (except for k*=3)
- Rotatable (for k= 4,7) or nearly so

**Drawbacks:**
- Not as flexible as CCD which allows:
  1. Factorial with center points (stop here if no curvature)
  2. Second block of axial (star) points only if needed

*\( k = \) number of factors

Box-Behnken discussion

**Quote from client A:**
“*I use the Box-Behnken design because it does not have points at the corners of the design space, so I don’t have to worry about those high-high-high or low-low-low factor combinations that potentially don’t work for my process.*”

**Quote from client B:**
“*I never use the Box-Behnken because it does not put points at those extreme combinations of the design space. The Central Composite design fills my process space better.*”

Choose the design that fits the problem!!
Agenda

- Fundamentals of an RSM design
- Central Composite design
- Box-Behnken design
- **Optimal design**
- Wrap Up & Peek at DX13

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**Optimal (custom) Design**

**Description:**
- Computer-generated design to fit a selected model. Include lack of fit points and replicate points for robustness (defaults).

**Advantages:**
- Customize the polynomial model
- Add constraints to fit an irregular-shaped design space
- Good design properties if software defaults used

**Drawbacks:**
- Different point layout each time design generated
- You don’t control the number of levels (unless discrete factors)
- Points may be at inconvenient values (may need to round)
Optimal Design
Examples – 2 factor, quadratic model

1. Select **polynomial** - that will likely approximate the actual response surface. (Refer back to the pictures – which one most likely?)
   - Default is a *quadratic model*.

2. Select the **optimality** criteria (see next slides).
   - Default is *I-optimal for response surface design*.

3. Select **point selection** method (see next slides).
   - Default is *Both Exchanges, with several designs built using point exchange and several built using coordinate exchange. Most optimal design is displayed to the experimenter*.

**Recommendation: Use the software defaults!!!**

Keys to RSM Design 25

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Keys to RSM Design 26
Optimality: D-optimal

Goal: D-optimal design minimizes the determinant of the \((X'X)^{-1}\) matrix. This minimizes the volume of the confidence ellipsoid for the coefficients and maximizes information about the polynomial coefficients.

Uncorrelated Coefficients

\[
\beta_1 \quad \beta_2
\]

Correlated Coefficients

\[
\beta_1 \quad \beta_2
\]

Note: the confidence ellipsoid is not a standard error plot.

Optimality: I-optimal

An I-optimal design seeks to minimize the integral of the prediction variance across the design space. These designs are built algorithmically to provide lower integrated prediction variance across the design space. This equates to minimizing the area under the fraction of design space (FDS) curve.

Keys to RSM Design

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D-optimal versus I-optimal
One Factor 12 run Design

One factor twelve run quadratic model designs:

D-optimal

I-optimal

Keys to RSM Design

Optimality Choice

What you need to remember:

- D-optimal is precise estimation of model coefficients
  
  *Best for factorial designs that detect effects.*

- I-optimal is precise estimation of the response
  
  *Best for response surface designs that optimize predictions.*

These are the Design-Expert software default settings.
Design Point Selection algorithm

Start with an initial selection of design points and then switch points in and out, keeping the set with the highest optimality score. Points are selected and switched 1 at a time, then 2 at a time, etc., based on either:

Point Exchange or Coordinate Exchange

1. To increase the chances of finding the global optimum, a number of designs are built. Using the best (both exchange) option:
   - Half the designs are built using point exchange.
   - Half the designs are built using coordinate exchange.

2. The most optimal of these builds is selected as the final design.

3. “Best” (DX12 & earlier) or “Both Exchanges” (DX13) is our recommended point selection algorithm.

Design Point Selection
Best/Both Exchange Algorithm

Keys to RSM Design

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Optimal (custom) Design Summary

- Flexible design options
- Factors can be
  - numeric – continuous
  - numeric – discrete (1, 4, 7)
  - categoric – classes/names
- Multilinear constraints can be added to cut off a portion of the design space that would not provide measurable results.
- Polynomial models – linear, quadratic, cubic, custom, etc.

While “flexibility” is great, follow good statistical design principles!

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Choosing a Response Surface Design

<table>
<thead>
<tr>
<th>Criteria</th>
<th>Central Composite</th>
<th>Box-Behnken</th>
<th>Optimal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Factor levels</td>
<td>5, 3 optional</td>
<td>3</td>
<td>varies</td>
</tr>
<tr>
<td>Design Space</td>
<td>Axial points located outside factorial box</td>
<td>Factorial cube doesn’t include corners</td>
<td>Defined by factor limits, not limited to cube</td>
</tr>
<tr>
<td>Includes Lack of Fit</td>
<td>Yes</td>
<td>Yes</td>
<td>With defaults</td>
</tr>
<tr>
<td>Includes Replicates</td>
<td>Yes – center point</td>
<td>Yes – center point</td>
<td>With defaults, chosen by optimality</td>
</tr>
<tr>
<td>Low Prediction Error</td>
<td>Yes</td>
<td>Yes</td>
<td>With defaults</td>
</tr>
<tr>
<td>Choose when:</td>
<td>Region of interest is a cube</td>
<td>Region of interest is a sphere</td>
<td>Region of interest is custom</td>
</tr>
</tbody>
</table>

Keys to RSM Design

Final Notes

*All of these designs are statistically sound, and likely more efficient than what an experimenter would create by hand.*

Choose the design that fits the problem!
Many new, user-requested features!

• Modify Design Space Wizard
• Round Columns
• Poisson Regression
• Multiple Analyses
• Import Data Wizard
• Box Plot, Post-Build Edit Constraints, and more!

Modify Design-Space Augment Wizard
Design-Expert 13 Preview

Round Columns

Keys to RSM Design

Continuing Education


**Keys to Analyzing Response Surface Designs** – February 10

The follow-up to today’s webinar dives into the analysis of RSM designs. Learn more about the automated model selection methods and the keys that confirm a good analysis.

**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.
Stat-Ease Training:
Sharpen Up Your DOE Skills

Modern DOE for Process Optimization
Mixture Design for Optimal Formulations

<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>

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Contact: [workshops@statease.com](mailto:workshops@statease.com)

Resources*

3rd edition 2015

2nd edition 2016

1st edition 2018

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

Questions? Email shari@statease.com