Keys to Analyzing a Response Surface Design

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Making the most of this learning opportunity

Hide the Control Panel
Mute your line

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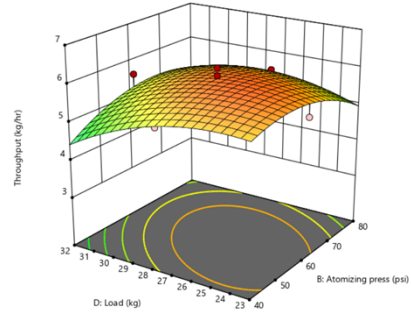
Note: The slides and a recording of this webinar will be posted on the Webinars page of the Stat-Ease website within a few days.

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)

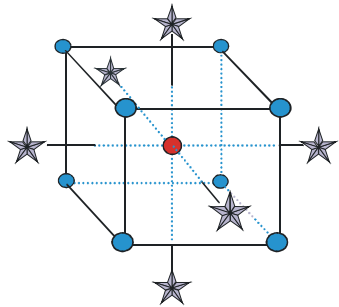Central composite design runs were conducted in two blocks:

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

Configure | Fit Summary | Model | ANOVA | Diagnostics | Model Graphs

1. Configure: Start with no transformation, click **Start Analysis**.
2. Fit Summary: Comparative statistics on polynomial models. *Do not select an aliased model: There are not enough runs to estimate all the coefficients!*
3. Model: Choose best (suggested) model for in-depth analysis. *Return here for model reduction.*
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*.*

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Response Surface Methods Case
Fit Summary

Source	Sequential p-value	Lack of Fit p-value	Adjusted R²	Predicted R²	
Linear	0.1640	0.0442	0.1374	-0.4682	
2FI	0.0083	0.1442	0.5803	0.3691	
Quadratic	**0.0017**	**0.8574**	**0.8881**	**0.7891**	**Suggested**
Cubic	0.8538	0.4836	0.8396	-3.6399	**Aliased**

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.
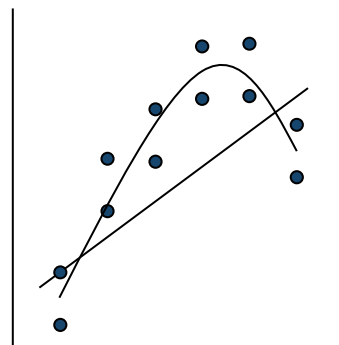
Lack of Fit
Six Replicated Design Points

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. *(Hint: No replicates = No lack of fit test)*

Response Surface Methods Case
Model Tab

Process Order: Quadratic | Auto Select...

Add Term

m	The term will be included in the model.
⚠	Indicates the term is aliased with another term, or was not estimated in the Fit Summary calculations. Including the term in the model is not recommended.
🔒	A user-forced term. Automatic model selection will always produce a model that includes this term.
🔒	Indicates that the term is required to be in the model by the program.

Model terms:
m Intercept
m A-time
m B-temperature
m C-catalyst
m AB
m AC
m BC
m A²
m B²
m C²
m ABC

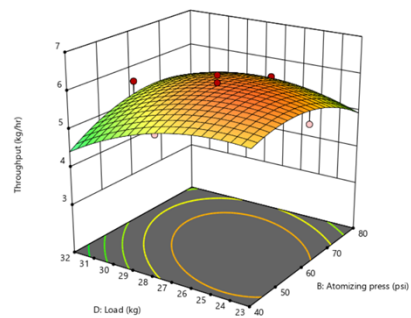*Suggested model is the default – usually okay to start there.*

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Response Surface Methods Case
ANOVA for Quadratic Model

Source	Sum of Squares	df	Mean Square	F-value	p-value	
Block	64.53	1	64.53			
Model	2561.82	9	284.65	16.87	0.0001	significant
A-time	14.44	1	14.44	0.8561	0.3790	
B-temperature	222.96	1	222.96	13.21	0.0054	
C-catalyst	525.64	1	525.64	31.15	0.0003	
AB	36.13	1	36.13	2.14	0.1774	
AC	1035.12	1	1035.12	61.35	< 0.0001	
BC	120.12	1	120.12	7.12	0.0257	
A^2	51.76	1	51.76	3.07	0.1138	
B^2	119.19	1	119.19	7.06	0.0261	
C^2	397.61	1	397.61	23.57	0.0009	
Residual	151.85	9	16.87			
Lack of Fit	46.60	5	9.32	0.3542	0.8574	not significant
Pure Error	105.25	4	26.31			
Cor Total	2778.20	19				

Response Surface Methods Case
Post-ANOVA (Fit Statistics)

Std. Dev.	4.11		**R^2**	0.9440
Mean	78.30		**Adjusted R^2**	0.8881
C.V. %	5.25		**Predicted R^2**	0.7891
			Adeq Precision	16.2944

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

Adjusted R^2: the amount of variation in the data, that is explained by the model. (higher is better)

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

Response Surface Methods Case
Prediction Equations

In Terms of **Coded** Factors:			In Terms of **Actual** Factors:		
Conversion	=		Conversion	=	
+81.60			+1026.77403		
+1.03	* A		-11.56883	* time	
+4.04	* B		-18.70551	* temperature	
+6.20	* C		+44.50242	* catalyst	
+2.13	* AB		+0.085000	* time * temperature	
+11.37	* AC		+4.55000	* time * catalyst	
-3.87	* BC		-1.55000	* temperature * catalyst	
-1.90	* A^2		-0.075839	* $time^2$	
+2.88	* B^2		+0.11508	* $temperature^2$	
-5.25	* C^2		-21.01890	* $catalyst^2$	

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.
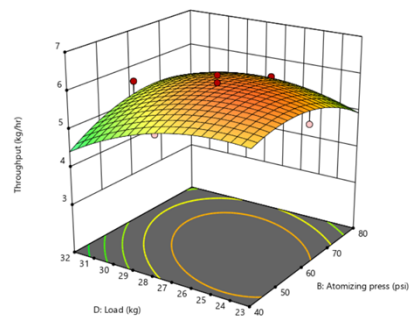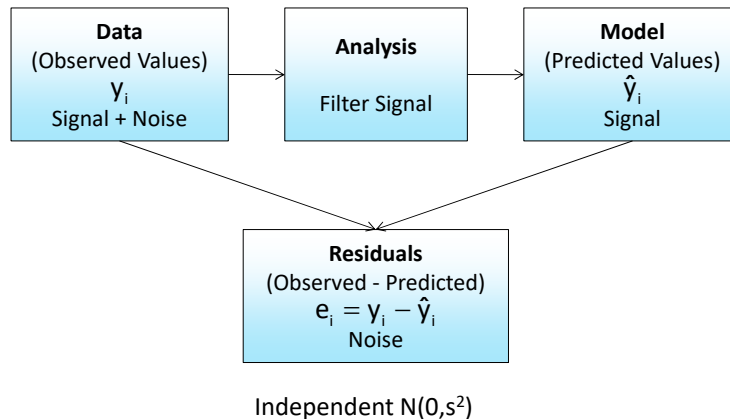

Agenda

Response Surface Analysis Steps

➢ Fit Summary

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➢ Wrap Up

| 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 $N(0, s^2)$

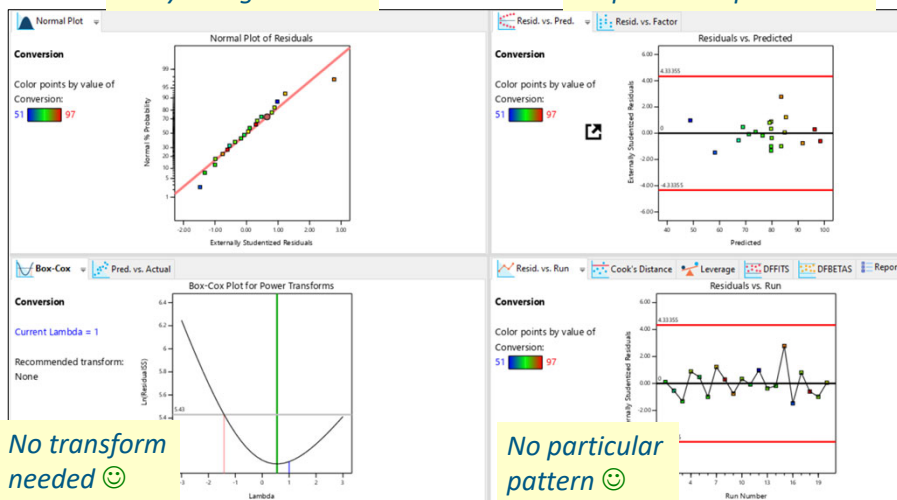Keys to Analyzing an RSM Design   15

Response Surface Methods Case
Diagnostics – validate ANOVA

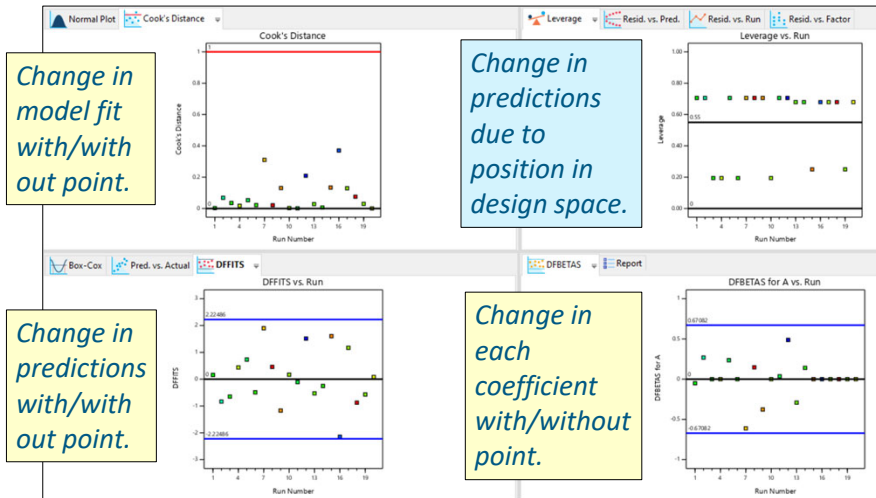*Fairly straight line* ☺   *No particular pattern* ☺

Normal Plot
Normal Plot of Residuals
Conversion
Color points by value of Conversion:
51   97

Resid. vs. Pred.   Resid. vs. Factor
Residuals vs. Predicted
Conversion
Color points by value of Conversion:
51   97

Box-Cox   Pred. vs. Actual
Box-Cox Plot for Power Transforms
Conversion
Current Lambda = 1
Recommended transform: None

Resid. vs. Run   Cook's Distance   Leverage   DFFITS   DFBETAS   Report
Residuals vs. Run
Conversion
Color points by value of Conversion:
51   97

No transform needed ☺   *No particular pattern* ☺

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Response Surface Methods Case
*Influence – measures influence of each point*

Change in model fit with/with out point.

Change in predictions due to position in design space.

Change in predictions with/with out point.

Change in each coefficient with/without point.

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Agenda

Response Surface Analysis Steps

➢ Fit Summary

➢ ANOVA & Statistics

➢ Diagnostics

➢ **Model Reduction**

➢ Confirmation

➢ Wrap Up
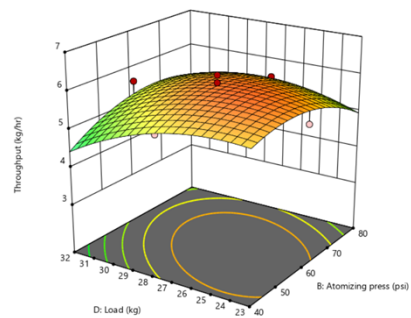
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Response Surface Methods Case
Backing up: ANOVA – remove non-significant terms

Source	Sum of Squares	df	Mean Square	F-value	p-value	
Block	64.53	1	64.53			
Model	2561.82	9	284.65	16.87	0.0001	significant
A-time	14.44	1	14.44	0.8561	0.3790	(needed for hierarchy)
B-temperature	222.96	1	222.96	13.21	0.0054	
C-catalyst	525.64	1	525.64	31.15	0.0003	
AB	36.13	1	36.13	2.14	0.1774	
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Algorithmic Model Reduction

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

Criterion	Selection method
p-values (smaller better)	Forward, **Backward**, Stepwise
AICc (lower better)	**Forward, Backward**
BIC (lower better)	Forward, Backward
Adj R-squared (higher better)	All Hierarchical

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!

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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
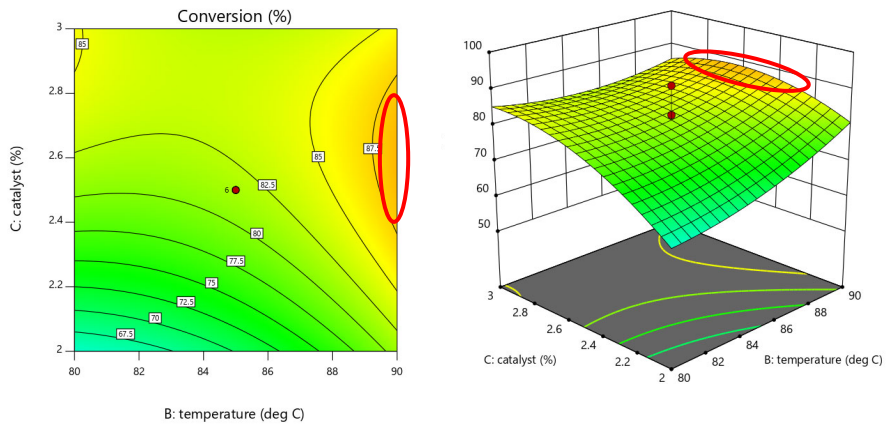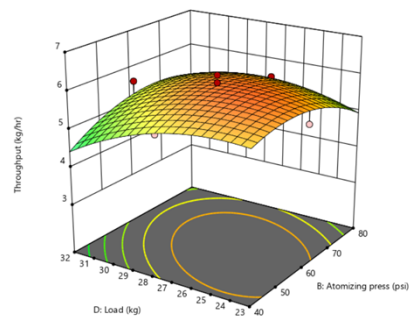
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Response Surface Analysis Steps

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➢ **Confirmation**

➢ Wrap Up

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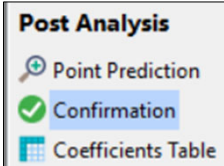
Response Surface Methods Case
Last Step: Confirmation

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.

Post Analysis
- Point Prediction
- ✅ Confirmation
- Coefficients Table

Response Surface Methods Case
Last Step: Confirmation

Confirmation Location #1 ⬇ Factors

Confirmation Location #1

	time	temperature	catalyst
	50	90	3

Enter the process conditions (location) for the runs.

Response data

Runs: 4

Enter the run data.

	Conversion
	92.3
	88
	98.6
	91.5

Response Surface Methods Case
Last Step: Confirmation

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

Confirmation

Two-sided   Confidence = 95%

Solution 1 of 49 Response	Predicted Mean	Predicted Median	Observed	Std Dev	n	SE Pred	95% PI low	Data Mean	95% PI high
Conversion	96.8139	96.8139		4.66845	4	4.1401	87.7016	92.6	105.926

(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.
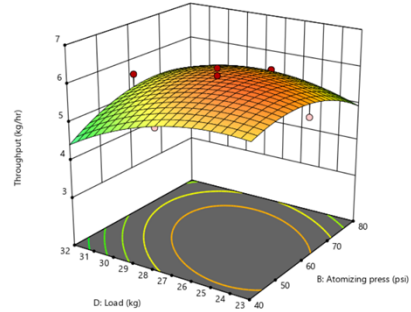
Agenda

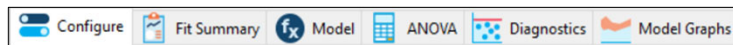**Response Surface Analysis Steps**

➢ Fit Summary

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➢ **Wrap Up**

Keys to Analyzing an RSM Design

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Response Surface Methods Case
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7. Confirmation: Verify the model predictions with confirmation runs*.*

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Final Remarks

| Configure | Fit Summary | Model | ANOVA | Diagnostics | Model Graphs |
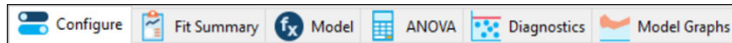
All statistical analysis should be guided by subject matter knowledge.

- Does it make sense that the given terms are significant?
- Do the model graphs reflect the actual process?
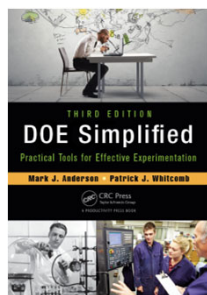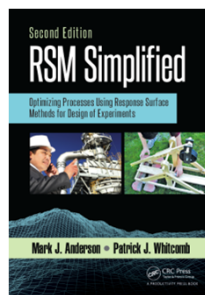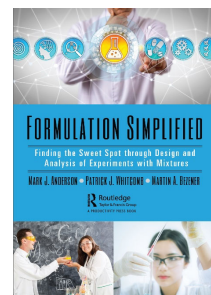- Do the confirmation runs verify the analysis?

Resources*

* Taylor & Francis/CRC/
Productivity Press
New York, NY.

Self-study options for learning more

YouTube Channel: www.youtube.com/c/StatisticsMadeEasybyStatEase

Playlist: New to DOE?

A collection of webinars on basic to intermediate-level topics.

Stat-Ease Academy: www.statease.com/training/academy/

Self-paced online courses covering the basics of factorial and fractional-factorial designs.

Thank you for listening!

Questions? Email stathelp@statease.com