Innovative Mixture-Process Models and Designs

Dr. Geoff Vining

1

Outline:

- Important Background
- Origin of the Ideas Underlying the Designs
- "Selling" John Cornell
- Comments on Resulting Analysis
- NASA Reliability Computer Experiment

2

Important Background

- Virginia Tech Connection
  - My PhD: 1988, Virginia Tech (Ray Myers)
  - First Academic Position: 1988, University of Florida
    - John Cornell – Virginia Tech 1968 (Advisor: IJ Good!)
    - Andre Khuri – Virginia Tech 1976 (Ray Myers)
    - Week of Short-Courses
  - Doug Montgomery
    - Virginia Tech 1969 (Ray Myers, Not PhD Advisor))
    - Teaching Short-Courses for Doug

3

- My Initial Work: Robust Parameter Design
  - Motivation: Fit of Cap to Barrel of Pens
  - Real Problem: Faber-Castell 1981-1985
- Right Time, Right Place: Taguchi Phenomenon
  - Control Factors
  - Noise Factors
  - "Crossed" Control with Noise Experiment.
- Initial Interest: Efficient Analysis of Results

4

- Work with My Mentors
  - Myers, Khuri, Vining 1992: Taguchi Alternatives
  - Cornell: Evaluating Mixture Predictive Capability
  - Personal Introduction to Mixture Experiments
  - Fish Patty Data
    - 3 Mixture Components
    - 3 Process Variables
    - Crossed Experiment
    - If Need to Fractionate: Always Fractionate Process Exp.

5

Origin of the Basic KCV Ideas

- Mixtures Short-Course (mid 1990's)
  - Used Doug Montgomery's Notes
  - Example of Mixture-Process from the Notes
    - Used Ratios of the Mixture Components
    - Built Second-Order Surfaces
    - Design Not Efficient over Experimental Region
- Scott Kowalski Starting His Dissertation

6

- Basic Issues: John's World
  - Mixture Experiment More Important than Process
    - Process Variables: Basically Noise
    - Little Real Interest in Mixture-Process Interactions
- Reflection of the R&D-Production Divide
  - Corporate R&D "Owns" Formulation
  - Production Only the Operating Conditions
  - Interactions: How Formula Impacts Operation

7

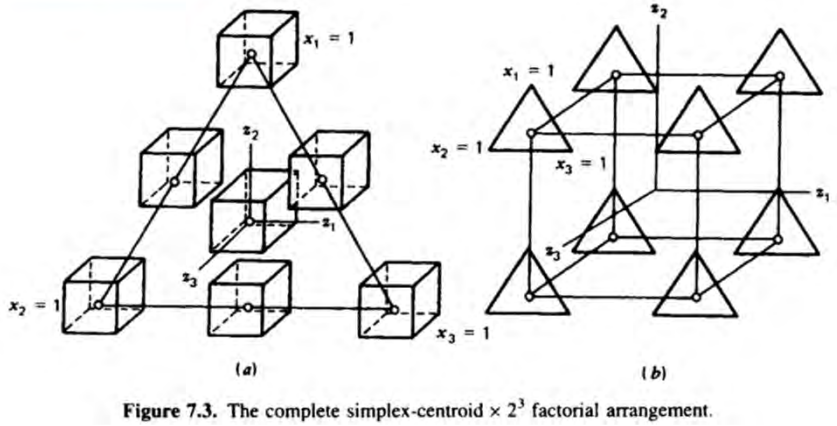

Figure 7.3. The complete simplex-centroid × 2^3 factorial arrangement.

8

StatEase
statistics made easy
Make the most from every experiment!

- Full Model – 56 Terms:

$$y(\mathbf{x},\mathbf{z}) = \sum_{i=1}^{3}\gamma_i^0 x_i + \sum\sum_{i<j}^{3}\gamma_{ij}^0 x_i x_j + \gamma_{123}^0 x_1 x_2 x_3 + \sum_{l=1}^{3}\left[\sum_{i=1}^{3}\gamma_i^l x_i + \sum\sum_{i<j}^{3}\gamma_{ij}^l x_i x_j + \gamma_{123}^l x_1 x_2 x_3\right] z_l + \sum\sum_{l<m}^{3}\left[\sum_{i=1}^{3}\gamma_i^{lm} x_i + \sum\sum_{i<j}^{3}\gamma_{ij}^{lm} x_i x_j + \gamma_{123}^{lm} x_1 x_2 x_3\right] z_l z_m + \left[\sum_{i=1}^{3}\gamma_i^{123} x_i + \sum\sum_{i<j}^{3}\gamma_{ij}^{123} x_i x_j + \gamma_{123}^{123} x_1 x_2 x_3\right] z_1 z_2 z_3 + \varepsilon \quad (7.4)$$

9

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- Fractional Factorial Model:

$$y(\mathbf{x},\mathbf{z}) = \sum_{i=1}^{3}\gamma_i^0 x_i + \sum\sum_{i<j}^{3}\gamma_{ij}^0 x_i x_j + \gamma_{123}^0 x_1 x_2 x_3 + \sum_{l=1}^{3}\left[\sum_{i=1}^{3}\gamma_i^l x_i + \sum\sum_{i<j}^{3}\gamma_{ij}^l x_i x_j + \gamma_{123}^l x_1 x_2 x_3\right] z_l + \varepsilon \quad (7.50)$$

10

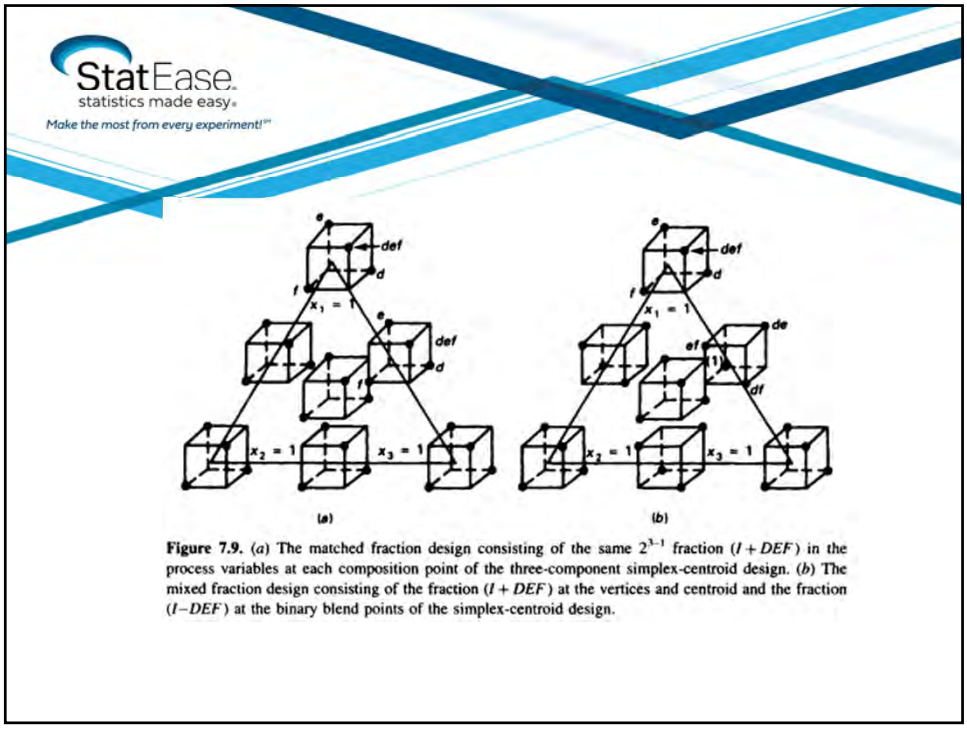


Figure 7.9. (*a*) The matched fraction design consisting of the same 2^{3-1} fraction ($I + DEF$) in the process variables at each composition point of the three-component simplex-centroid design. (*b*) The mixed fraction design consisting of the fraction ($I + DEF$) at the vertices and centroid and the fraction ($I - DEF$) at the binary blend points of the simplex-centroid design.

11

Common Reduced Model

$$y(\boldsymbol{x}, \boldsymbol{z}) = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{123} x_1 x_2 x_3 + \gamma_1 z_1 + \gamma_2 z_2 + \gamma_{12} z_1 z_2$$

There are no mixture by process interactions.

$$\gamma z = \gamma * 1 * z = \gamma(x_1 + x_2 + x_3)z = \gamma x_1 z + \gamma x_2 z + \gamma x_3 z$$

γ is an "average" value of the individual interactions

12

Selling John Cornell

- My Process for Mentoring PhD Students
  - Frequent Meetings with the Committee
  - Short Student Presentations
  - Get Past "Formal" Examinations
  - Focus on Collaboration
- Scott Was the Guinea Pig!
- Preparation for John Was Critical!

13

Scott's Presentation Structure

- Start with True Second-Order Model in Both
- Show Impact of the Mixture Constraint
- Highlight Resulting Model
- Show Figures of the Proposed Design Strategy
- Emphasize Robustness of the Design!

14

- Second-Order Model (3 Mixture, 2 Process):

$$y(\boldsymbol{x},\boldsymbol{z}) = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{123} x_1 x_2 x_3 + \gamma_{11} x_1 z_1 + \gamma_{21} x_2 z_1 + \gamma_{31} x_3 z_1 + \gamma_{12} x_1 z_2 + \gamma_{22} x_2 z_2 + \gamma_{32} x_3 z_2 + + \alpha_{11} z_1^2 + \alpha_{22} z_2^2 + \alpha_{12} z_1 z_2$$

- Actually, a Special Cubic in the Mixture!

15

- If There Are No Mixture-Process Interactions:

$$y(\boldsymbol{x},\boldsymbol{z}) = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 +$$

$$\beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{123} x_1 x_2 x_3 +$$

$$\gamma_1 z_1 + \gamma_2 z_2 + \gamma_3 z_3 +$$

$$\alpha_{11} z_1^2 + \alpha_{22} z_2^2 + \alpha_{12} z_1 z_2$$

16

- John's Reaction
  - For John, This Was a Formal Examination
  - Jumps to the Board Once Scott Proposed Model
  - Made Clear Not Going in Correct Direction
- My Reaction to John, "Just Sit Down!"
- Scott then Presented Basic *Design* Structure

17

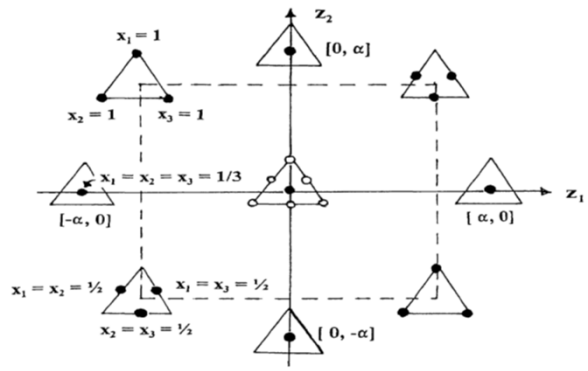


Figure 1. Two Central Composite Designs for Three Mixture Components and Two Process Variables. • Defines the 17-Point Design C: ○ Represents the Six Additional Points of Design F.

18

- John's Reaction to the Design: **Wow!**
  - Expected a Blind Optimal Design Application
  - Radical Idea: Fractionate the Mixture Portion!
  - Immediately Saw the Projection Properties
  - Saw Benefit in Overall Design Size
- *John Was Second Author on the Two Papers!*

19

Analysis of Mixture-Process Interaction:

- Consider the Test for the Mixture-Process Interactions Involving z_1:

$$H_0: \gamma_{11} = \gamma_{21} = \gamma_{31} = \gamma_1$$

- The Test Reduces to Comparing One γ_{j1} to the Average of the Other Two.
- A Basic "Two-Sample" t-Test.

20

- Result of Basic Mixture Constraint:
  - Mixture "Pure-Blend" Terms Remain Required
  - If One Mixture-Process Interaction is Important, Model Requires All with that Process Variable
- KCV Models Are Truly Second-Order
  - Often Higher for the Mixture Components
  - Often Have Better Interpretation than Traditional

21

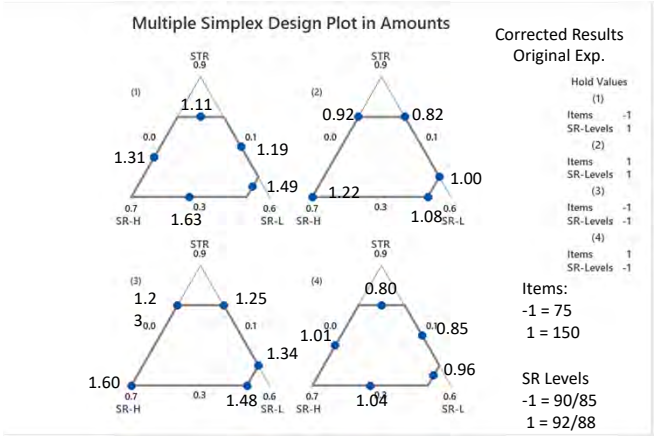
NASA Computer Experiment

- Understand What Impacts Reliability at Use
- Carbon Over-Wrapped Pressure Vessels
- Real Experiment, but Cannot Discuss Details
- Similar to a Mixture-Amount Problem
- NASA-SBU (Sensitive but Not Classified)

22

- Three Mixture Components:
  - STR: $.3 \leq x_1 \leq .7$
  - SR-H: $.1 \leq x_2 \leq .7$
  - SR-L: $0 \leq x_3 \leq .3$
- Two Process Variables:
  - Items: Numeric 75 - 150
  - Test-Plan: Categorical -1, +1

23



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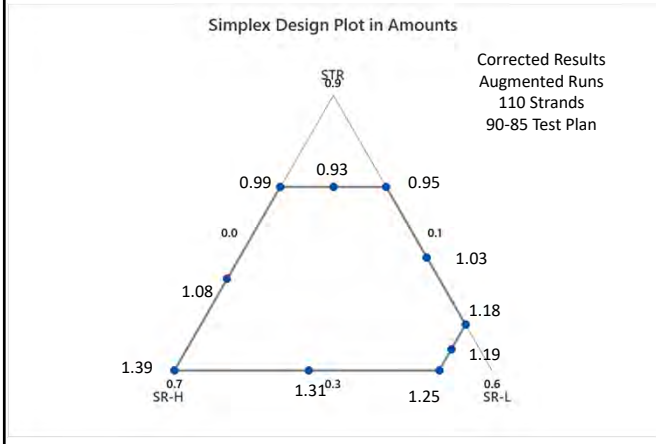


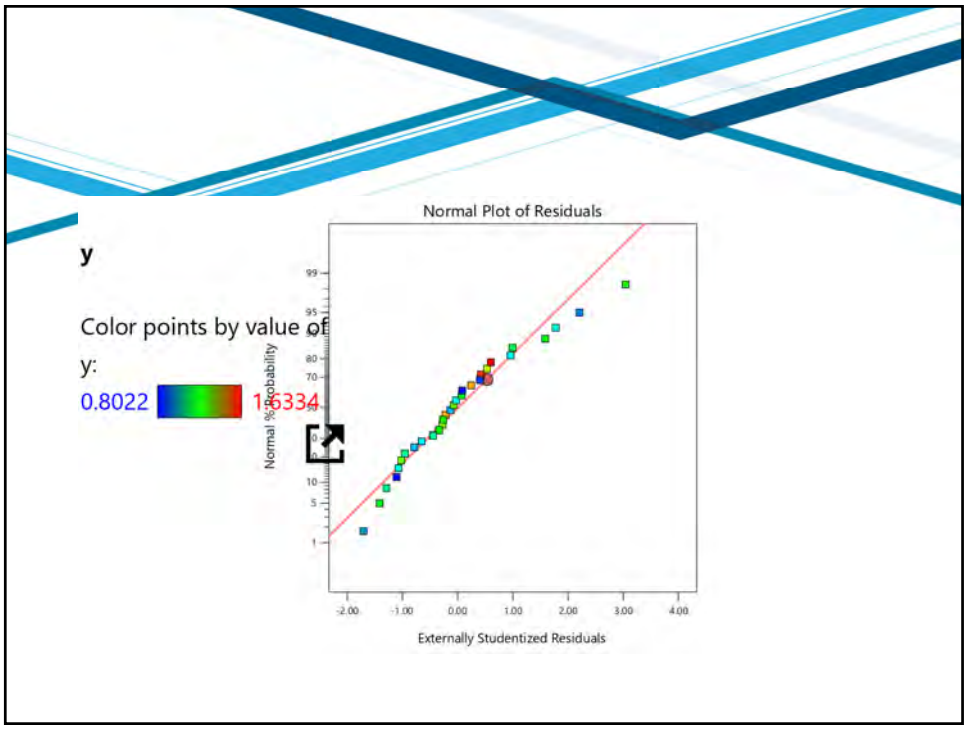
25

Source	Sum of Squares	df	Mean Square	F-value	p-value	
Model	1.40	10	0.1401	58.29	< 0.0001	significant
[1]Linear Mixture	0.5806	2	0.2903	120.83	< 0.0001	
AB	0.0163	1	0.0163	6.79	0.0174	
AC	0.0123	1	0.0123	5.11	0.0357	
AD	0.0387	1	0.0387	16.12	0.0007	
AE	0.0038	1	0.0038	1.59	0.2231	
BD	0.1503	1	0.1503	62.56	< 0.0001	
BE	0.0051	1	0.0051	2.11	0.1628	
CD	0.2596	1	0.2596	108.07	< 0.0001	
CE	0.0099	1	0.0099	4.11	0.0568	
Residual	0.0456	19	0.0024			
Cor Total	1.45	29				

26

Component	Coefficient Estimate	df	Standard Error	95% CI Low	95% CI High	VIF
A-A	0.9975	1	0.0780	0.8344	1.16	12.54
B-B	1.40	1	0.0259	1.35	1.46	1.64
C-C	1.27	1	0.0258	1.22	1.33	2.27
AB	-0.5595	1	0.2147	-1.01	-0.1101	6.40
AC	-0.4962	1	0.2194	-0.9555	-0.0369	8.71
AD	-0.1230	1	0.0306	-0.1871	-0.0589	1.29
AE	-0.0334	1	0.0265	-0.0890	0.0221	1.45
BD	-0.2137	1	0.0270	-0.2702	-0.1571	1.19
BE	0.0340	1	0.0234	-0.0150	0.0830	1.34
CD	-0.2391	1	0.0230	-0.2872	-0.1909	1.20
CE	0.0404	1	0.0199	-0.0013	0.0821	1.36

27



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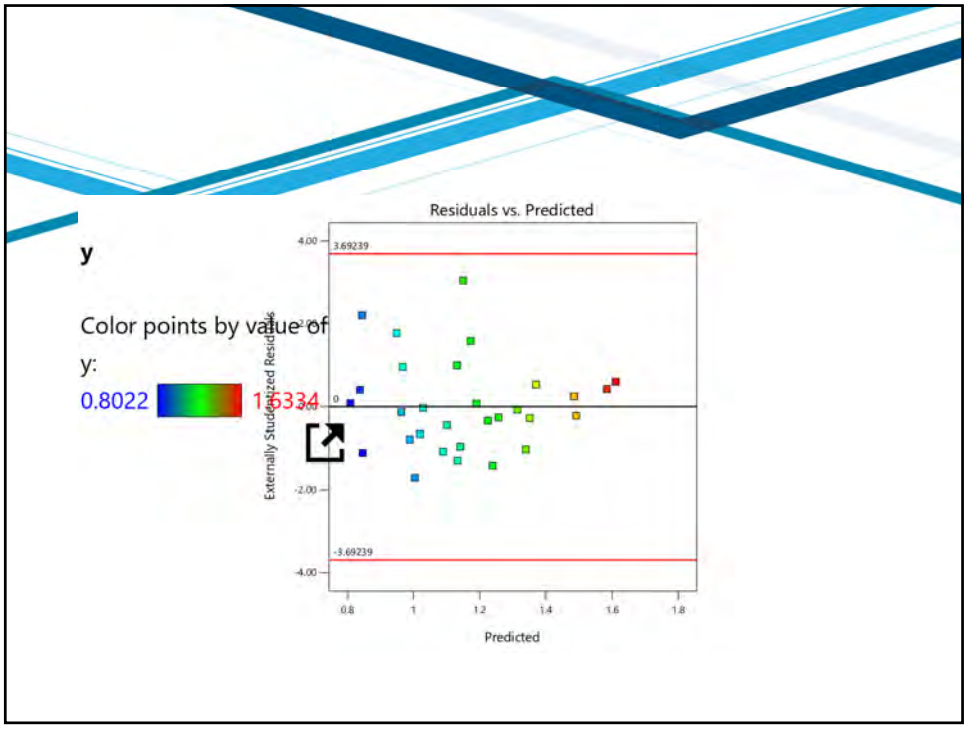

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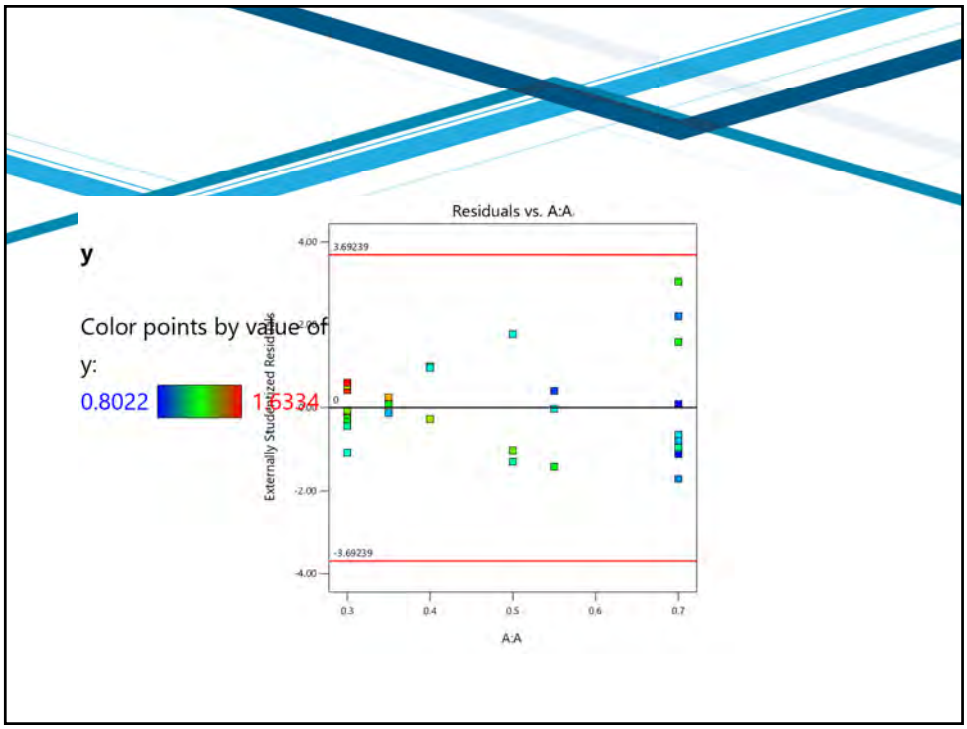

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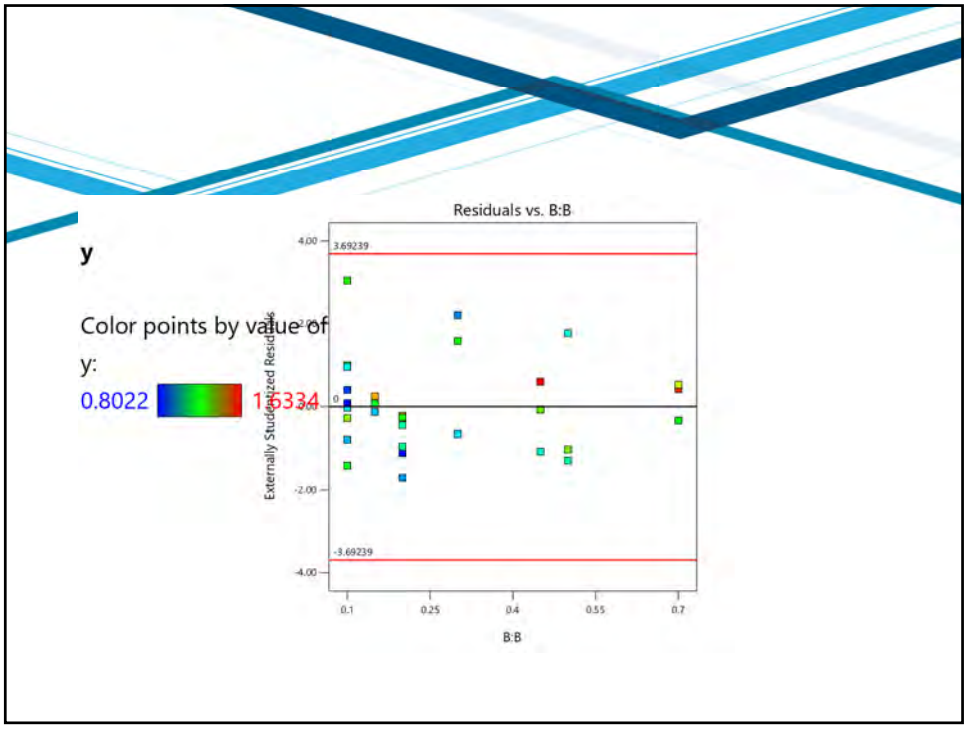

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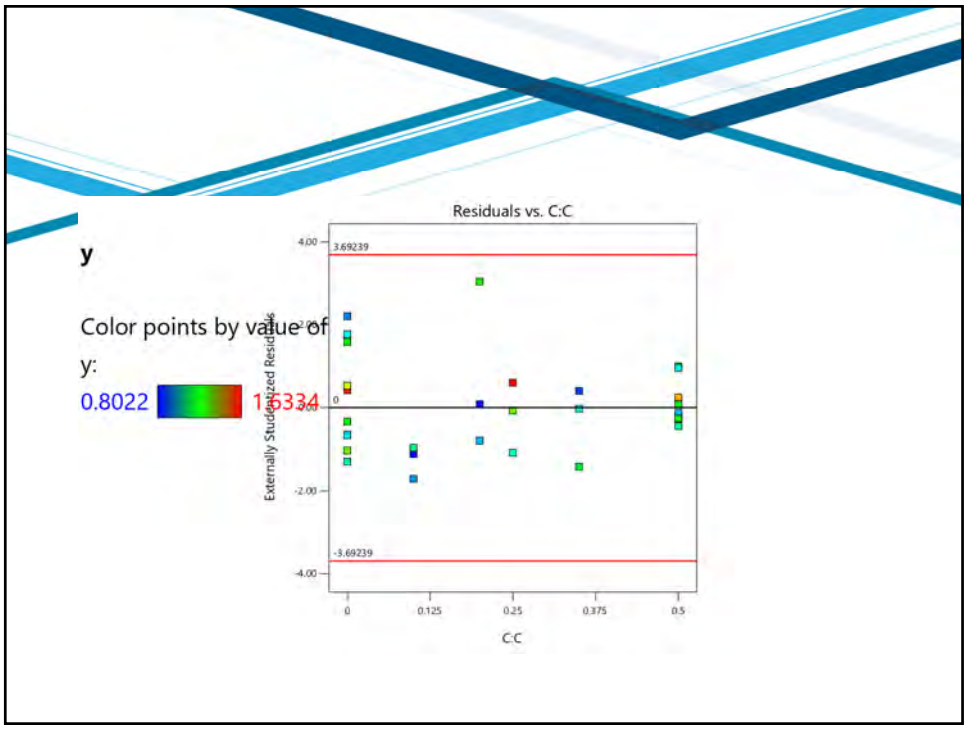

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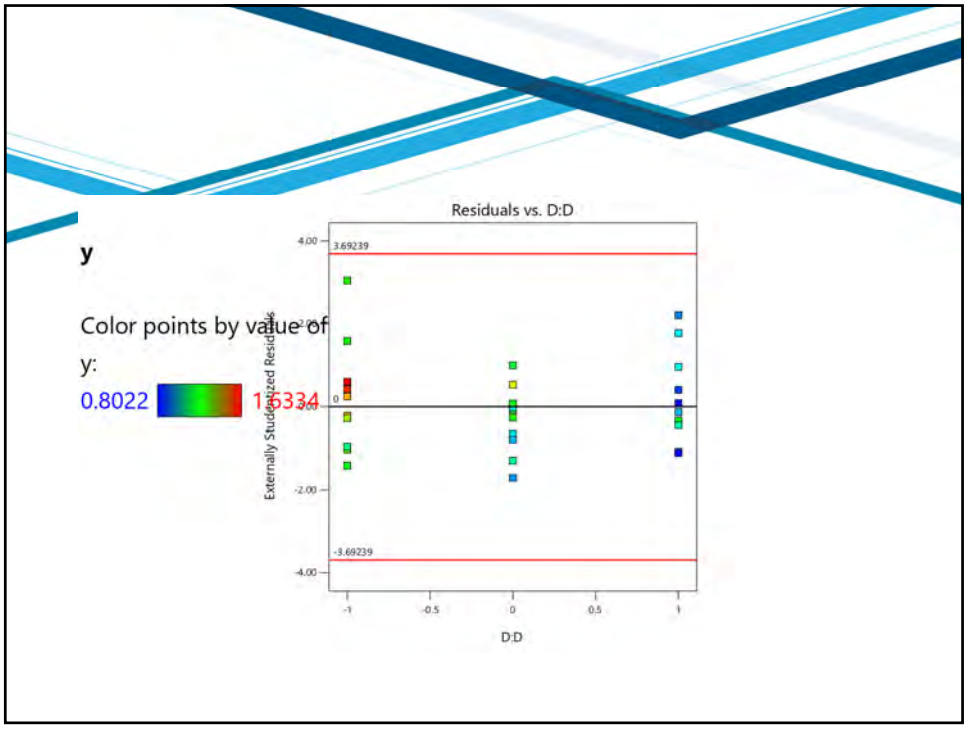

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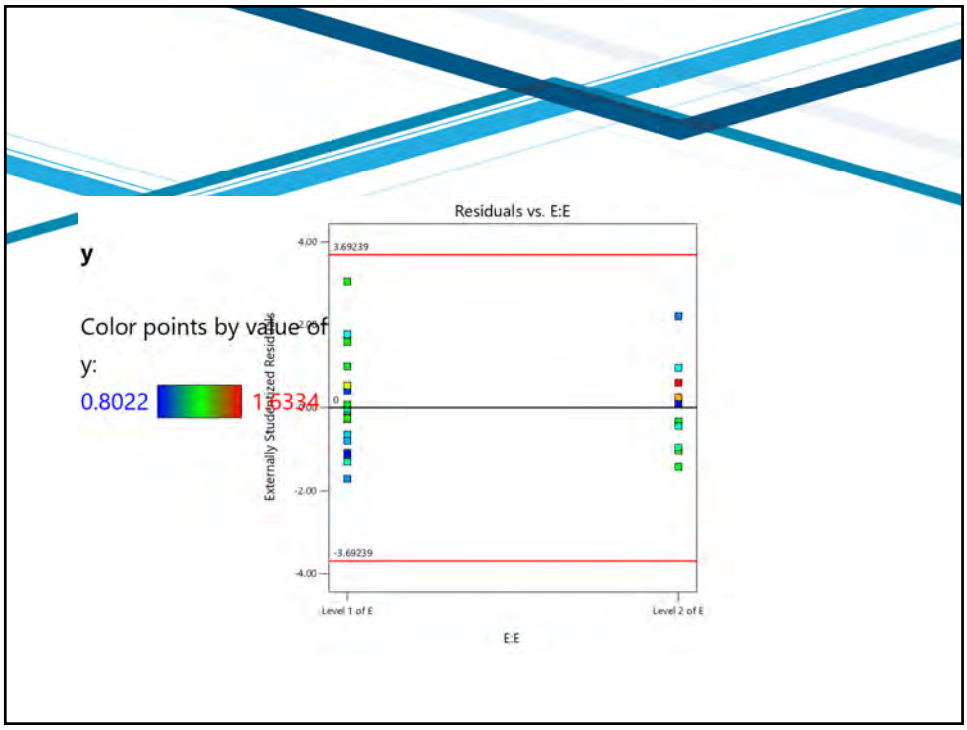

34