The Art of Augmentation
Adding Runs to Existing Designs

Shari Kraber, MS Applied Statistics
Senior Client Success Manager
Stat-Ease, Inc.

shari@statease.com

January 2023

Maximizing this educational opportunity

Welcome everyone! To make the most from this webinar:

- Attendees on mute

- Questions addressed afterward

- Send further questions to stathelp@statease.com

Presentation posted: www.statease.com/webinars/ and
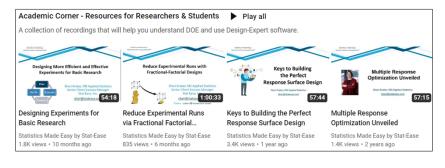
▶ YouTube   Statistics Made Easy by Stat-Ease

Stat-Ease YouTube Channel

Easy source for more content: **StatisticsMadeEasybyStatEase**

On this channel, explore playlists on DOE topics:

Academic Corner - Resources for Researchers & Students ▶ Play all

A collection of recordings that will help you understand DOE and use Design-Expert software.

Designing Experiments for Basic Research	Reduce Experimental Runs via Fractional Factorial...	Keys to Building the Perfect Response Surface Design	Multiple Response Optimization Unveiled
Statistics Made Easy by Stat-Ease	Statistics Made Easy by Stat-Ease	Statistics Made Easy by Stat-Ease	Statistics Made Easy by Stat-Ease
1.8K views • 10 months ago	835 views • 6 months ago	3.4K views • 1 year ago	1.4K views • 2 years ago

The Art of Design Augmentation

Augmentation is an **ART**, as well as a science. You need to first understand your existing data – what information does it provide, what is it missing? Then choose more runs that satisfy your goals.

- Do you want to estimate a higher-order polynomial?
- Do you want to fill out the design space or cover a specific area more thoroughly?
- Do you want to reduce the standard error of predictions in a specific area?

Software can help choose runs, but ultimately you need to use subject matter knowledge and an understanding of your goals to decide the best augmentation path.

Agenda: Art of Design Augmentation

- ➤ **Understanding the structure of a traditional DOE**
- ➤ Goals of Design Augmentation
- ➤ Case 1: Existing Data
  - ➤ Evaluate Current Data
  - ➤ Optimal Augmentation
- ➤ Case 2: Augmenting OFAT to CCD
  - ➤ Evaluate Current Data
  - ➤ Custom Factorial Augmentation
- ➤ Summary
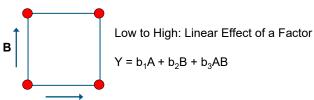

Structure of a traditional DOE
Background knowledge

Experimentation Goal: Improve a product or process

Design of experiments (DOE) uses a specific pattern/layout of factor combinations so that a statistical relationship can be established between the input factors and the output responses.

How? Fit a polynomial model to the data that estimates the factor versus response relationship and makes reliable predictions of future performance.

Low to High: Linear Effect of a Factor

$$Y = b_1A + b_2B + b_3AB$$

B
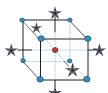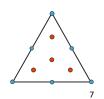
A

Types of DOE's

Factorial – <u>Two levels</u> (low/high) for each factor allows estimation of main effects and interactions for either a screening or characterization study. Minimal work for maximum information.

Response surface – <u>Three+ levels</u> for each factor allows estimation of quadratic (or higher-order) polynomials to model non-linear factor-response relationships.

Mixture* – Model formulations where the responses are dependent on the proportions of the mixture components. Required to properly model the dependencies between the components.

*Jan 18 Webinar – Crash Course in Mixture DOE

Agenda: Art of Design Augmentation

➢ Understanding the structure of a traditional DOE

➢ **Goals of Design Augmentation**

➢ Case 1: Existing Data

  ➢ Evaluate Current Data

  ➢ Optimal Augmentation

➢ Case 2: Augmenting OFAT to CCD

  ➢ Evaluate Current Data

  ➢ Custom Factorial Augmentation

➢ Summary

Possible Goals of Augmentation

Add runs in order to:

1. Estimate a higher-order polynomial (original runs may have aliasing)
   a. Estimate main effects cleanly
   b. Estimate two-factor interactions cleanly
   c. Estimate non-linear (quadratic) effects
2. Improve the modeling in a particular part of the design space
   a. Reduce the standard error of predictions
   b. Confirm model fit

Augmentation: Add runs that fill out the design space appropriately to meet your goals.

Agenda: Art of Design Augmentation

➢ Understanding the structure of a traditional DOE
➢ Goals of Design Augmentation
➢ **Case 1: Existing Data**
  ➢ **Evaluate Current Data**
  ➢ Optimal Augmentation
➢ Case 2: Augmenting OFAT to CCD
  ➢ Evaluate Current Data
  ➢ Custom Factorial Augmentation
➢ Summary

Step 1: Evaluating Current Data

Evaluate the current data using **Design Evaluation**:

1. Check **aliasing**:

    • What can be estimated now?

    • Which additional terms do you want to estimate?

    • How many more runs can you afford?

2. Graph the data – **Custom Graphs** and/or **Contour plot**:

    • Are there areas of the design space that you are more interested in? (may want to manually add some runs)

Step 2: Choosing an Augmentation method

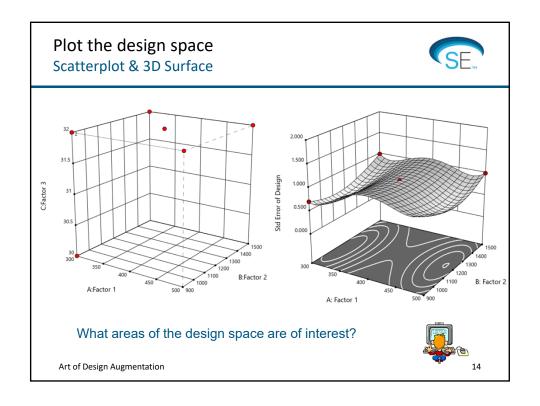**Starting from a response surface DOE or existing data (focus today):**

1. RSM Optimal – adds runs based on the additional terms selected

Starting from a 2-level factorial design (not reviewing here):

1. Foldover – adds the "opposite" set of runs

2. Semi-foldover – adds 50% more runs

3. Factorial Optimal – adds runs based on the additional terms selected

4. Central Composite – adds axial points and center points to a 2-level factorial design to estimate a quadratic model

6

Example 1: Existing data
Evaluate the existing aliases

The original set of runs done by an R&D scientist:

Run	A:Factor 1	B:Factor 2	C:Factor 3	Response
1	300	900	32	287
2	300	1500	32	265
3	500	900	32	438
4	500	1500	32	474
5	400	1200	32	547
6	300	900	32	268
7	300	900	30	448

Alias Matrix

Estimated Term	Aliased Terms
Intercept	= Intercept + AC + BC + C²
A	= A + AC
B	= B + BC
C	= C - AC - BC
AB	= AB
A²	= A² + B²

There are 4 aliased terms for a quadratic model: AC, BC, B^2, C^2

Factor C only has 1 run at the low level (30).

Art of Design Augmentation

13

Plot the design space
Scatterplot & 3D Surface

What areas of the design space are of interest?

Art of Design Augmentation

14

Agenda: Art of Design Augmentation

- ➤ Understanding the structure of a traditional DOE
- ➤ Goals of Design Augmentation
- ➤ **Case 1: Existing Data**
  - ➤ Evaluate Current Data
  - ➤ **Optimal Augmentation**
- ➤ Case 2: Augmenting OFAT to CCD
  - ➤ Evaluate Current Data
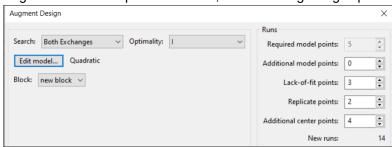 - ➤ Custom Factorial Augmentation
- ➤ Summary

What additional information?
Augment design to a specific model

Augment to fit a full quadratic model, in the existing design space.
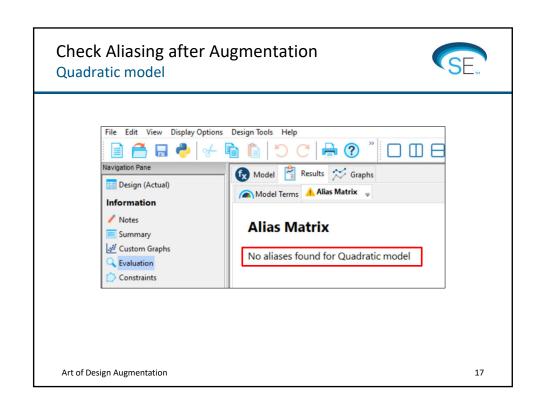

Edit model: change to Quadratic – 5 required points to fit model (inc. block)
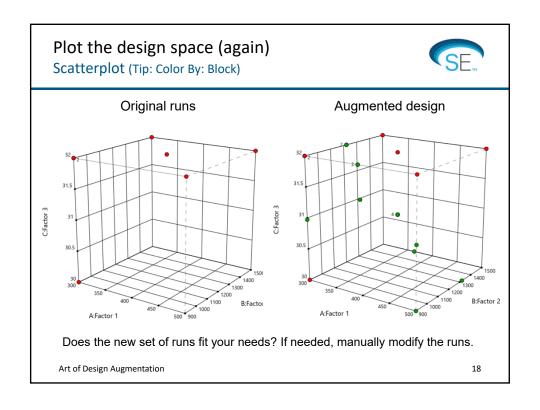**Lack of fit points:** added points in between the model points
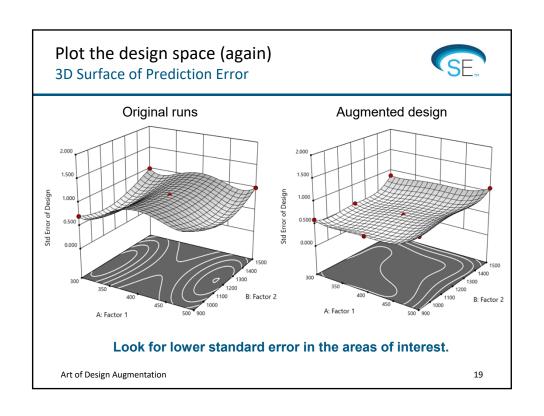**Replicate points:** required for a lack of fit test and reduce prediction error
Center points: add points to reduce the standard error in the center
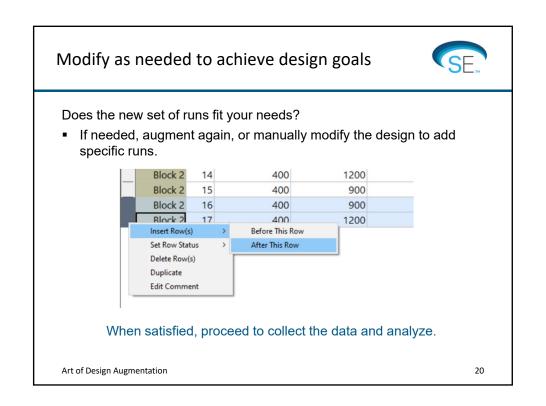
Check Aliasing after Augmentation
Quadratic model

Plot the design space (again)
Scatterplot (Tip: Color By: Block)

Original runs | Augmented design

Does the new set of runs fit your needs? If needed, manually modify the runs.

Plot the design space (again)
3D Surface of Prediction Error

Original runs   Augmented design

Look for lower standard error in the areas of interest.

Modify as needed to achieve design goals

Does the new set of runs fit your needs?

- If needed, augment again, or manually modify the design to add specific runs.

Block 2	14	400	1200
Block 2	15	400	900
Block 2	16	400	900
Block 2	17	400	1200

Insert Row(s)   >   Before This Row
Set Row Status   >   After This Row
Delete Row(s)
Duplicate
Edit Comment

When satisfied, proceed to collect the data and analyze.

Agenda: Art of Design Augmentation

- ➢ Understanding the structure of a traditional DOE
- ➢ Goals of Design Augmentation
- ➢ Case 1: Existing Data
  - ➢ Evaluate Current Data
  - ➢ Optimal Augmentation
- ➢ **Case 2: Augmenting OFAT to CCD**
  - ➢ **Evaluate Current Data**
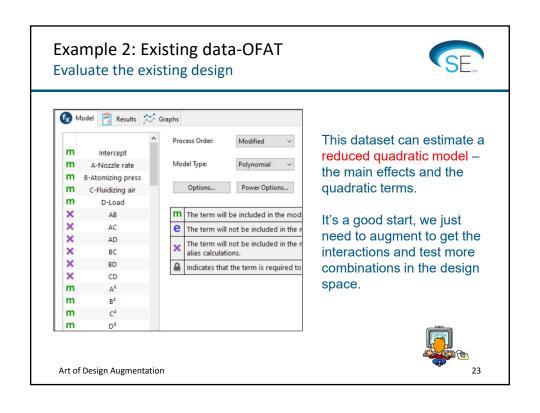 - ➢ Custom Factorial Augmentation
- ➢ Summary

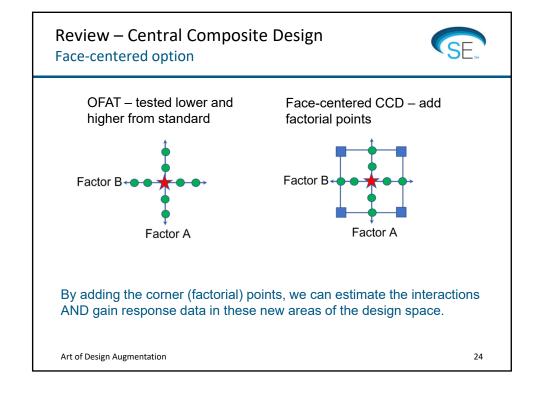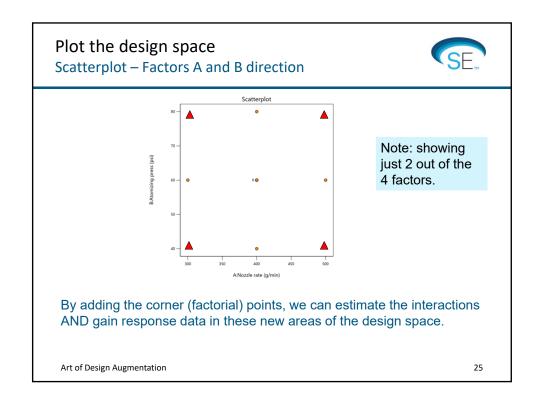## Example 2: Existing data-OFAT (4 factors)
Evaluate the existing design

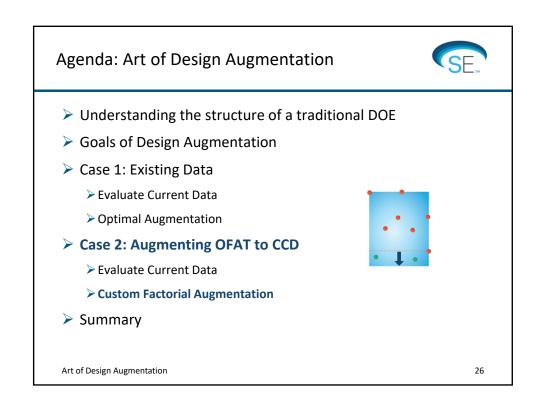| Run	A:Nozzle rate	B:Atomizing press	C:Fluidizing air	D:Load
	g/min	psi	scfm	kg
1	400	60	700	27.5
2	400	60	700	27.5
3	400	60	700	27.5
4	400	60	700	27.5
5	400	60	700	32
6	400	60	700	23
7	400	60	800	27.5
8	400	60	600	27.5
9	400	80	700	27.5
10	400	40	700	27.5
11	500	60	700	27.5
12	300	60	700	27.5

Four control/center points, followed by a low/high test for each factor, while holding the other factors constant (OFAT)!

Example 2: Existing data-OFAT
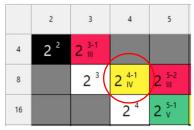### Evaluate the existing design

This dataset can estimate a **reduced quadratic model** – the main effects and the quadratic terms.

It's a good start, we just need to augment to get the interactions and test more combinations in the design space.

Review – Central Composite Design
Face-centered option

OFAT – tested lower and higher from standard

Face-centered CCD – add factorial points

By adding the corner (factorial) points, we can estimate the interactions AND gain response data in these new areas of the design space.

Plot the design space
Scatterplot – Factors A and B direction

Note: showing just 2 out of the 4 factors.

By adding the corner (factorial) points, we can estimate the interactions AND gain response data in these new areas of the design space.

Agenda: Art of Design Augmentation

- ➤ Understanding the structure of a traditional DOE
- ➤ Goals of Design Augmentation
- ➤ Case 1: Existing Data
  - ➤ Evaluate Current Data
  - ➤ Optimal Augmentation
- ➤ **Case 2: Augmenting OFAT to CCD**
  - ➤ Evaluate Current Data
  - ➤ **Custom Factorial Augmentation**
- ➤ Summary

What additional information?
Augment design to a specific model

- Current 4-factor design has axial and center points (typical OFAT design where experimenter is testing "a little lower and higher" for each factor).

- 2^4 factorial design = 16 runs (full factorial design)

- 2^{4-1} design = 8 runs (Resolution IV half-fraction factorial design)
  Considering this information, then combined with the existing runs, 8 more runs may be just enough to fit a full quadratic model, in the existing design space! *(Note: more runs would improve statistics!)*

How can we select a specific type of point when augmenting?

What additional information?
Augment design with specific points (factorial)

Augment to add factorial points (vertices).

Edit model: set to Quadratic – 7 required points to fit model

Additional model points: set to 1 for a total of 8 model points

Search method: Point Exchange

Points allowed: only Vertices

Check Evaluation & Graphs after Augmenting
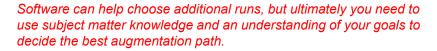
Confirm runs meet your needs!

1. Evaluation – check aliasing for desired model
2. Evaluation – check Standard Error graphs (Contour or 3D Surface)
3. Custom Graphs – build scatter plot of factors and view layout of new points

   Hint: Color by Block, check multiple views

If you find deficiencies:

   a. Manually edit runs or,
   b. Manually add more runs

Software can help choose additional runs, but ultimately you need to use subject matter knowledge and an understanding of your goals to decide the best augmentation path.

Agenda: Art of Design Augmentation

➤ Understanding the structure of a traditional DOE

➤ Goals of Design Augmentation

➤ Case 1: Existing Data

   ➤ Evaluate Current Data

   ➤ Optimal Augmentation

➤ Case 2: Augmenting OFAT to CCD

   ➤ Evaluate Current Data

   ➤ Custom Factorial Augmentation

➤ **Summary**

Summary: Augmentation of a data set

1. What does the current data set look like? (**Design Evaluation**)
   a. What polynomial terms can it estimate?
   b. Are there gaps in the data? (**Create pictures**)
   c. Compare to statistically-strong DOE's to determine a path
2. What is the most efficient way to estimate more effects?

Start with:	Augment method:
Fractional factorial	Foldover or Semi-fold
Response Surface	Optimal
One factor at a time	Custom point selection or Optimal
Historical data	Optimal

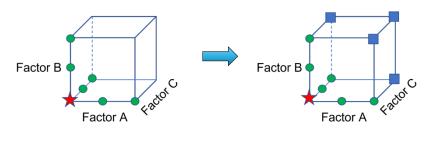Tip: Do 3-5 **more** runs than the minimum to get good statistics.

Summary: Augmentation of a data set

3. What does the new data set look like? (**Design Evaluation**)
   a. What polynomial terms can it estimate?
   b. Are there gaps in the data? (**Create pictures**)
4. Modify until it meets your needs. Then collect the data and analyze!

Modern DOE for Process Optimization

Mixture Design for Optimal Formulations

Individuals	Teams (6+ people)
Improve your DOE skills	Choose your date & time
Topics applicable to both novice and advanced practitioners	Add company case studies

Learn more: **www.statease.com**

Contact: **workshops@statease.com**

Art of Design Augmentation   33

Thank you for listening!

Questions? Email shari@statease.com