MORS

Contractor Disclosure Form 712A – Deadline: 2 June 2014

MORS Symposium

16-19 June 2014, Hilton Mark Center, Alexandria, VA

Fax completed form to 703-933-9066 or email to liz@mors.org

Abstract 594

PART I **Author Request** - The following author(s) request authority to disclose the following presentation at the MORS Symposium with subsequent publication in the MORS Final Report, and posting on the MORS website, if applicable.

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Title of Presentation:

Definitive Screening Designs - Run Fewer Trials and Get More Information than Using Fractional Factorial DOE Methods

This presentation is: ☐ SECRET ☐ SECRET//REL TO FVEY ☐ CONFIDENTIAL ☐ CONFIDENTIAL//REL TO FVEY

■ UNCLASSIFIED ☐ Other ____________ and will be presented in:

■ Tutorial ☐ List all WG(s) #:

This work was performed in connection with a government contract.	☐ YES (Complete Parts I, II, & III)
This presentation is based on material developed by the author as part of company-approved research e.g. IR&D and was NOT done under a government contract.	☐ YES (Complete Parts I, II & III)
This presentation was NOT done under a government contract, contains no government information, is my own work and is approved for public release.	■ YES (Complete Part I only)

jmp

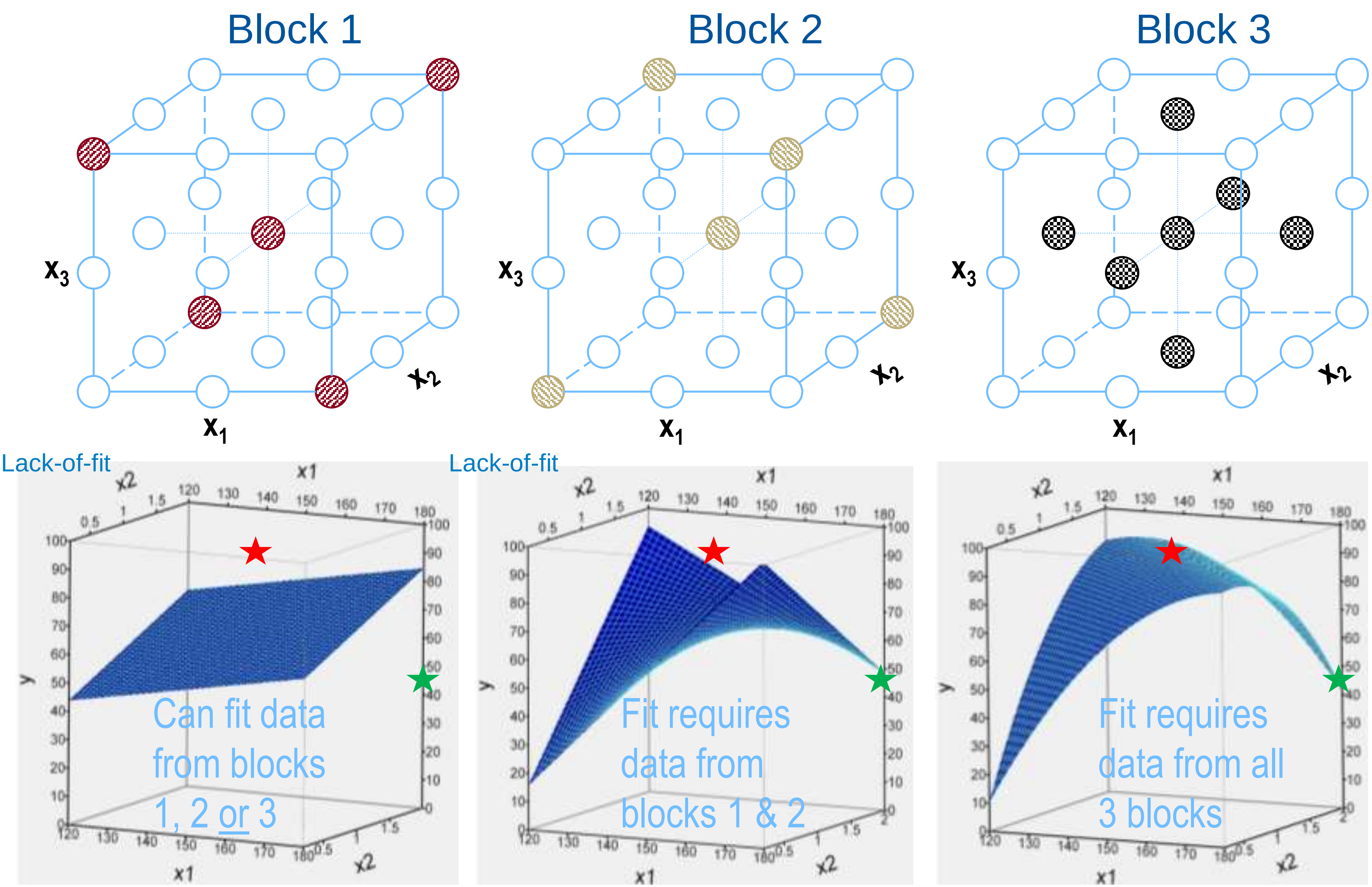
sas THE POWER TO KNOW.

DESIGN OF EXPERIMENTS: USING DEFINITIVE SCREENING DESIGNS TO GET MORE INFORMATION FROM FEWER TRIALS

June17, 2014
82nd MORSS
Alexandria, VA

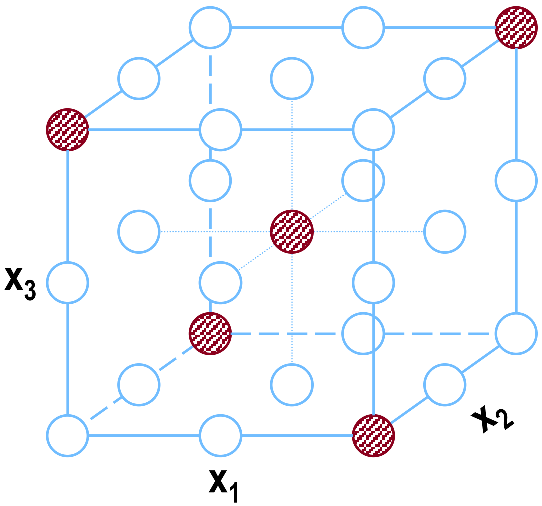
Tom Donnelly, PhD
Systems Engineer & Co-insurrectionist
JMP Federal Government Team

CLASSIC RESPONSE-SURFACE DOE IN A NUTSHELL



POLYNOMIAL MODELS USED TO CALCULATE SURFACES

Block 1

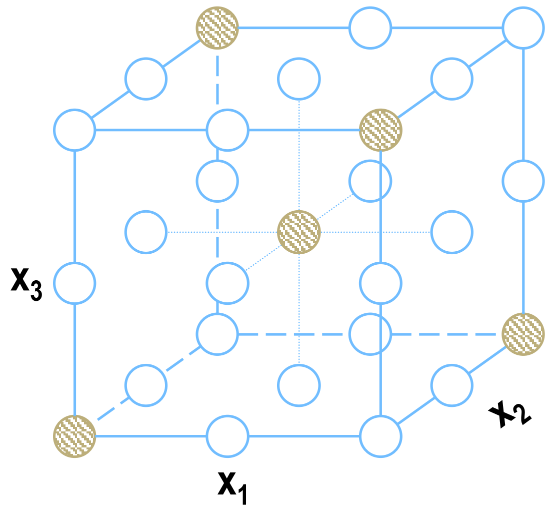


$$y = a_0 + a_1x_1 + a_2x_2 + a_3x_3$$

Run this block 1st to:

(i) estimate the main effects*
(ii) use center point to check for curvature.

Block 2

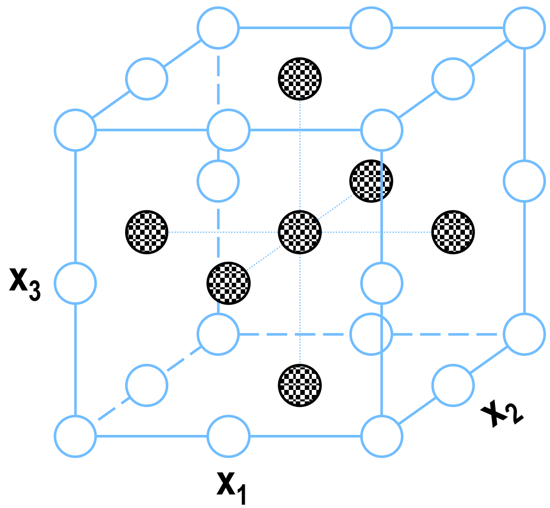


$$y = a_0 + a_1x_1 + a_2x_2 + a_3x_3$$
$$+ a_{12}x_1x_2 + a_{13}x_1x_3 + a_{23}x_2x_3$$

Run this block 2nd to:

(i) repeat main effects estimate,
(ii) check if process has shifted
(iii) add interaction effects to model <u>if needed.</u>

Block 3

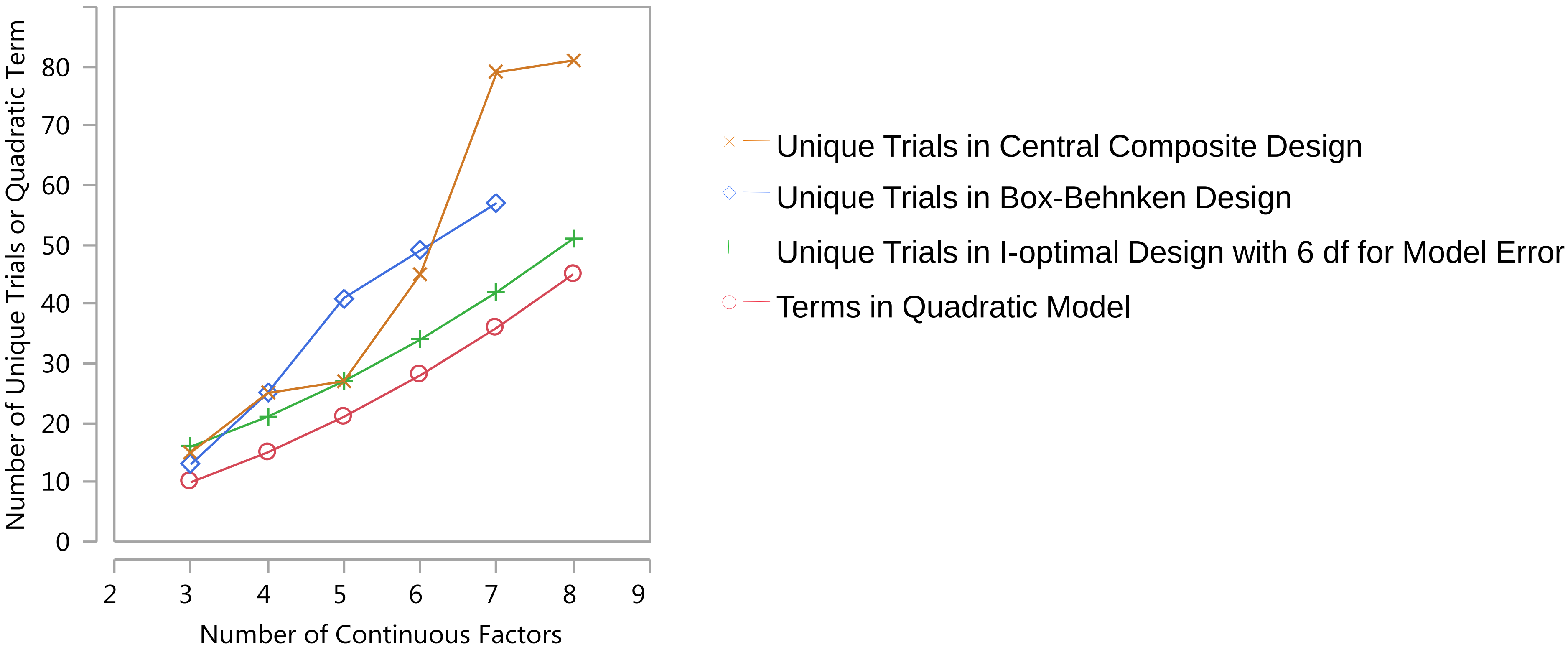


$$y = a_0 + a_1x_1 + a_2x_2 + a_3x_3$$
$$+ a_{12}x_1x_2 + a_{13}x_1x_3 + a_{23}x_2x_3$$
$$+ a_{11}x_1^2 + a_{22}x_2^2 + a_{33}x_3^2$$

Run this block 3rd to:

(i) repeat main effects estimate,
(ii) check if process has shifted
(iii) add curvature effects to model <u>if needed.</u>

NUMBER OF UNIQUE TRIALS FOR 3 RESPONSE-SURFACE DESIGNS AND NUMBER OF QUADRATIC MODEL TERMS VS. NUMBER OF CONTINUOUS FACTORS



If generally running 3, 4 or 5-factor fractional-factorial designs…

1. How many interactions are you not investigating?
2. How many more trials needed to fit curvature?
3. Consider two stages: Definitive Screening + Augmentation

- ***Definitive Screening Designs***
  - Efficiently estimate main and quadratic effects for no more and **often fewer trials than traditional designs**
  - If only a few factors are important the design may collapse into a **"one-shot"** design that supports a response-surface model
  - If many factors are important the design can be **augmented** to support a response-surface model
  - Case study for a **10-variable process** shows that it can be **optimized in just 23 unique trials**

Definitive Screening Designs

- For continuous factors only - three levels

Jones, B., and C. J. Nachtsheim (2011). “A Class of Three-Level Designs for Definitive Screening in the Presence of Second-Order Effects," Journal of Quality Technology, 43 pp. 1-14

- Construction via Conference Matrices

Xiao, L, Lin, D. K.J., and B. Fengshan (2012). “Constructing Definitive Screening Designs Using Conference Matrices,” Journal of Quality Technology, 44, pp. 1-7.

- For continuous factors AND two-level categorical factors

Jones, B., and C. J. Nachtsheim (2013). “Definitive Screening Designs with Added Two-Level Categorical Factors,” Journal of Quality Technology, 45 pp. 121-129

A Class of Three-Level Designs for Definitive Screening in the Presence of Second-Order Effects

BRADLEY JONES

SAS Institute, Cary, NC 27513

CHRISTOPHER J. NACHTSHEIM

Carlson School of Management, University of Minnesota, Minneapolis, MN 55455

Journal of Quality Technology *Vol. 43, No. 1, January 2011*

PAPER AND CATALOGUE OF DEFINITIVE SCREENING DESIGNS FOR 4 TO 30 FACTORS AVAILABLE AT ASQ WEBSITE:
HTTP://ASQ.ORG/QIC/DISPLAY-ITEM/INDEX.HTML?ITEM=33051

IN ORIGINAL 2011 JQT PAPER - DESIGN SIZE IS 2M + 1

Run	m = 9	m = 10	m = 11	m = 12
1	0++++++++	0++-++++-+	0-+-----+-+	0--+-+-+++-+
2	0--------	0--+----+-	0+-+++++-+-	0++-+-+---+-
3	+0+-+--+-	+0-++-++--	-0--+----++	-0+++++++---
4	-0-+-++-+	-0+--+--++	+0++-++++--	+0-------+++
5	-+0-+-+--	-+0---+---	--0++++---+	++0-++-++-++
6	+-0+-+-++	+-0+++-+++	++0----+++-	--0+--+--+--
7	--+0+---+	-++0+--++-	---0-++-++-	+--0+-+-+--+
8	++-0-+++-	+--0-++--+	+++0+--+--+	-++0-+-+-++-
9	+-+-0++--	----0++++-	+--+0+-++++	++++0-++++++
10	-+-+0--++	++++0----+	-++-0-+----	----0+------
11	----+0+++	-+-++0+-++	--++-0-+-+-	+-+-+0++-+-+
12	++++-0---	+-+--0-+--	++--+0+-+-+	-+-+-0--+-+-
13	++--++0-+	++----0+++	---++-0++--	++++-+0----+
14	--++--0+-	--++++0---	+++--+0--++	----+-0++++-
15	---+++-0-	++++-++0+-	-+++--+0+++	--+++--0--++
16	+++---+0+	----+--0-+	+---++-0---	++---++0++--
17	-++--+-+0	++--++--0-	-+---+-+0-+	+-++++--0++-
18	+--++-+-0	--++--++0+	+-+++-+-0+-	-+----++0--+
19	000000000	+-+-+-+-+0	+-----++-0+	++-++--+-0--
20		-+-+-+-+-0	-+++++--+0-	--+--++-+0++
21		0000000000	++-+------0	-+-++++--+0+
22			--+-++++++0	+-+----++-0-
23			00000000000	+--+-+++--+0
24				-++-+---++-0
25				000000000000

DEFINITIVE SCREENING DESIGNS FROM CONFERENCE MATRICES XIAO, BAI AND LIN (JQT, 2012)

The D-efficiency is 92.3%, higher than 89.8% for the design given in Jones and Nachtsheim (2011).

$$
\mathrm{D} = \begin{pmatrix} \mathrm{C} \\ -\mathrm{C} \\ 0 \end{pmatrix} =
\begin{array}{c}
\begin{array}{cccccccccccc} x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & x_7 & x_8 & x_9 & x_{10} & x_{11} & x_{12} \end{array} \\
\left(\begin{array}{rrrrrrrrrrrr}
0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 0 & -1 & -1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 & 1 \\
1 & 1 & 0 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 \\
1 & 1 & -1 & 0 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\
1 & 1 & -1 & -1 & 0 & 1 & -1 & 1 & 1 & 1 & -1 & -1 \\
1 & 1 & 1 & -1 & -1 & 0 & 1 & 1 & -1 & -1 & 1 & -1 \\
1 & -1 & -1 & 1 & 1 & -1 & 0 & 1 & 1 & -1 & 1 & -1 \\
1 & 1 & 1 & 1 & -1 & -1 & -1 & 0 & 1 & -1 & -1 & 1 \\
1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 0 & 1 & 1 & -1 \\
1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 & -1 & 0 & -1 & 1 \\
1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 0 & 1 \\
1 & -1 & 1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 & 0 \\
\hline
0 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\
-1 & 0 & 1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 & -1 & -1 \\
-1 & -1 & 0 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & 1 \\
-1 & -1 & 1 & 0 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 \\
-1 & -1 & 1 & 1 & 0 & -1 & 1 & -1 & -1 & -1 & 1 & 1 \\
-1 & -1 & -1 & 1 & 1 & 0 & -1 & -1 & 1 & 1 & -1 & 1 \\
-1 & 1 & 1 & -1 & -1 & 1 & 0 & -1 & -1 & 1 & -1 & 1 \\
-1 & -1 & -1 & -1 & 1 & 1 & 1 & 0 & -1 & 1 & 1 & -1 \\
-1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & 0 & -1 & -1 & 1 \\
-1 & 1 & 1 & -1 & 1 & -1 & -1 & -1 & 1 & 0 & 1 & -1 \\
-1 & 1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & 0 & -1 \\
-1 & 1 & -1 & 1 & -1 & -1 & -1 & 1 & -1 & 1 & 1 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}\right)
\end{array}
$$

http://www.newton.ac.uk/programmes/DAE/seminars/090209001.pdf

CONFERENCE MATRIX METHOD IN 2012 JQT PAPER
DESIGN SIZE IS 2M + 3 FOR ODD M
DESIGN SIZE IS 2M + 1 FOR EVEN M

7-FACTOR – DSD17

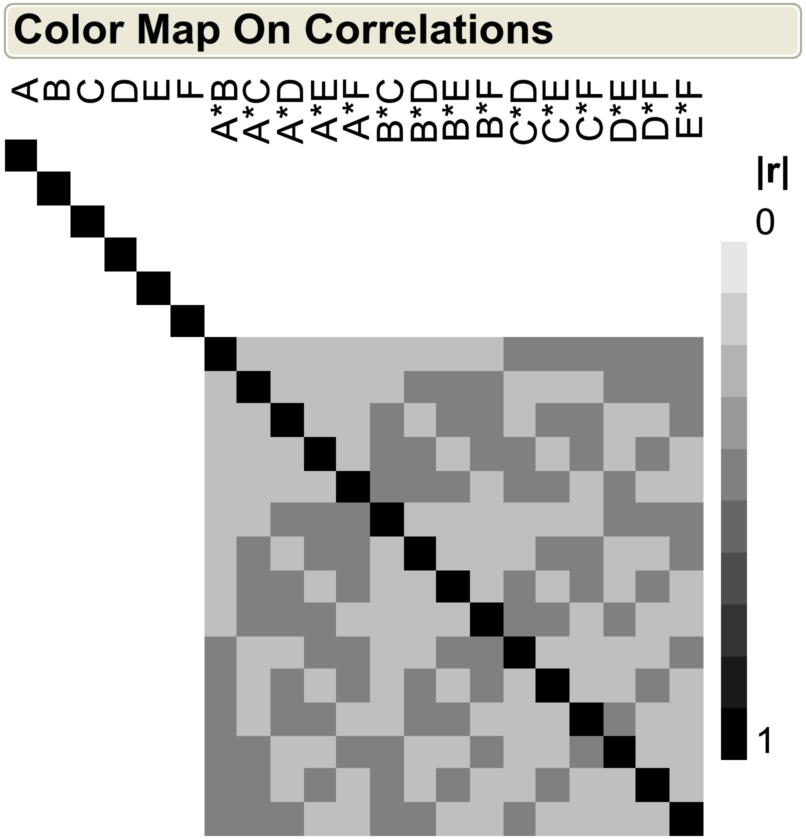
	A	B	C	D	E	F	G
1	0	1	1	1	1	1	1
2	0	-1	-1	-1	-1	-1	-1
3	1	0	-1	-1	1	-1	1
4	-1	0	1	1	-1	1	-1
5	1	1	0	-1	-1	1	-1
6	-1	-1	0	1	1	-1	1
7	1	1	1	0	-1	-1	1
8	-1	-1	-1	0	1	1	-1
9	1	-1	1	1	0	-1	-1
10	-1	1	-1	-1	0	1	1
11	1	1	-1	1	1	0	-1
12	-1	-1	1	-1	-1	0	1
13	1	-1	1	-1	1	1	0
14	-1	1	-1	1	-1	-1	0
15	1	-1	-1	1	-1	1	1
16	-1	1	1	-1	1	-1	-1
17	0	0	0	0	0	0	0

8-FACTOR – DSD17

	A	B	C	D	E	F	G	H
1	0	1	1	1	1	1	1	1
2	0	-1	-1	-1	-1	-1	-1	-1
3	1	0	-1	-1	1	-1	1	1
4	-1	0	1	1	-1	1	-1	-1
5	1	1	0	-1	-1	1	-1	1
6	-1	-1	0	1	1	-1	1	-1
7	1	1	1	0	-1	-1	1	-1
8	-1	-1	-1	0	1	1	-1	1
9	1	-1	1	1	0	-1	-1	1
10	-1	1	-1	-1	0	1	1	-1
11	1	1	-1	1	1	0	-1	-1
12	-1	-1	1	-1	-1	0	1	1
13	1	-1	1	-1	1	1	0	-1
14	-1	1	-1	1	-1	-1	0	1
15	1	-1	-1	1	-1	1	1	0
16	-1	1	1	-1	1	-1	-1	0
17	0	0	0	0	0	0	0	0

6-FACTOR, 13-TRIAL, DEFINITIVE SCREENING DESIGN

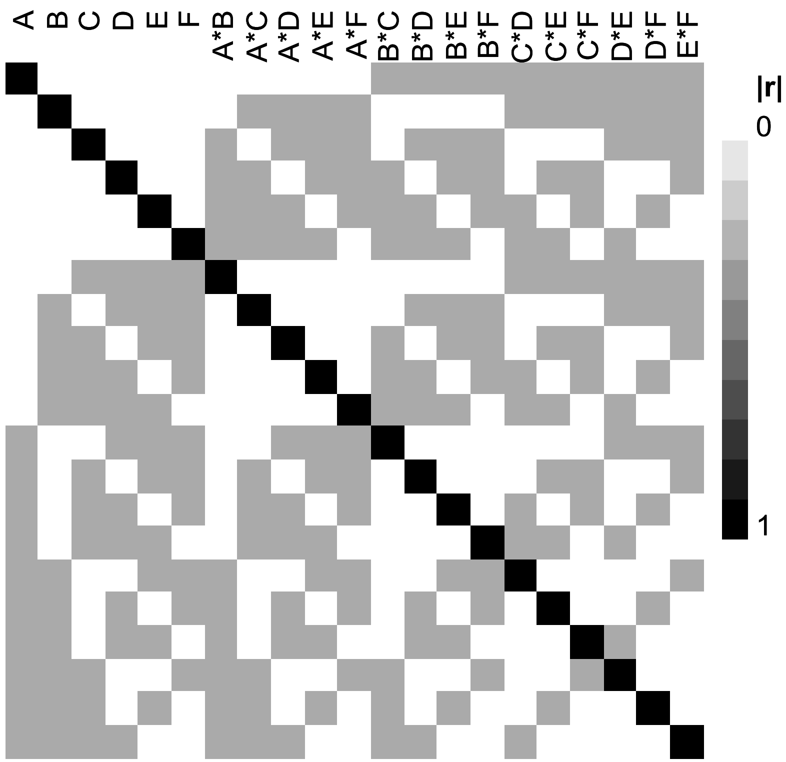
	A	B	C	D	E	F
1	0	1	-1	-1	-1	-1
2	0	-1	1	1	1	1
3	1	0	-1	1	1	-1
4	-1	0	1	-1	-1	1
5	-1	-1	0	1	-1	-1
6	1	1	0	-1	1	1
7	-1	1	1	0	1	-1
8	1	-1	-1	0	-1	1
9	1	-1	1	-1	0	-1
10	-1	1	-1	1	0	1
11	1	1	1	1	-1	0
12	-1	-1	-1	-1	1	0
13	0	0	0	0	0	0



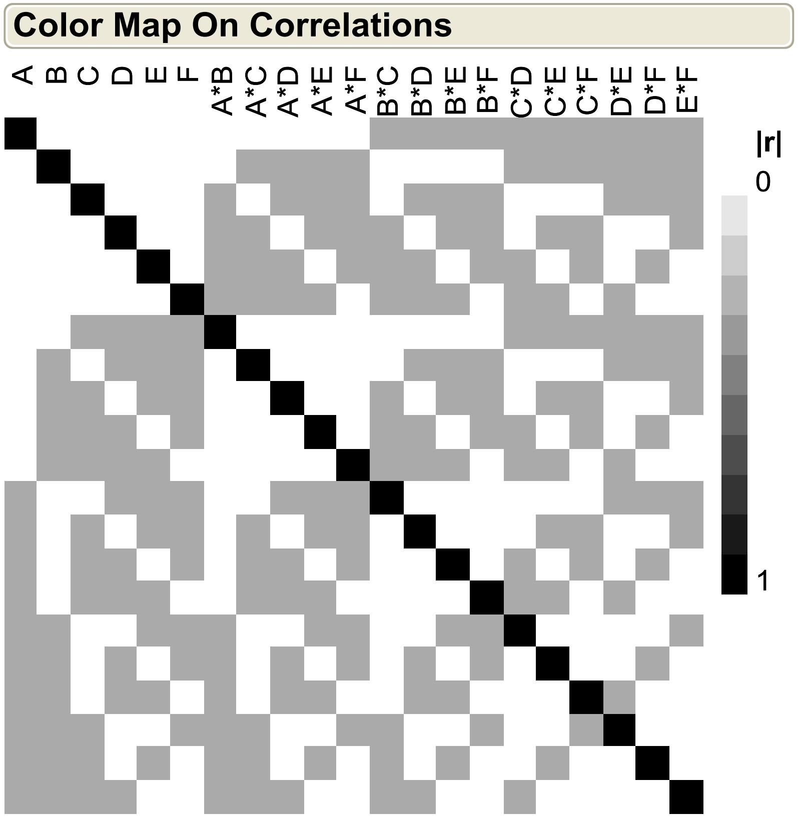
6-FACTOR, 12-TRIAL, PLACKETT-BURMAN DESIGN

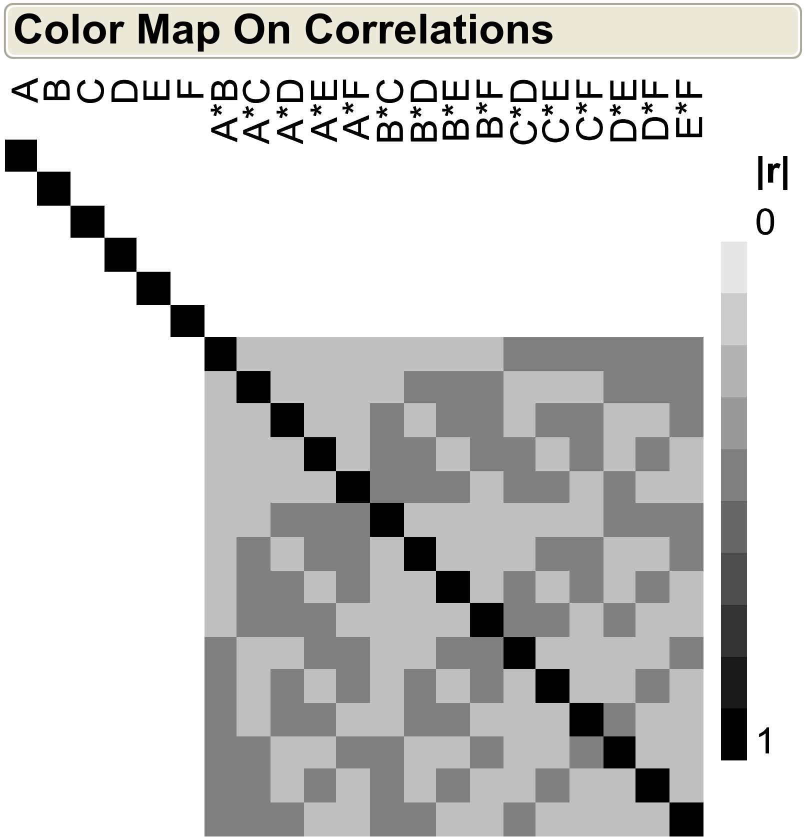
	A	B	C	D	E	F
1	1	-1	1	-1	1	1
2	-1	-1	1	-1	-1	1
3	1	1	1	-1	-1	-1
4	-1	1	-1	-1	1	-1
5	-1	-1	-1	-1	1	-1
6	1	-1	1	1	1	-1
7	1	1	-1	-1	-1	1
8	1	1	-1	1	1	1
9	-1	-1	-1	1	-1	1
10	1	-1	-1	1	-1	-1
11	-1	1	1	1	-1	-1
12	-1	1	1	1	1	1

Color Map On Correlations



COLOR MAPS FOR 6-FACTOR, PLACKETT-BURMAN (LEFT) AND DEFINITIVE SCREENING DESIGN (RIGHT)





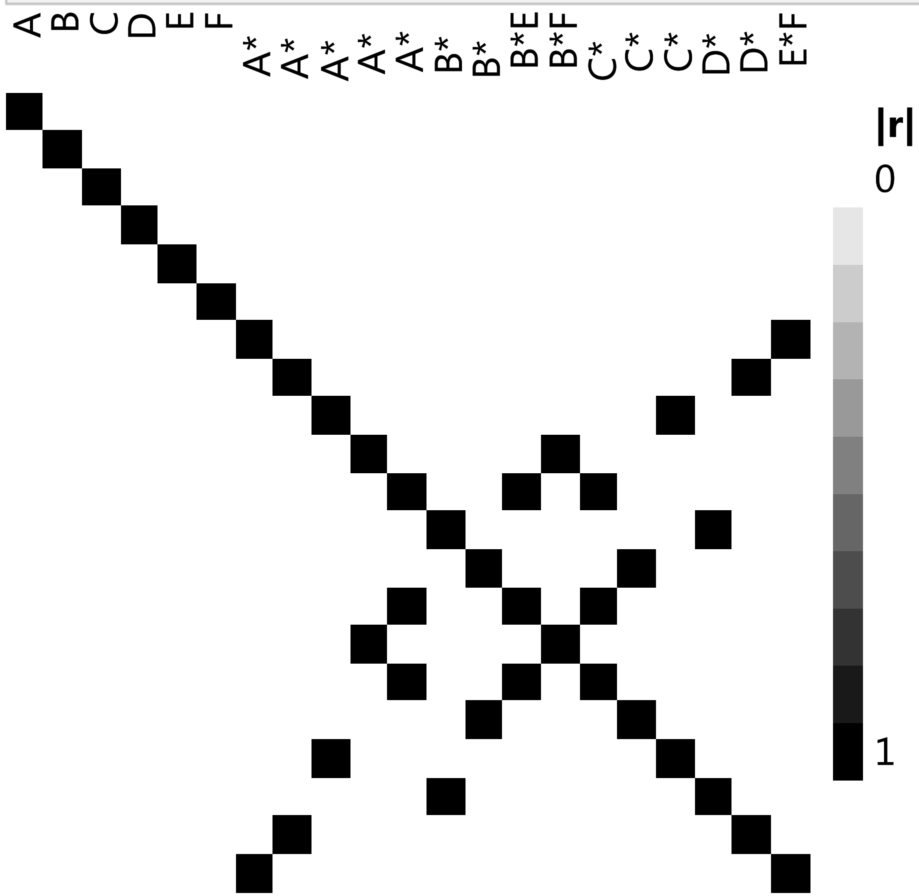
Including center point with Plackett-Burman, these two designs are both 13 trials

Same size BUT Definitive Screening can test for curvature in each factor

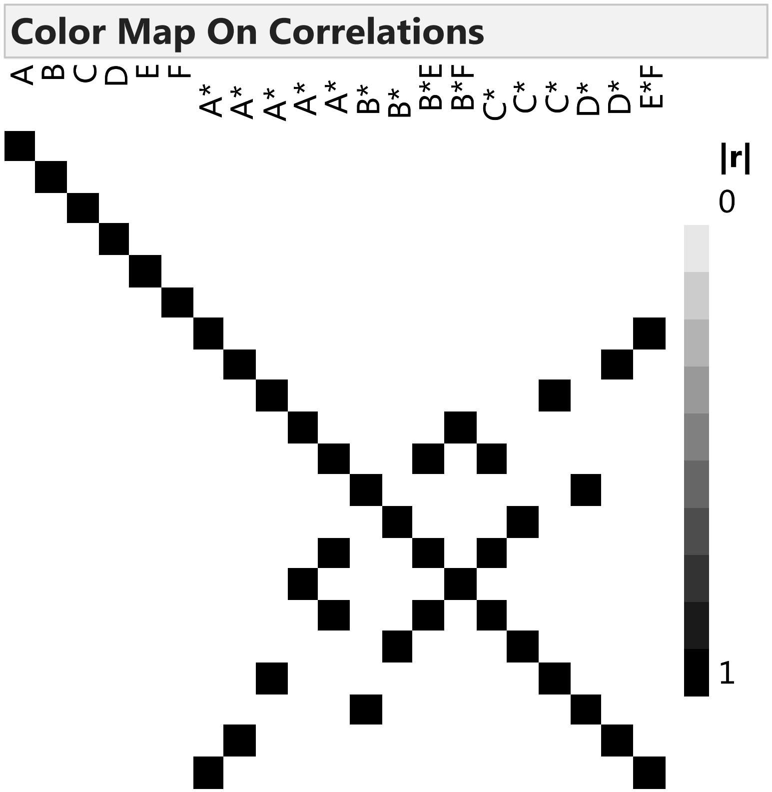
6-FACTOR, 16-TRIAL, REGULAR FRACTIONAL FACTORIAL

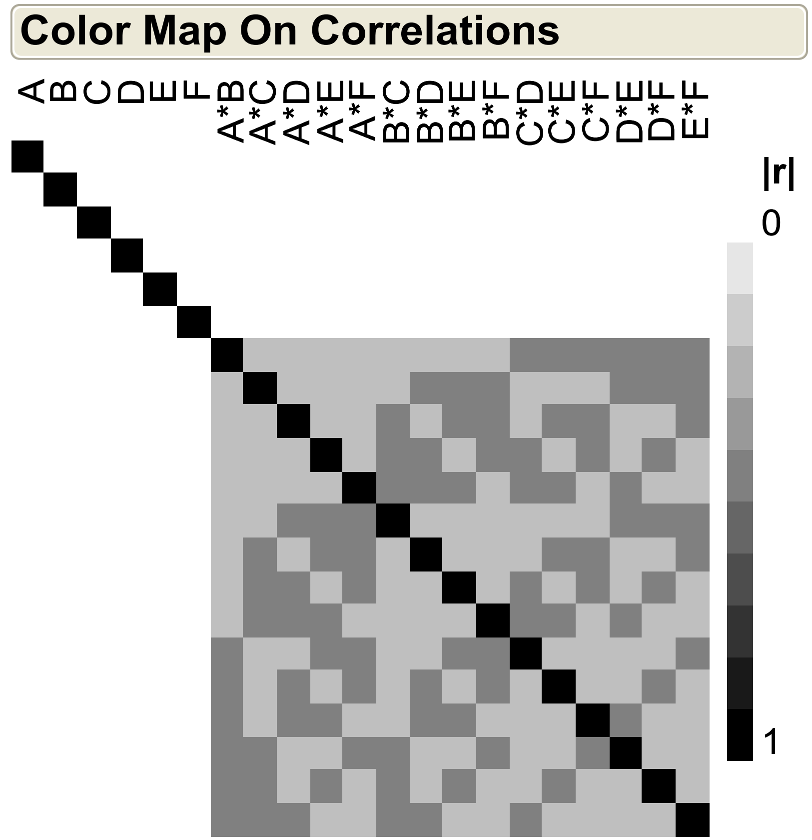
	Pattern	A	B	C	D	E	F
1	−−−−−−	-1	-1	-1	-1	-1	-1
2	−−−+++	-1	-1	-1	1	1	1
3	−−+−++	-1	-1	1	-1	1	1
4	−−++−−	-1	-1	1	1	-1	-1
5	−+−−+−	-1	1	-1	-1	1	-1
6	−+−+−+	-1	1	-1	1	-1	1
7	−++−−+	-1	1	1	-1	-1	1
8	−++++−	-1	1	1	1	1	-1
9	+−−−−+	1	-1	-1	-1	-1	1
10	+−−++−	1	-1	-1	1	1	-1
11	+−+−+−	1	-1	1	-1	1	-1
12	+−++−+	1	-1	1	1	-1	1
13	++−−++	1	1	-1	-1	1	1
14	++−+−−	1	1	-1	1	-1	-1
15	+++−−−	1	1	1	-1	-1	-1
16	++++++	1	1	1	1	1	1

Color Map On Correlations



COLOR MAPS FOR 6-FACTOR, FRACTIONAL FACTORIAL (LEFT) AND DEFINITIVE SCREENING DESIGN (RIGHT)





Including center point with FF increases size to 17 trials - 13-trial Definitive Screening Design is **4 fewer tests AND can test for curvature in each factor**

DO WE GIVE UP NOTHING?

- Relative to same size classic 2-level screening designs
  - Confidence intervals increase – typically ≤10%
  - Standard error increases – typically ≤ 10%
  - Power is reduced for main effects – typically ≤ 10% (when comparing just ME)
  - Power for squared terms is “low”
    - » Still better than power for single center point test for curvature
    - » Power is same as much larger Central Composite Design supporting full quadratic model

ANY OTHER WEAKNESSES?

- Factor range for screening may not include optimum
  - So follow on design will be over different ranges – really can’t augment
  - This is more likely with early product development than with mature systems

CONFIDENCE INTERVAL, STANDARD ERROR & MAIN EFFECTS POWER FOR 6-FACTOR DESIGNS:

PLACKETT-BURMAN 12 + CP
DEFINITIVE SCREENING DESIGN 13
FRACTIONAL-FACTORIAL 16 + CP
DEFINITIVE SCREENING DESIGN 17

PB12+CP

Estimation Efficiency

Parameter	Fractional Increase in CI Length	Relative Std Error of Parameters
Intercept	0	0.277
X1	0.041	0.289
X2	0.041	0.289
X3	0.041	0.289
X4	0.041	0.289
X5	0.041	0.289
X6	0.041	0.289

Power Analysis

Significance Level 0.05

Anticipated RMSE 1

Parameter	Anticipated Coefficients	Power
Intercept	1	0.85
X1	1	0.821
X2	1	0.821
X3	1	0.821
X4	1	0.821
X5	1	0.821
X6	1	0.821

FF16+CP

Estimation Efficiency

Parameter	Fractional Increase in CI Length	Relative Std Error of Parameters
Intercept	0	0.243
X1	0.031	0.25
X2	0.031	0.25
X3	0.031	0.25
X4	0.031	0.25
X5	0.031	0.25
X6	0.031	0.25

Power Analysis

Significance Level 0.05

Anticipated RMSE 1

Parameter	Anticipated Coefficients	Power
Intercept	1	0.959
X1	1	0.949
X2	1	0.949
X3	1	0.949
X4	1	0.949
X5	1	0.949
X6	1	0.949

DSD13

Estimation Efficiency

Parameter	Fractional Increase in CI Length	Relative Std Error of Parameters
Intercept	0	0.277
X1	0.14	0.316
X2	0.14	0.316
X3	0.14	0.316
X4	0.14	0.316
X5	0.14	0.316
X6	0.14	0.316

+ 10% + 9%

Power Analysis

Significance Level 0.05

Anticipated RMSE 1

Parameter	Anticipated Coefficients	Power
Intercept	1	0.85
X1	1	0.75
X2	1	0.75
X3	1	0.75
X4	1	0.75
X5	1	0.75
X6	1	0.75

- 9%

DSD17

Estimation Efficiency

Parameter	Fractional Increase in CI Length	Relative Std Error of Parameters
Intercept	0	0.243
X1	0.102	0.267
X2	0.102	0.267
X3	0.102	0.267
X4	0.102	0.267
X5	0.102	0.267
X6	0.102	0.267

+ 7% + 7%

Power Analysis

Significance Level 0.05

Anticipated RMSE 1

Parameter	Anticipated Coefficients	Power
Intercept	1	0.959
X1	1	0.92
X2	1	0.92
X3	1	0.92
X4	1	0.92
X5	1	0.92
X6	1	0.92

- 3%

QUADRATIC TERM POWER FOR TEN 6-FACTOR DESIGNS – SCREENING & RSM

DSD13 — **0.10**

Power Analysis

Significance Level 0.05
Anticipated RMSE 1

Parameter	Anticipated Coefficients	Power
Intercept	1	0.073
X1	1	0.196
X2	1	0.196
X3	1	0.196
X4	1	0.196
X5	1	0.196
X6	1	0.196
X1*X1	1	0.096
X2*X2	-1	0.096
X3*X3	1	0.096
X4*X4	-1	0.096
X5*X5	1	0.096
X6*X6	-1	0.096

DSD17 — **0.21**

Power Analysis

Significance Level 0.05
Anticipated RMSE 1

Parameter	Anticipated Coefficients	Power
Intercept	1	0.13
X1	1	0.796
X2	1	0.796
X3	1	0.796
X4	1	0.796
X5	1	0.796
X6	1	0.796
X1*X1	1	0.211
X2*X2	-1	0.211
X3*X3	1	0.211
X4*X4	-1	0.211
X5*X5	1	0.211
X6*X6	-1	0.211

DSD21 — **0.26**

Power Analysis

Significance Level 0.05
Anticipated RMSE 1

Parameter	Anticipated Coefficients	Power
Intercept	1	0.159
X1	1	0.959
X2	1	0.959
X3	1	0.959
X4	1	0.959
X5	1	0.959
X6	1	0.959
X1*X1	1	0.261
X2*X2	-1	0.261
X3*X3	1	0.261
X4*X4	-1	0.261
X5*X5	1	0.261
X6*X6	-1	0.261

2X DSD13 — **0.49**

Power Analysis

Significance Level 0.05
Anticipated RMSE 1

Parameter	Anticipated Coefficients	Power
Intercept	1	0.259
X1	1	0.985
X2	1	0.985
X3	1	0.985
X4	1	0.985
X5	1	0.985
X6	1	0.985
X1*X1	1	0.488
X2*X2	-1	0.488
X3*X3	1	0.488
X4*X4	-1	0.488
X5*X5	1	0.488
X6*X6	-1	0.488

AUGMENT DSD17 TO I-OPT34 — **0.58**

Power Analysis

Significance Level 0.05
Anticipated RMSE 1

Parameter	Anticipated Coefficients	Power
Intercept	1	0.39
X1	1	0.994
X2	1	0.996
X3	1	0.996
X4	1	0.996
X5	1	0.993
X6	1	0.993
X1*X1	1	0.583
X2*X2	-1	0.587
X3*X3	1	0.568
X4*X4	-1	0.623
X5*X5	1	0.574
X6*X6	-1	0.559

PB12+CP — **0.12**

Power Analysis

Significance Level 0.05
Anticipated RMSE 1

Parameter	Anticipated Coefficients	Power
Intercept	1	0.13
X1	1	0.789
X2	1	0.789
X3	1	0.789
X4	1	0.789
X5	1	0.789
X6	1	0.789
X1*X1	1	0.124

FF16+CP — **0.14**

Power Analysis

Significance Level 0.05
Anticipated RMSE 1

Parameter	Anticipated Coefficients	Power
Intercept	1	0.146
X1	1	0.944
X2	1	0.944
X3	1	0.944
X4	1	0.944
X5	1	0.944
X6	1	0.944
X1*X1	1	0.14

CCD45 — **0.32**

Power Analysis

Significance Level 0.05
Anticipated RMSE 1

Parameter	Anticipated Coefficients	Power
Intercept	1	0.839
X1	1	1
X2	1	1
X3	1	1
X4	1	1
X5	1	1
X6	1	1
X1*X1	1	0.321
X2*X2	1	0.321
X3*X3	1	0.321
X4*X4	1	0.321
X5*X5	1	0.321
X6*X6	1	0.321

BB49 — **0.61**

Power Analysis

Significance Level 0.05
Anticipated RMSE 1

Parameter	Anticipated Coefficients	Power
Intercept	1	0.164
X1	1	0.997
X2	1	0.997
X3	1	0.997
X4	1	0.997
X5	1	0.997
X6	1	0.997
X1*X1	1	0.608
X2*X2	-1	0.608
X3*X3	1	0.608
X4*X4	-1	0.608
X5*X5	1	0.608
X6*X6	-1	0.608

I-OPT34 — **0.63**

Power Analysis

Significance Level 0.05
Anticipated RMSE 1

Parameter	Anticipated Coefficients	Power
Intercept	1	0.466
X1	1	0.995
X2	1	0.991
X3	1	0.992
X4	1	0.995
X5	1	0.989
X6	1	0.991
X1*X1	1	0.597
X2*X2	-1	0.659
X3*X3	1	0.693
X4*X4	-1	0.631
X5*X5	1	0.594
X6*X6	-1	0.621

POWER FOR 6 MAIN EFFECTS & 6 QUADRATIC TERMS FOR ALL TERMS VS. ONE QUAD TERM AT A TIME

DSD13 — **0.10**

Power Analysis

Significance Level 0.05

Anticipated RMSE 1

Parameter	Anticipated Coefficients	Power
Intercept	1	0.073
X1	1	0.196
X2	1	0.196
X3	1	0.196
X4	1	0.196
X5	1	0.196
X6	1	0.196
X1*X1	1	0.096
X2*X2	-1	0.096
X3*X3	1	0.096
X4*X4	-1	0.096
X5*X5	1	0.096
X6*X6	-1	0.096

DSD13 — **0.24**

Power Analysis

Significance Level 0.05

Anticipated RMSE 1

Parameter	Anticipated Coefficients	Power
Intercept	1	0.291
X1	1	0.716
X2	1	0.716
X3	1	0.716
X4	1	0.716
X5	1	0.716
X6	1	0.716
X1*X1	1	0.236

PB12+CP — **0.12**

Power Analysis

Significance Level 0.05

Anticipated RMSE 1

Parameter	Anticipated Coefficients	Power
Intercept	1	0.13
X1	1	0.789
X2	1	0.789
X3	1	0.789
X4	1	0.789
X5	1	0.789
X6	1	0.789
X1*X1	1	0.124

DSD17 — **0.21**

Power Analysis

Significance Level 0.05

Anticipated RMSE 1

Parameter	Anticipated Coefficients	Power
Intercept	1	0.13
X1	1	0.796
X2	1	0.796
X3	1	0.796
X4	1	0.796
X5	1	0.796
X6	1	0.796
X1*X1	1	0.211
X2*X2	-1	0.211
X3*X3	1	0.211
X4*X4	-1	0.211
X5*X5	1	0.211
X6*X6	-1	0.211

DSD17 — **0.29**

Power Analysis

Significance Level 0.05

Anticipated RMSE 1

Parameter	Anticipated Coefficients	Power
Intercept	1	0.341
X1	1	0.913
X2	1	0.913
X3	1	0.913
X4	1	0.913
X5	1	0.913
X6	1	0.913
X1*X1	1	0.29

FF16+CP — **0.14**

Power Analysis

Significance Level 0.05

Anticipated RMSE 1

Parameter	Anticipated Coefficients	Power
Intercept	1	0.146
X1	1	0.944
X2	1	0.944
X3	1	0.944
X4	1	0.944
X5	1	0.944
X6	1	0.944
X1*X1	1	0.14

July 22, 2010

Secretary Chu Announces Six Projects to Convert Captured CO_2 Emissions from Industrial Sources into Useful Products

$106 Million Recovery Act Investment will Reduce CO_2 Emissions and Mitigate Climate Change

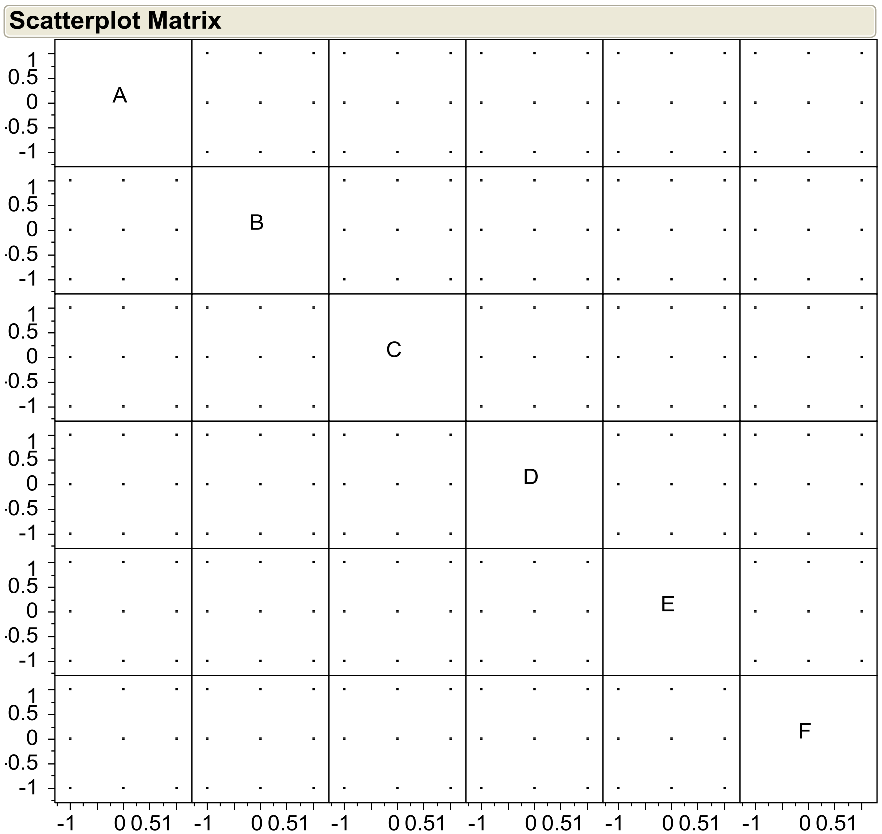
Washington, D.C. - U.S. Energy Secretary Steven Chu announced today the selections of six projects that aim to find ways of converting captured carbon dioxide (CO_2) emissions from industrial sources into useful products such as fuel, plastics, cement, and fertilizers. Funded with $106 million from the American Recovery and Reinvestment Act -matched with $156 million in private cost-share -today's selections demonstrate the potential opportunity to use CO_2 as an inexpensive raw material that can help reduce carbon dioxide emissions while producing useful by-products that Americans can use.

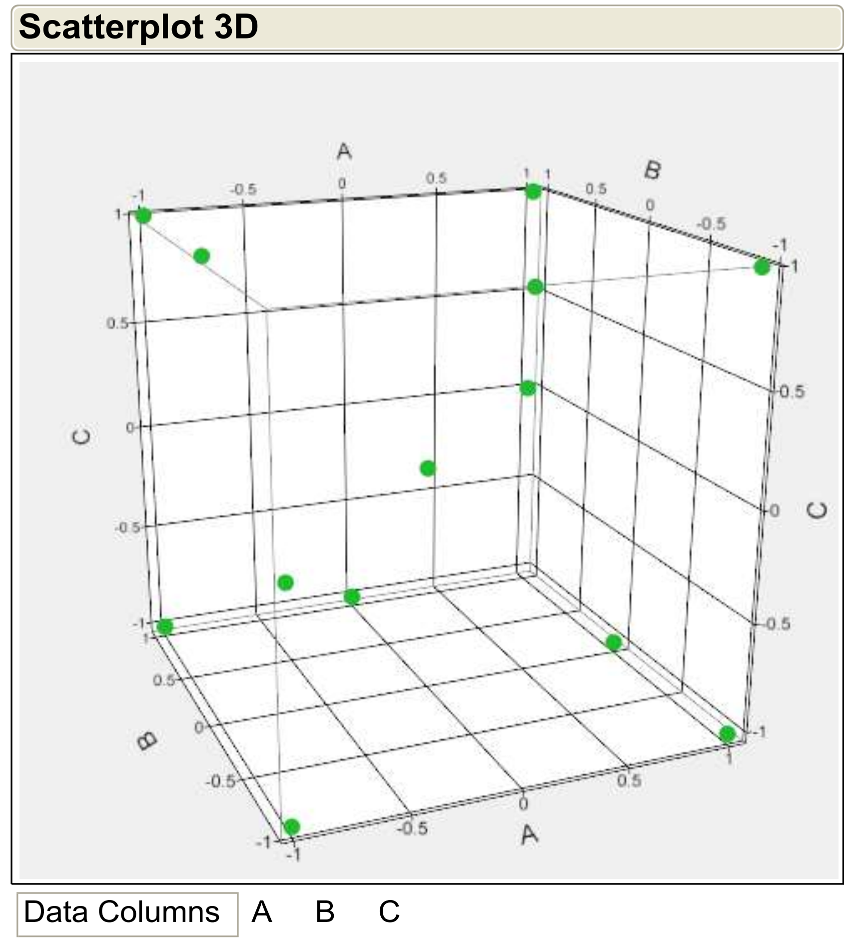
"These innovative projects convert carbon pollution from a climate threat to an economic resource," said Secretary Chu. "This is part of our broad commitment to unleash the American innovation machine and build the thriving, clean energy economy of the future."

23/1	Yield @ Time t	A	B	C	D	E	F	G	H	I	J
1	1.38	-1	1	1	0	1	-1	1	-1	1	1
2	6.44	1	-1	-1	-1	1	-1	1	1	0	1
3	5.96	-1	-1	1	-1	-1	1	-1	1	1	0
4	4.34	0	-1	1	1	1	1	1	1	-1	-1
5	10.46	-1	-1	-1	-1	-1	0	1	-1	-1	-1
6	6.95	-1	-1	1	-1	1	-1	-1	0	-1	-1
7	8.58	1	0	-1	1	1	-1	-1	-1	1	-1
8	2.69	0	1	-1	-1	-1	-1	-1	-1	1	1
9	4.3	-1	1	-1	1	0	-1	-1	1	-1	1
10	0.77	1	-1	1	-1	0	1	1	-1	1	-1
11	2.87	-1	1	1	1	-1	1	-1	-1	0	-1
12	1.01	1	1	1	1	1	0	-1	1	1	1
13	9.47	-1	-1	-1	1	1	1	0	-1	1	1
14	7.49	0	0	0	0	0	0	0	0	0	0
15	0.98	1	1	-1	1	1	-1	1	-1	-1	0
16	0.86	1	1	1	-1	-1	-1	0	1	-1	-1
17	1.25	-1	1	-1	-1	1	1	1	1	1	-1
18	1.03	1	-1	1	1	-1	-1	-1	-1	-1	1
19	1.07	1	1	0	-1	1	1	-1	-1	-1	1
20	7.33	0	0	0	0	0	0	0	0	0	0
21	2.61	1	-1	-1	0	-1	1	-1	1	-1	-1
22	11.39	-1	-1	0	1	-1	-1	1	1	1	-1
23	12.96	-1	0	1	-1	-1	1	1	1	-1	1
24	1.18	1	1	-1	1	-1	1	1	0	1	1

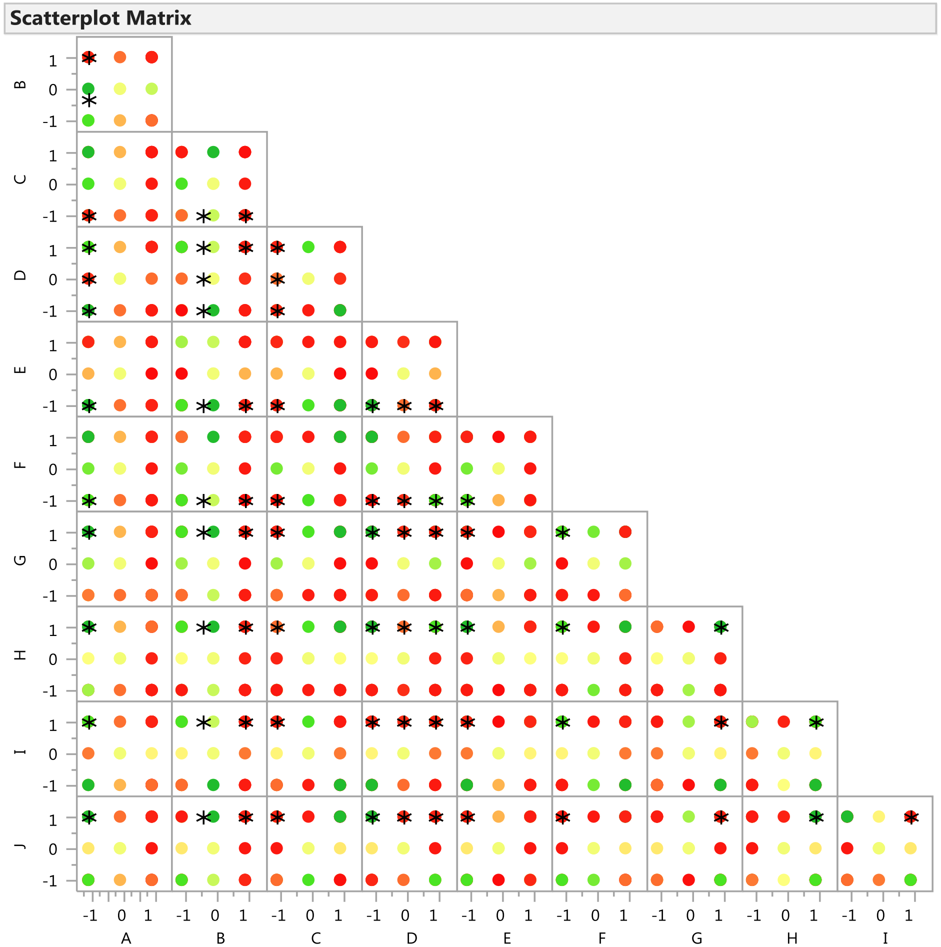
Original design was for 11 variables with 23 unique trials and the center point replicated once.

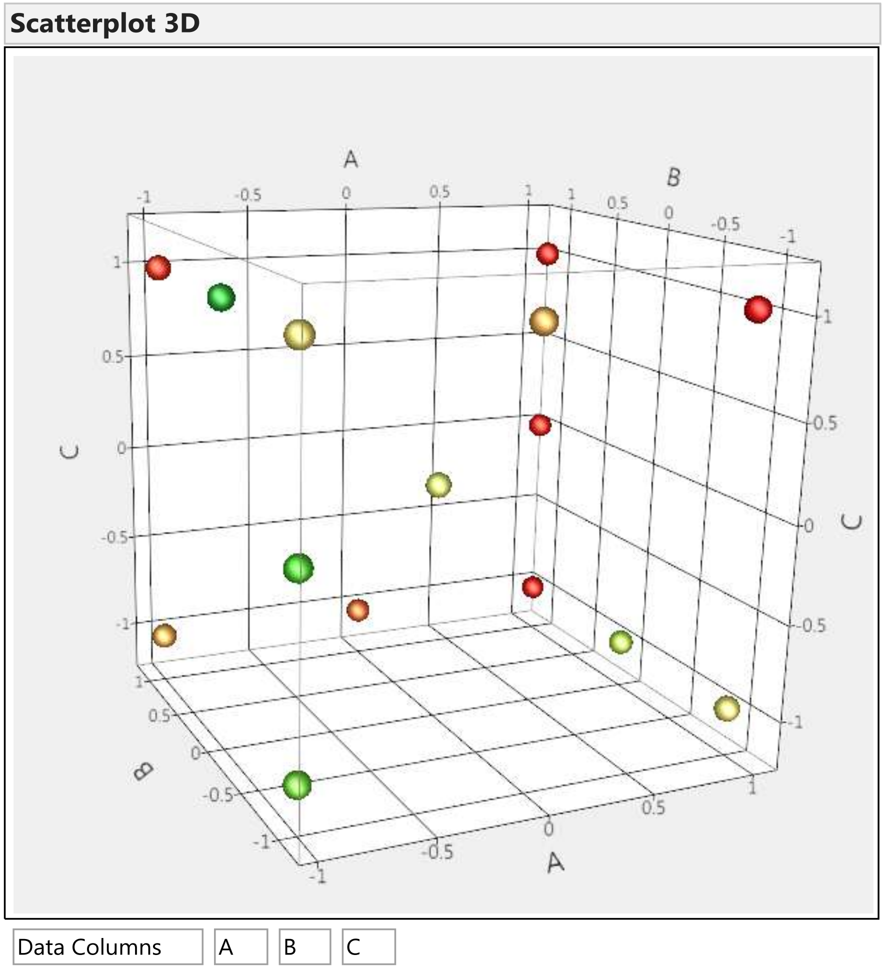
6-FACTOR DEFINITIVE SCREENING DESIGN, PROJECTION IN ALL 2-FACTOR COMBINATIONS (LEFT) AND PROJECTION IN FIRST THREE FACTORS (RIGHT)



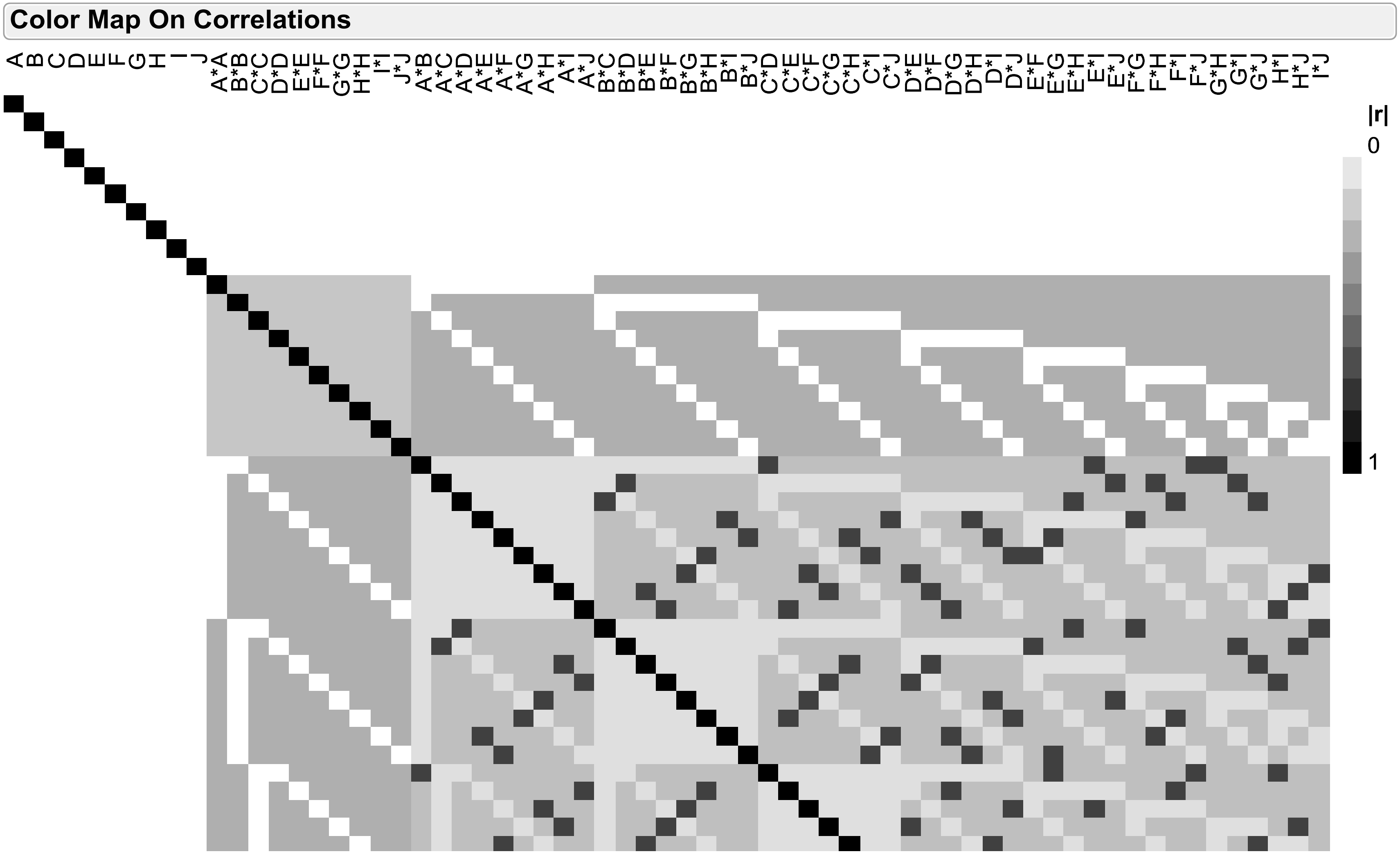


10-FACTOR DEFINITIVE SCREENING DESIGN, PROJECTION IN ALL 2-FACTOR COMBINATIONS (LEFT) AND PROJECTION IN FIRST THREE FACTORS (RIGHT)

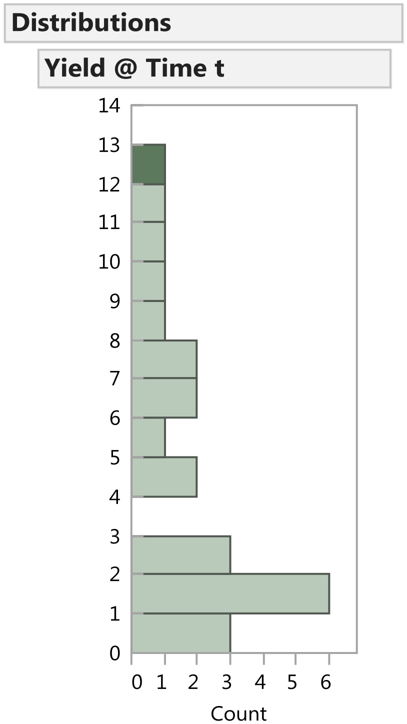


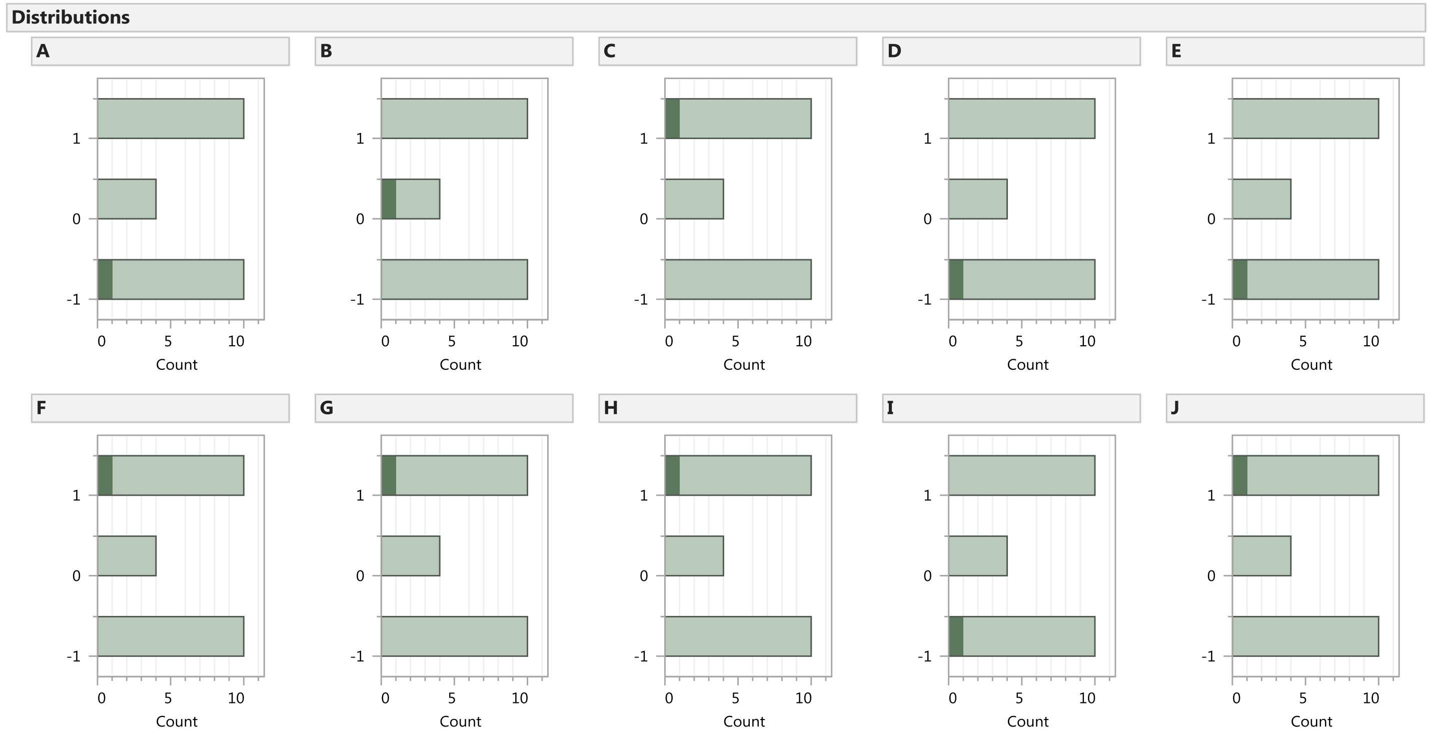


COLOR MAP FOR 10-FACTOR, 21-TRIAL, DEFINITIVE SCREENING DESIGN

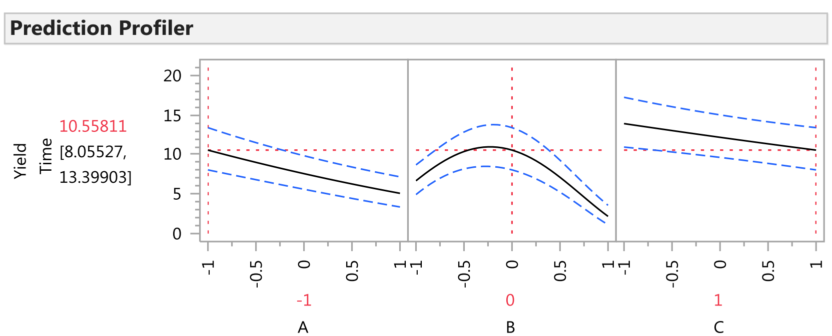


SETTINGS OF BEST OBSERVATION OF YIELD = 12.96

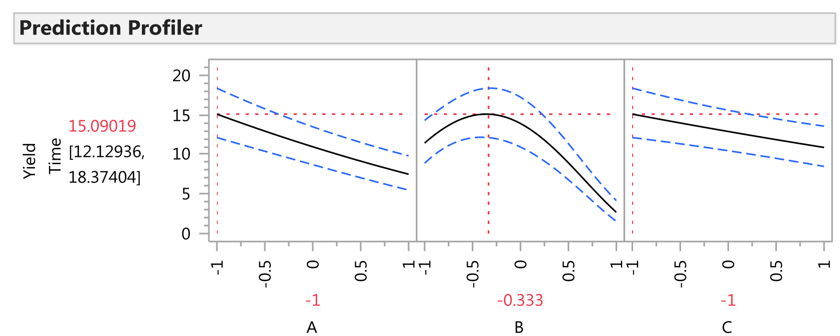




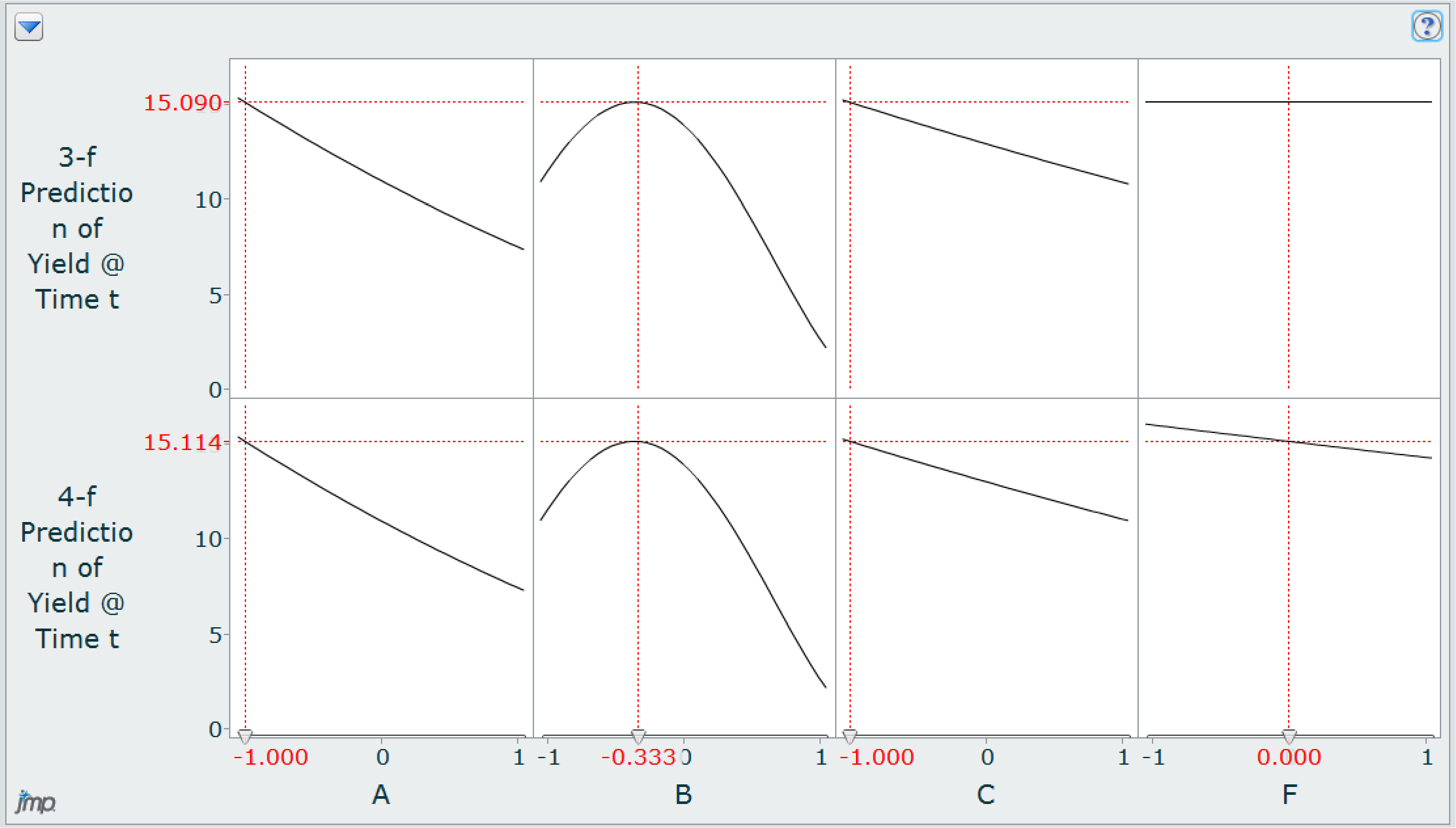
Prediction at settings of best observation



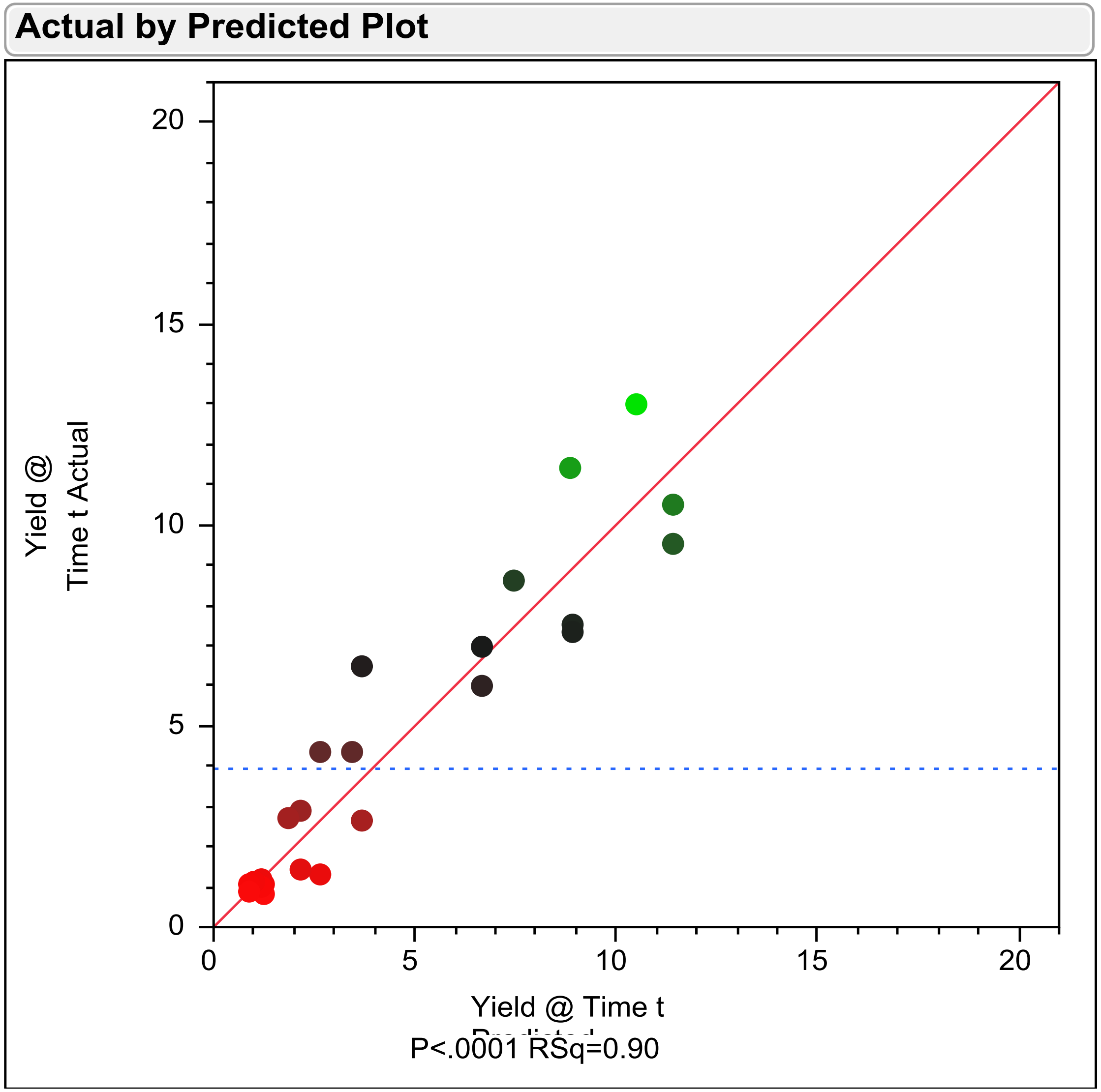
Prediction at best settings – run this checkpoint



PREDICTING WITH BEST 3-FACTOR AND 4-FACTOR MODELS

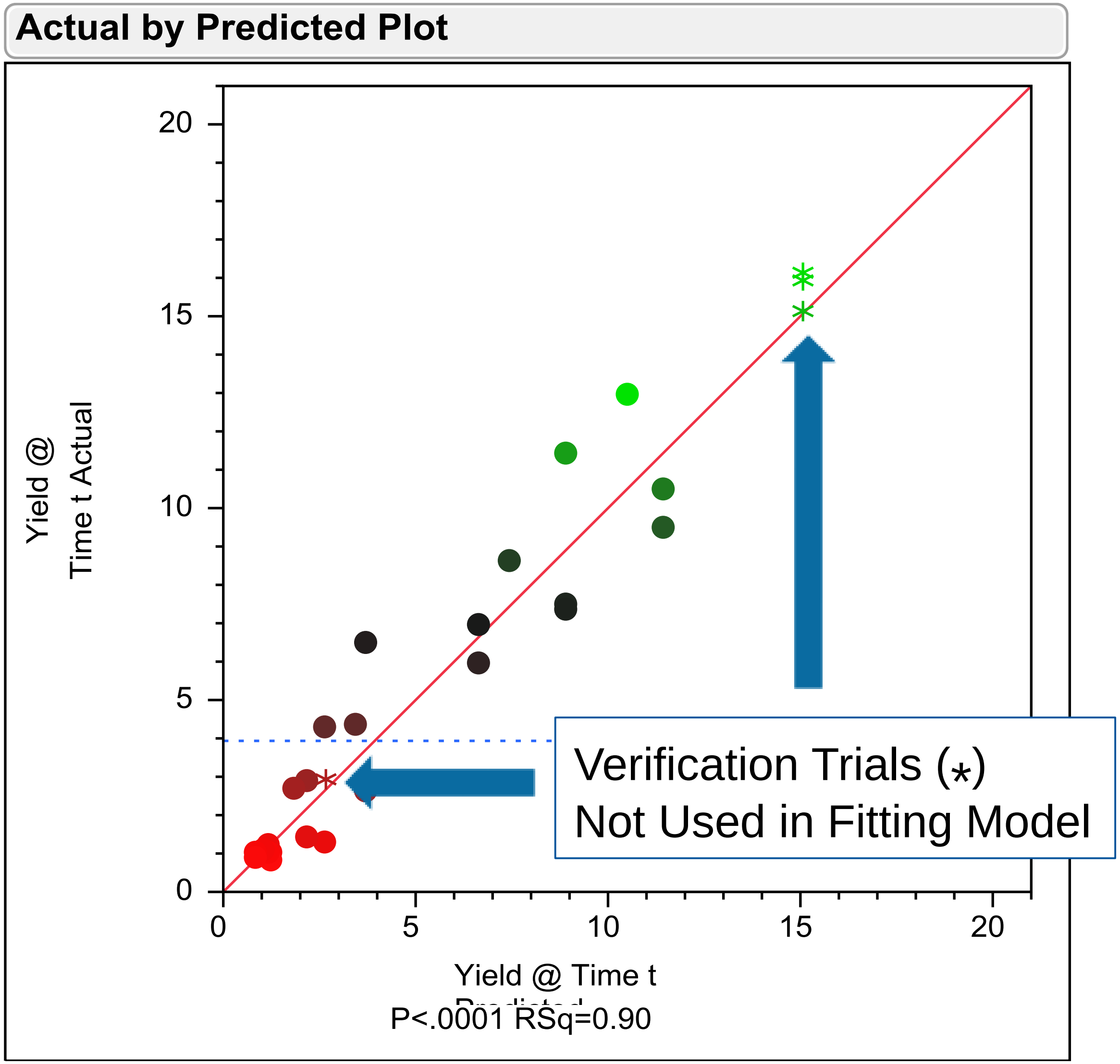


ACTUAL BY PREDICTED PLOT FOR FINAL 3-FACTOR MODEL FOR THE 24 DESIGN TRIALS



23/1	Yield @ Time t	A	B	C	D	E	F	G	H	I	J
1	1.38	-1	1	1	0	1	-1	1	-1	1	1
2	6.44	1	-1	-1	-1	1	-1	1	1	0	1
3	5.96	-1	-1	1	-1	-1	1	-1	1	1	0
4	4.34	0	-1	1	1	1	1	1	1	-1	-1
5	10.46	-1	-1	-1	-1	-1	0	1	-1	-1	-1
6	6.95	-1	-1	1	-1	1	-1	-1	0	-1	-1
7	8.58	1	0	-1	1	1	-1	-1	-1	1	-1
8	2.69	0	1	-1	-1	-1	-1	-1	-1	1	1
9	4.3	-1	1	-1	1	0	-1	-1	1	-1	1
10	0.77	1	-1	1	-1	0	1	1	-1	1	-1
11	2.87	-1	1	1	1	-1	1	-1	-1	0	-1
12	1.01	1	1	1	1	1	0	-1	1	1	1
13	9.47	-1	-1	-1	1	1	1	0	-1	1	1
14	7.49	0	0	0	0	0	0	0	0	0	0
15	0.98	1	1	-1	1	1	-1	1	-1	-1	0
16	0.86	1	1	1	-1	-1	-1	0	1	-1	-1
17	1.25	-1	1	-1	-1	1	1	1	1	1	-1
18	1.03	1	-1	1	1	-1	-1	-1	-1	-1	1
19	1.07	1	1	0	-1	1	1	-1	-1	-1	1
20	7.33	0	0	0	0	0	0	0	0	0	0
21	2.61	1	-1	-1	0	-1	1	-1	1	-1	-1
22	11.39	-1	-1	0	1	-1	-1	1	1	1	-1
23	12.96	-1	0	1	-1	-1	1	1	1	-1	1
24	1.18	1	1	-1	1	-1	1	1	0	1	1
25	15.93	-1	-0.333	-1	1	-1	-1	1	1	1	1
26	2.9	-1	1	-1	1	-1	-1	1	1	1	1
27	16.16	-1	-0.333	-1	-1	-1	-1	1	1	1	1
28	15.1	-1	-0.333	-1	0	-1	-1	1	1	1	1

ACTUAL BY PREDICTED PLOT FOR FINAL 3-FACTOR MODEL FOR THE 24 DESIGN TRIALS AND 4 VERIFICATION TRIALS



ANALYSIS STRATEGIES

- Conservative - treat designs like traditional screening
  - Fit main effects only (DSD is orthogonal in main effects)
  - Fit main effects + squared effects (DSD is orthogonal in squared terms too)
  - Use *factor sparsity* and *effect heredity* principles to propose final models

- Aggressive – use stepwise regression to pick best subsets of terms
  - Use AICc and BIC stopping criteria and pick “simpler model”
  - Use checkpoints validation R-square as stopping criteria to pick model
  - Use transformation to make error more uniform
    - square-root identified in plot of SSE vs. λ for Box-Cox transformation (i.e. $\lambda \approx 0.5$)
  - Fit ALL possible models

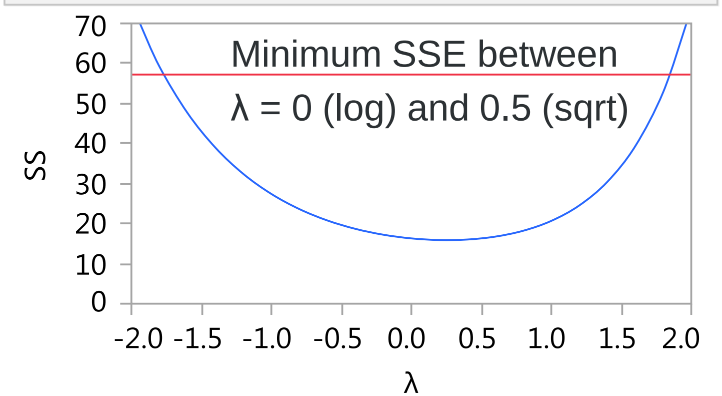
RANKED PARAMETER ESTIMATES

10 Main Effects (left) & 10 ME + 10 Squared Effects (right)

Sorted Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
A	-2.023428	0.791305	-2.56	0.0239 *
B	-2.030884	0.815352	-2.49	0.0271 *
C	-0.844283	0.791305	-1.07	0.3054
F	-0.453239	0.791305	-0.57	0.5766
J	0.3462584	0.815352	0.42	0.6780
G	0.3230058	0.799335	0.40	0.6927
H	0.2867159	0.788411	0.36	0.7220
E	-0.287384	0.791305	-0.36	0.7223
I	-0.155204	0.799335	-0.19	0.8490
D	0.1332841	0.788411	0.17	0.8684

Box-Cox Transformations

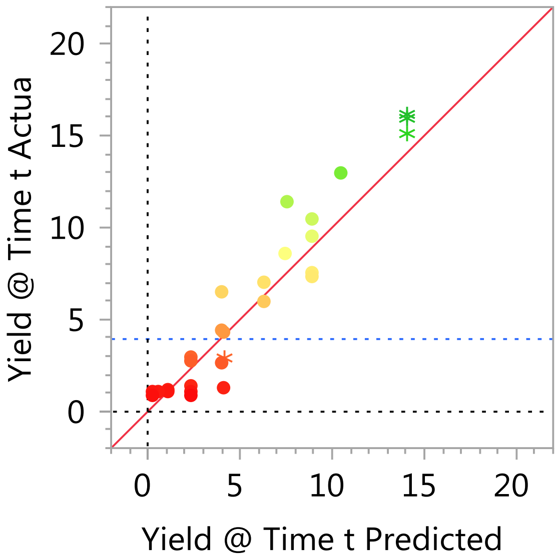


Sorted Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
B*B	-6.318587	1.774188	-3.56	0.0378 *
A	-2.023428	0.607403	-3.33	0.0447 *
B	-2.030884	0.625861	-3.24	0.0477 *
C	-0.844283	0.607403	-1.39	0.2587
D*D	2.456413	1.774188	1.38	0.2602
E*E	1.916413	1.774188	1.08	0.3592
C*C	-1.778587	1.774188	-1.00	0.3900
F	-0.453239	0.607403	-0.75	0.5097
F*F	-1.283587	1.774188	-0.72	0.5217
J	0.3462584	0.625861	0.55	0.6186
J*J	0.981413	1.774188	0.55	0.6187
A*A	0.936413	1.774188	0.53	0.6342
G	0.3230058	0.613566	0.53	0.6350
H	0.2867159	0.605181	0.47	0.6680
E	-0.287384	0.607403	-0.47	0.6684
G*G	-0.713587	1.774188	-0.40	0.7145
I	-0.155204	0.613566	-0.25	0.8166
D	0.1332841	0.605181	0.22	0.8398
H*H	0.386413	1.774188	0.22	0.8416
I*I	-0.203587	1.774188	-0.11	0.9159

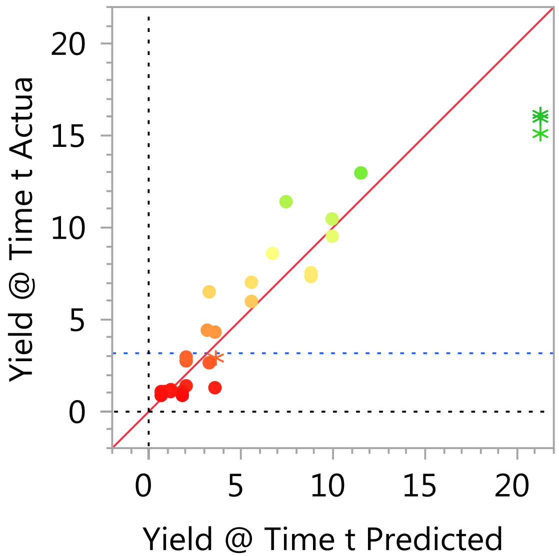
TRANSFORMATIONS SQRT, LOG, & NONE

Actual by Predicted Plot



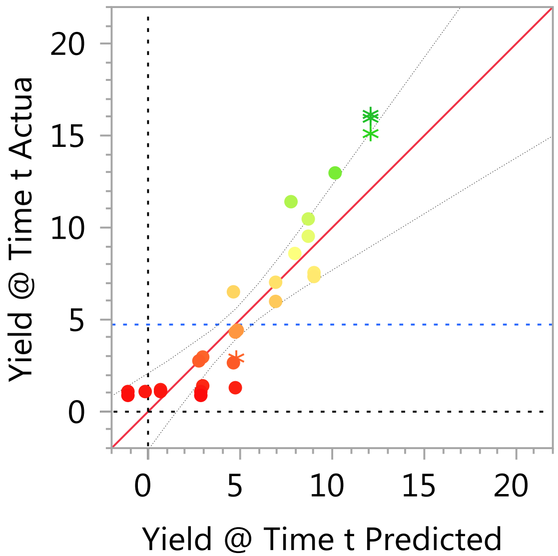
P<.0001 RSq=0.83
RMSE=0.4163

Actual by Predicted Plot



P<.0001 RSq=0.82
RMSE=0.4509

Actual by Predicted Plot



P<.0001 RSq=0.79
RMSE=1.9387

Summary of Fit

RSquare	0.825967
RSquare Adj	0.789328
Root Mean Square Error	0.416337
Mean of Response	1.983747
Observations (or Sum Wgt	24

Summary of Fit

RSquare	0.823029
RSquare Adj	0.785772
Root Mean Square Error	0.450888
Mean of Response	1.151951
Observations (or Sum Wgt	24

Summary of Fit

RSquare	0.789957
RSquare Adj	0.745738
Root Mean Square Error	1.938688
Mean of Response	4.72375
Observations (or Sum Wgt	24

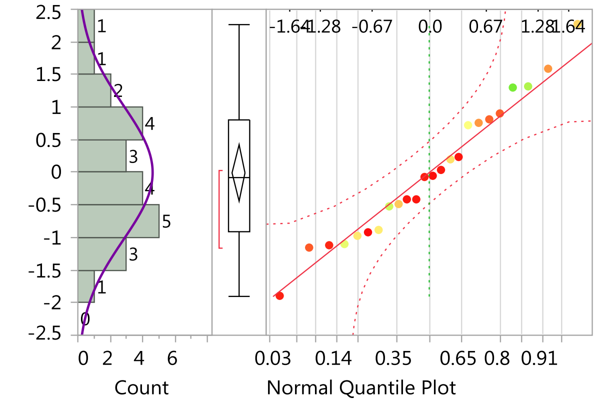
PLOTS OF RESIDUALS FOR DIFFERENT TRANSFORMATIONS

Model fit was reduced quadratic in A, B & C:

Yield = Intercept + A + B + C + B*B + A*B + B*C

Distributions

Studentized Resid Sqrt(Yield @ Time t) 2



Normal(-0.0045,1.03596)

Fitted Normal

Parameter Estimates

Type	Parameter	Estimate	Lower 95%	Upper 95%
Location	μ	-0.004478	-0.441926	0.4329688
Dispersio	σ	1.0359592	0.8051616	1.4532028

-2log(Likelihood) = 68.8047829349136

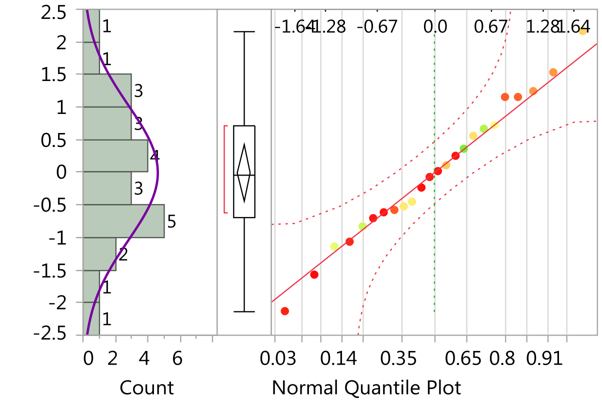
Goodness-of-Fit Test

Shapiro-Wilk W Test

W	Prob<W
0.972241	0.7224

Note: Ho = The data is from the Normal distribution. Small p-values reject Ho.

Studentized Resid Log(Yield @ Time t)



Normal(-0.008,1.03586)

Fitted Normal

Parameter Estimates

Type	Parameter	Estimate	Lower 95%	Upper 95%
Location	μ	-0.007981	-0.445387	0.4294258
Dispersio	σ	1.035863	0.8050868	1.4530679

-2log(Likelihood) = 68.8003267780461

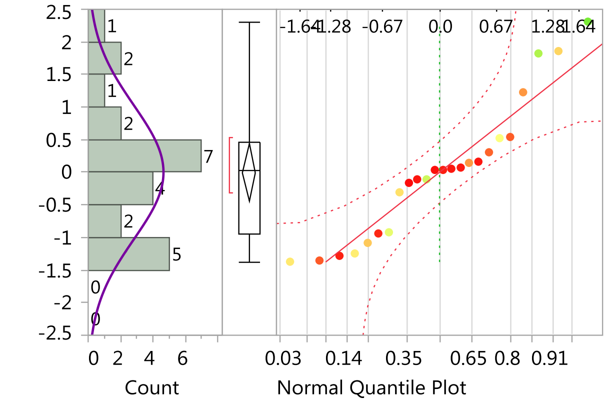
Goodness-of-Fit Test

Shapiro-Wilk W Test

W	Prob<W
0.992406	0.9994

Note: Ho = The data is from the Normal distribution. Small p-values reject Ho.

Studentized Resid Yield @ Time t



Normal(-0.0003,1.0284)

Fitted Normal

Parameter Estimates

Type	Parameter	Estimate	Lower 95%	Upper 95%
Location	μ	-0.000276	-0.434534	0.4339807
Dispersio	σ	1.0284046	0.79929	1.4426054

-2log(Likelihood) = 68.4534641248215

Goodness-of-Fit Test

Shapiro-Wilk W Test

W	Prob<W
0.918997	0.0555

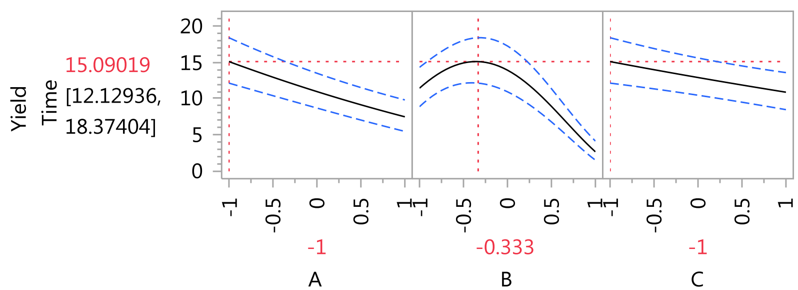
Note: Ho = The data is from the Normal distribution. Small p-values reject Ho.

STEPWISE 3-FACTOR MODEL (7 TERMS) - LEFT
FULL QUADRATIC 3-FACTOR MODEL (10 TERMS) - RIGHT

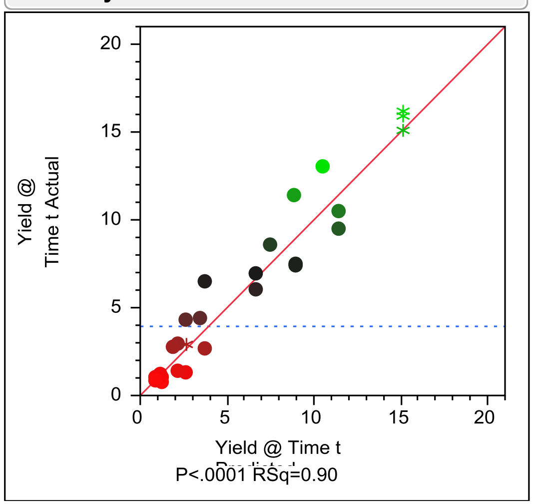
Sorted Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
B*B	-1.218717	0.182702	-6.67	<.0001 *
A	-0.496169	0.075133	-6.60	<.0001 *
B	-0.481867	0.075133	-6.41	<.0001 *
C	-0.240181	0.075133	-3.20	0.0053 *
A*B	0.2306449	0.078918	2.92	0.0095 *
C*B	0.1585526	0.078918	2.01	0.0607

Prediction Profiler



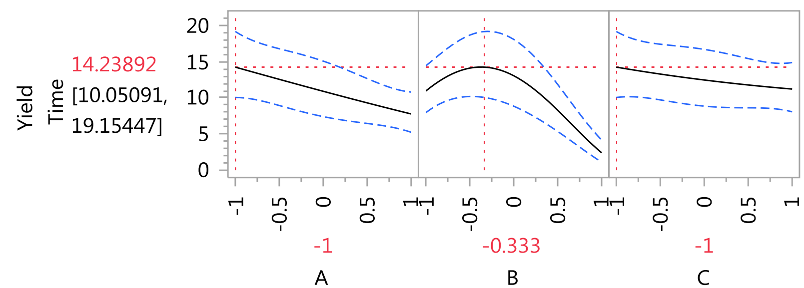
Actual by Predicted Plot



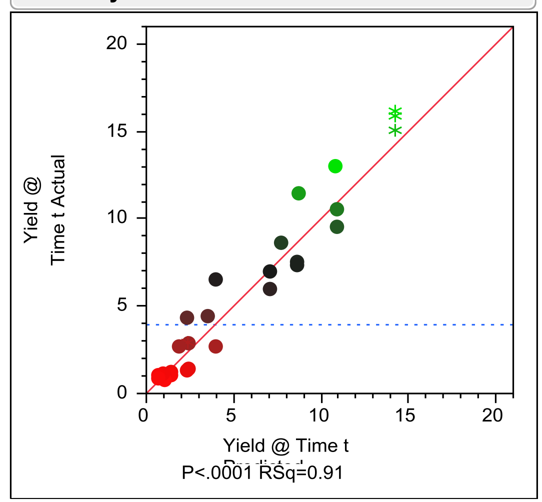
Sorted Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
A	-0.496169	0.080197	-6.19	<.0001 *
B	-0.481867	0.080197	-6.01	<.0001 *
B*B	-1.181941	0.233332	-5.07	0.0002 *
C	-0.240181	0.080197	-2.99	0.0096 *
A*B	0.2339616	0.087698	2.67	0.0184 *
C*B	0.1610152	0.087698	1.84	0.0877
A*C	-0.08124	0.087698	-0.93	0.3700
C*C	0.0307046	0.233332	0.13	0.8972
A*A	-0.021309	0.233332	-0.09	0.9285

Prediction Profiler

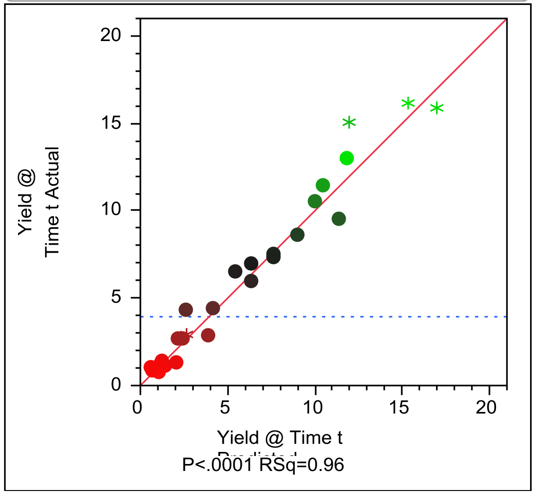


Actual by Predicted Plot

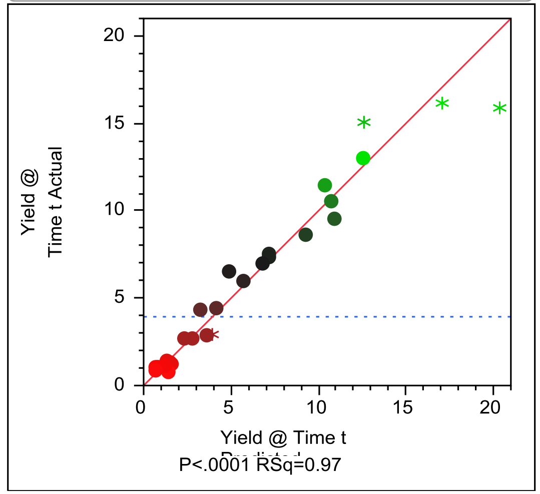


STEPWISE MODELS:
4-FACTOR (12 TERMS), 5-FACTOR (13 TERMS), 6-FACTOR (15 TERMS)

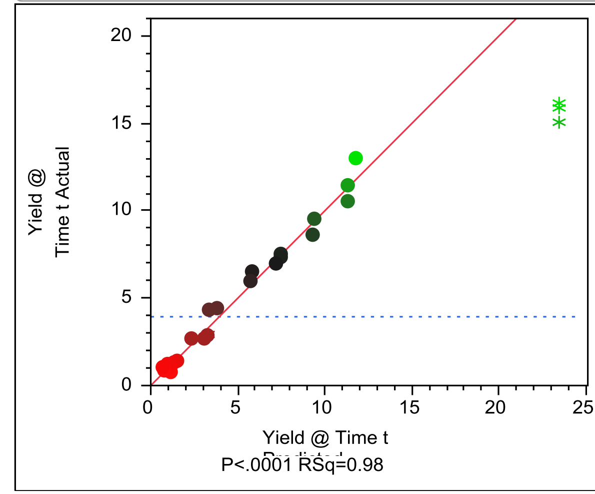
Actual by Predicted Plot



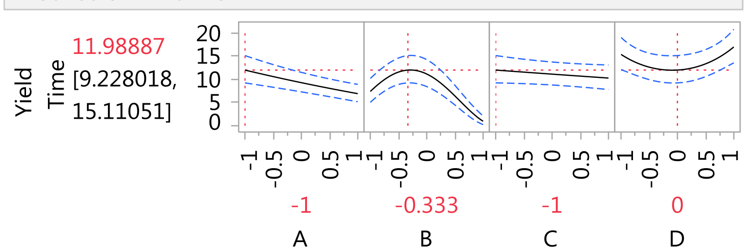
Actual by Predicted Plot



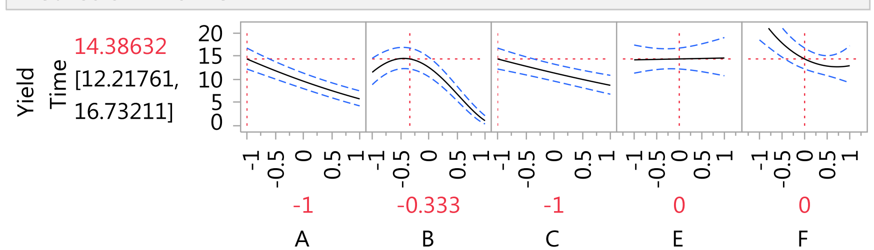
Actual by Predicted Plot



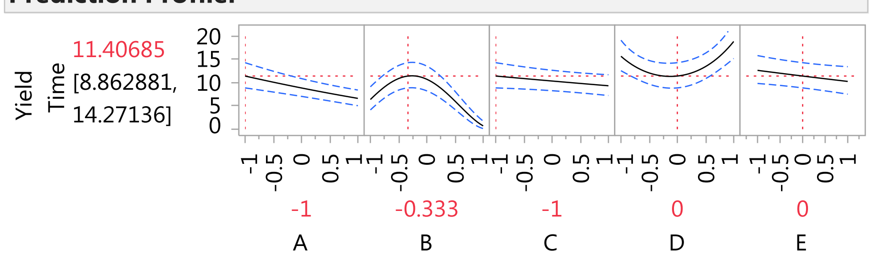
Prediction Profiler



Prediction Profiler



Prediction Profiler



AGGRESSIVE ANALYSES

- Stepwise using Main Effects and Squared Effects for all factors
  - Will show just the use of AICc & BIC stopping criteria –
    all stepwise approaches yield very similar results

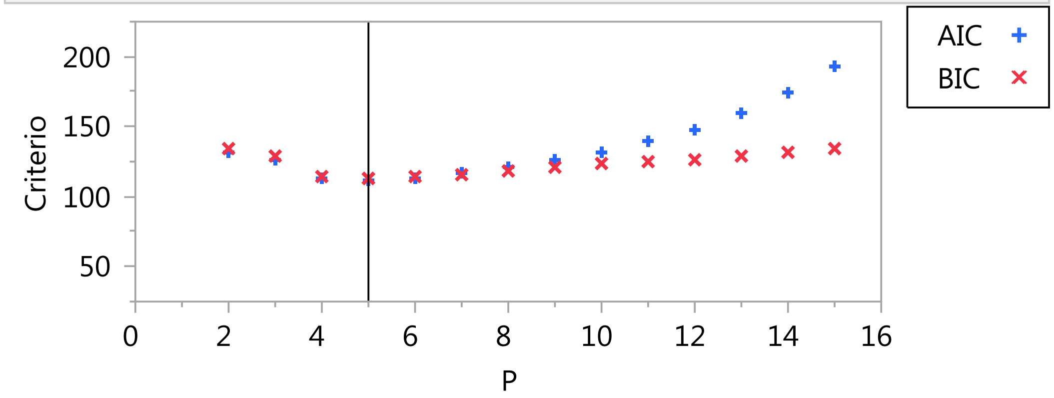
- Stepwise using full 10-factor, 66-term quadratic model
  1 intercept + 10 ME + 10 SQ + 45 2FI (2-factor interactions)
  - Use AICc & BIC stopping criteria and pick “simpler model” – Occam’s razor
  - Use max K-Fold R-square as stopping rule to pick model (no checkpoints)
  - Use max validation R-square for checkpoints as stopping rule to pick model
  - Fit ALL possible models

USE MIN AIC OR BIC CRITERION AS STOPPING RULE

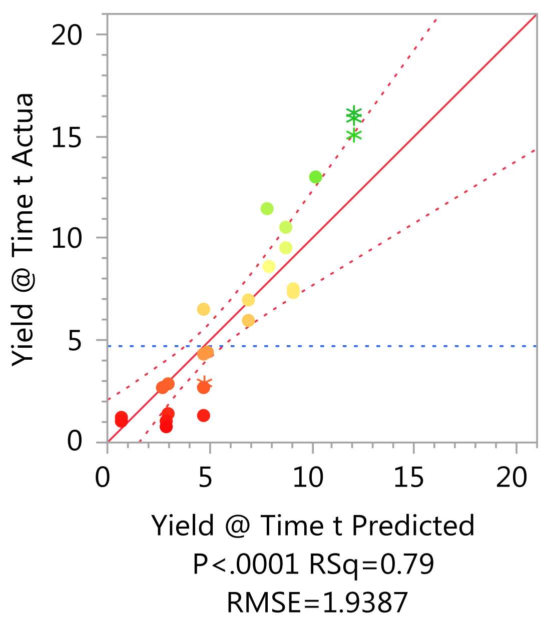
21 TERMS, ME + SQ

RAW RESPONSE VALUES USED

Criterion History



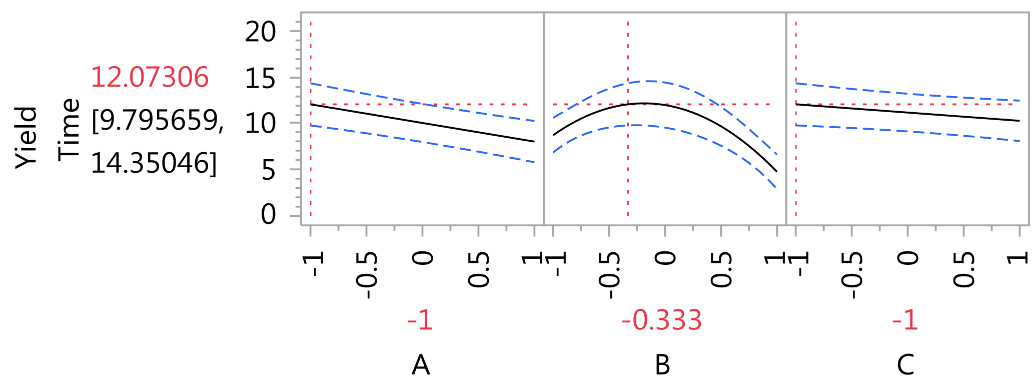
Actual by Predicted Plot



Sorted Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
B*B	-5.2395	1.061863	-4.93	<.0001 *
A	-2.014167	0.437499	-4.60	0.0002 *
B	-1.979167	0.437499	-4.52	0.0002 *
C	-0.890833	0.437499	-2.04	0.0559

Prediction Profiler

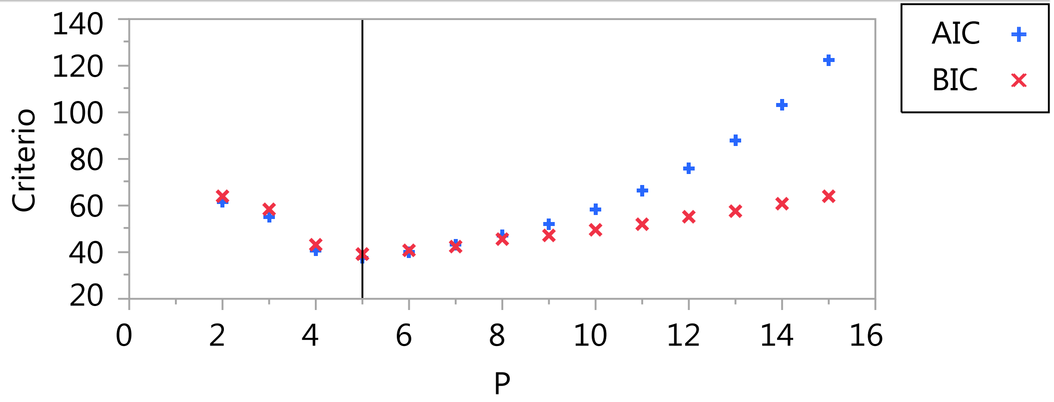


USE MIN AIC OR BIC CRITERION AS STOPPING RULE

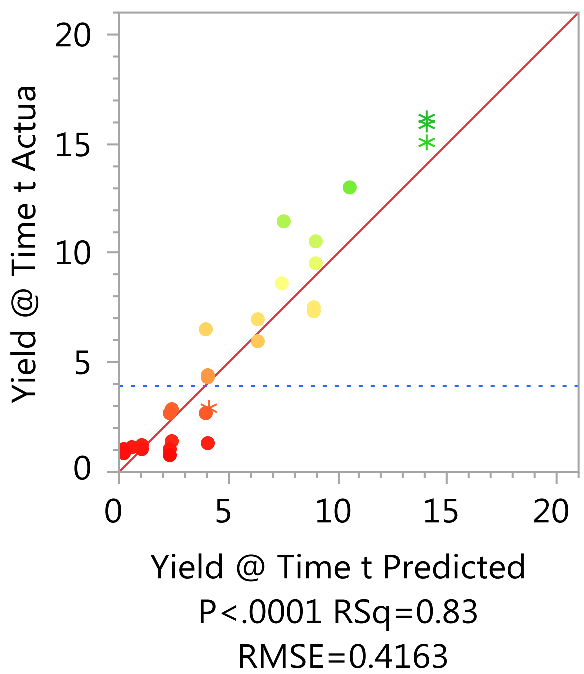
21 TERMS, ME + SQ

TRANSFORMED VALUES USED

Criterion History



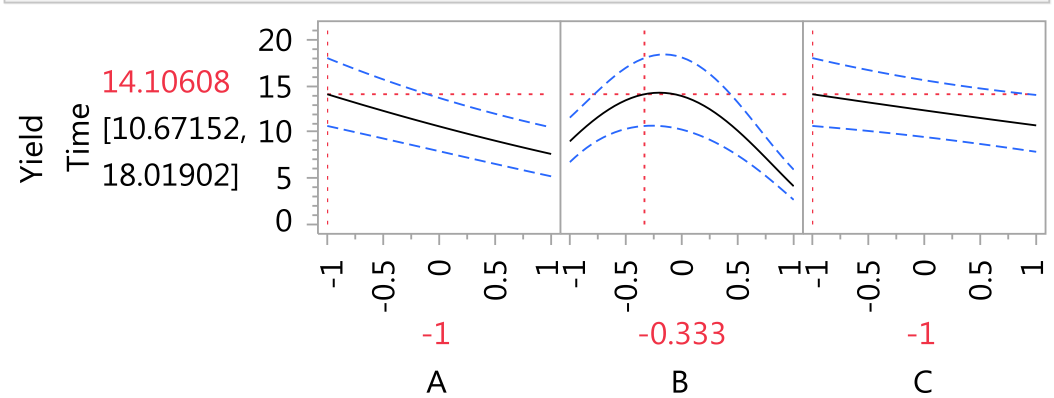
Actual by Predicted Plot



Sorted Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
B*B	-1.211508	0.228037	-5.31	<.0001 *
A	-0.496169	0.093954	-5.28	<.0001 *
B	-0.481867	0.093954	-5.13	<.0001 *
C	-0.240181	0.093954	-2.56	0.0193 *

Prediction Profiler

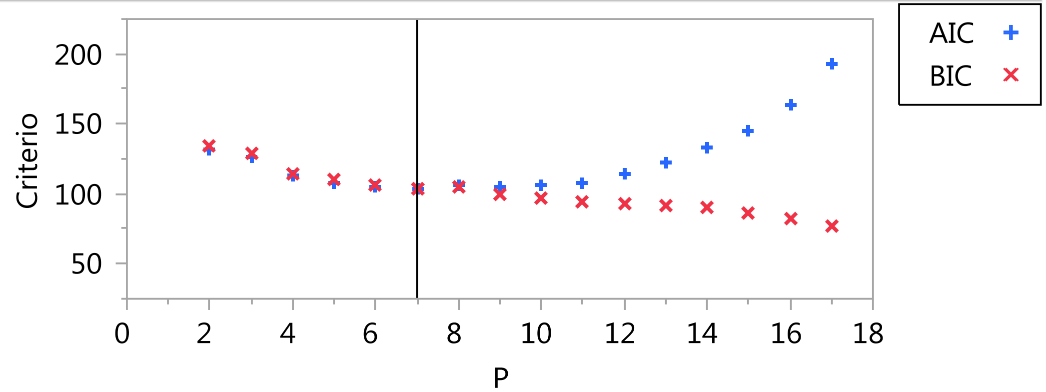


USE MIN AIC OR BIC CRITERION AS STOPPING RULE

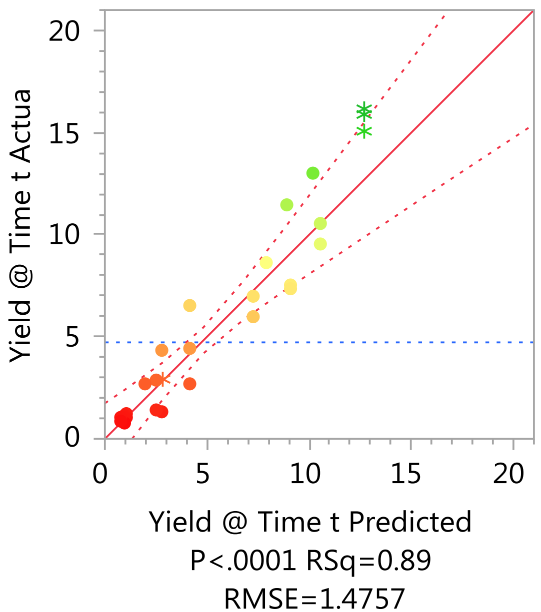
66 TERM QUADRATIC

RAW RESPONSE VALUES USED

Criterion History



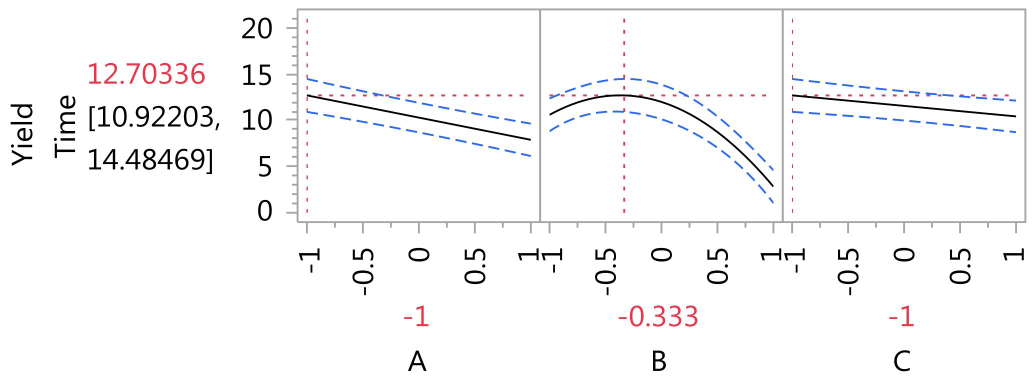
Actual by Predicted Plot



Sorted Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
B*B	-5.282841	0.809809	-6.52	<.0001 *
A	-2.014167	0.33302	-6.05	<.0001 *
B	-1.979167	0.33302	-5.94	<.0001 *
A*B	1.1703157	0.349799	3.35	0.0038 *
C	-0.890833	0.33302	-2.68	0.0160 *
B*C	0.7369066	0.349799	2.11	0.0503

Prediction Profiler

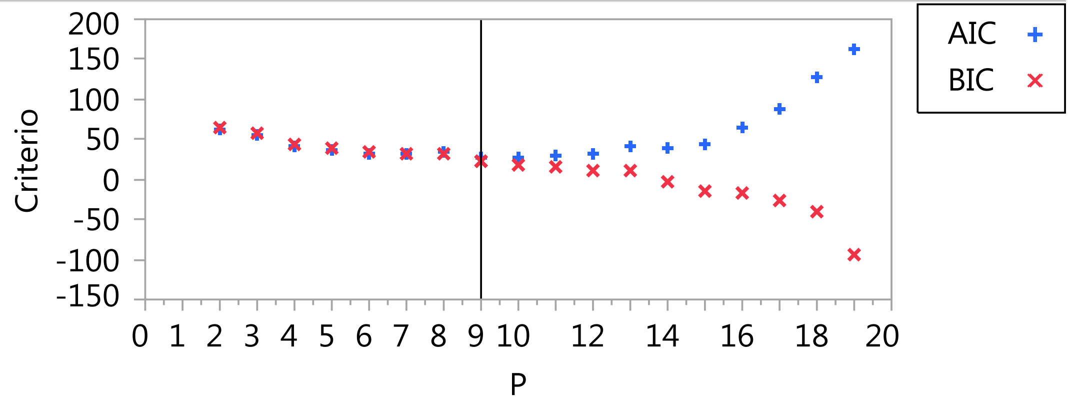


USE MIN AIC OR BIC CRITERION AS STOPPING RULE

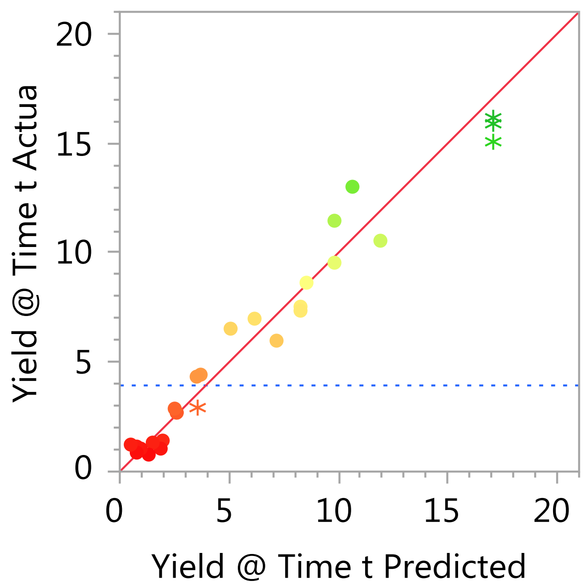
66 TERM QUADRATIC

TRANSFORMED VALUES USED

Criterion History



Actual by Predicted Plot

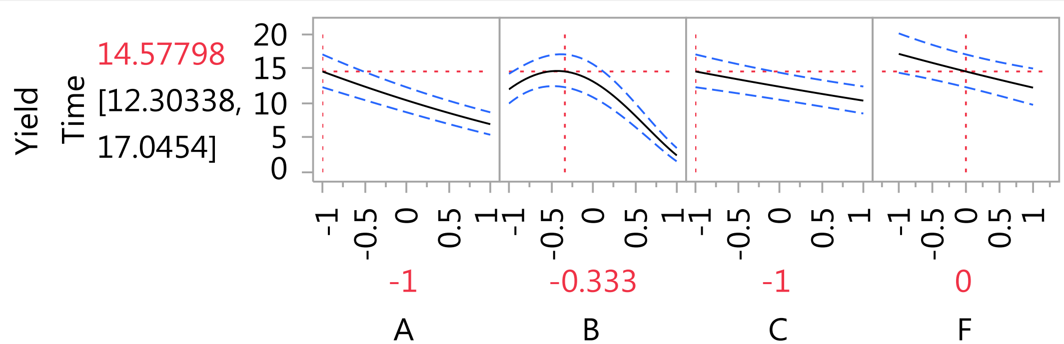


P<.0001 RSq=0.95
RMSE=0.2519

Sorted Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
A	-0.505343	0.057053	-8.86	<.0001 *
B	-0.491041	0.057053	-8.61	<.0001 *
B*B	-1.111685	0.141981	-7.83	<.0001 *
A*B	0.253637	0.060121	4.22	0.0007 *
C	-0.231007	0.057053	-4.05	0.0010 *
B*C	0.2053297	0.061367	3.35	0.0044 *
C*F	0.2093075	0.063209	3.31	0.0047 *
F	-0.110087	0.057053	-1.93	0.0728

Prediction Profiler

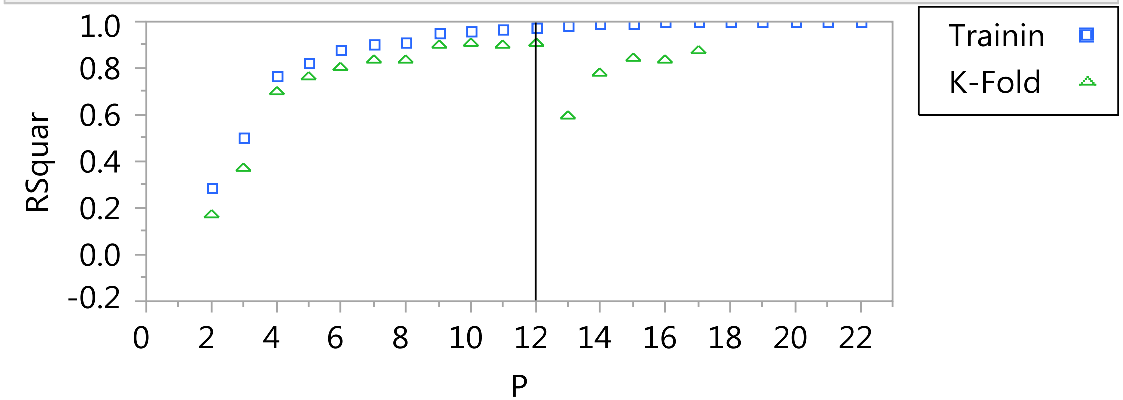


USE MAX K-FOLD R-SQUARE AS STOPPING RULE

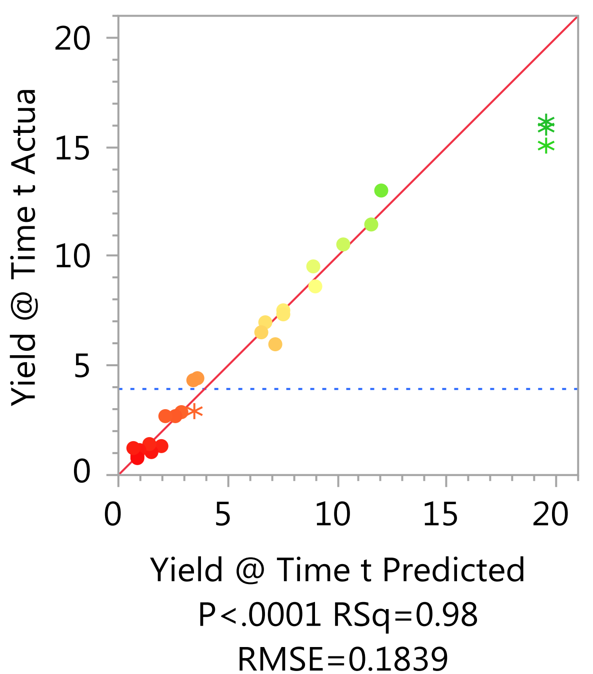
66 TERM QUADRATIC

TRANSFORMED VALUES USED

RSquare History



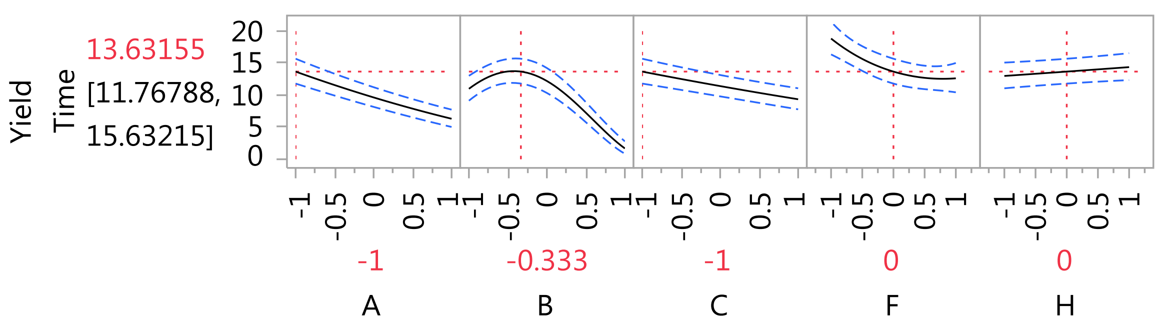
Actual by Predicted Plot



Sorted Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
A	-0.498201	0.041762	-11.93	<.0001 *
B	-0.483899	0.041762	-11.59	<.0001 *
B*B	-1.184839	0.114991	-10.30	<.0001 *
A*B	0.2798015	0.045426	6.16	<.0001 *
C	-0.238149	0.041762	-5.70	<.0001 *
B*C	0.2427713	0.047097	5.15	0.0002 *
C*F	0.2349251	0.047559	4.94	0.0003 *
F	-0.117229	0.041762	-2.81	0.0158 *
B*F	0.1203014	0.0449	2.68	0.0201 *
H	0.0928467	0.041762	2.22	0.0462 *
F*F	0.2478009	0.120097	2.06	0.0614

Prediction Profiler

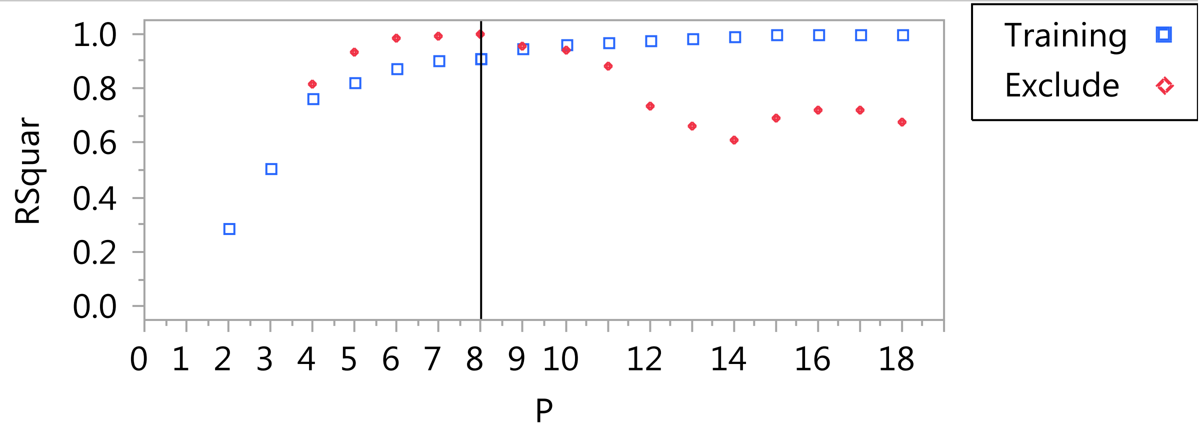


USE MAX VALIDATION R-SQUARE FOR 4 CHECKPOINTS AS STOPPING RULE

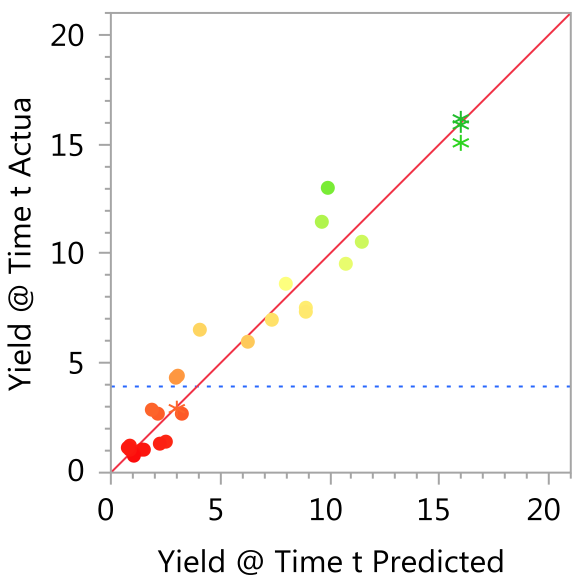
66 TERM QUADRATIC

TRANSFORMED VALUES USED

RSquare History



Actual by Predicted Plot

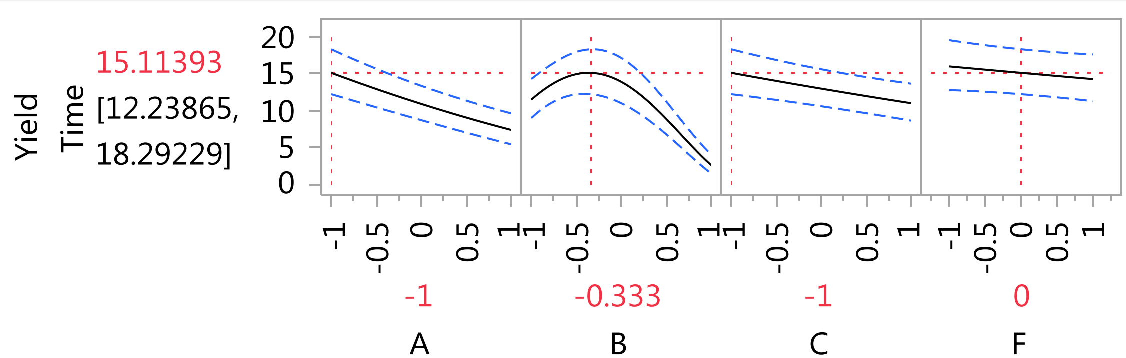


P<.0001 RSq=0.91
RMSE=0.3209

Sorted Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
A	-0.505343	0.072679	-6.95	<.0001 *
B*B	-1.218717	0.17612	-6.92	<.0001 *
B	-0.491041	0.072679	-6.76	<.0001 *
C	-0.231007	0.072679	-3.18	0.0058 *
A*B	0.2306449	0.076075	3.03	0.0079 *
B*C	0.1585526	0.076075	2.08	0.0535
F	-0.110087	0.072679	-1.51	0.1494

Prediction Profiler



FIT ALL POSSIBLE MODELS UP TO 8 TERMS

- 1-term A
- 2-term B, B*B
- 3-term A, B, B*B
- 4-term A, B, C, B*B
- 5-term A, B, C, A*B, B*B
- 6-term A, B, C, A*B, B*B, B*C
- 7-term A, B, C, G, A*B, B*B, B*G
- 8-term A, B, C, G, A*B, B*B, A*C, B*G

CO2 Capture Process - Fit Stepwise 2 - JMP Pro

Stepwise Fit for Sqrt(Yield @ Time t)

All Possible Models

Model	Number	RSquare	RMSE	AICc	BIC
B,F,H	3	0.2934	0.8177	67.4058	69.9628
A,E,(E--0.1429)*(E--0.1429)	3	0.2922	0.8184	67.4456	70.0025
A,B,C,B*B	4	0.8260	0.4163	37.3830	39.5102
A,B,A*B,B*B	4	0.8169	0.4270	38.5990	40.7262
A,B,F,B*B	4	0.7835	0.4644	42.6270	44.7542

4-term

CO2 Capture Process - Fit Stepwise 2 - JMP Pro

Stepwise Fit for Sqrt(Yield @ Time t)

All Possible Models

Model	Number	RSquare	RMSE	AICc	BIC
A,B,H,(H-0.14286)*(H-0.14286)	4	0.5358	0.6800	60.9300	63.0571
A,B,D,A*A	4	0.5352	0.6804	60.9587	63.0858
A,B,C,A*B,B*B	5	0.8768	0.3599	33.1552	34.4016
A,B,C,B*B,B*C	5	0.8504	0.3966	37.8124	39.0588
A,B,C,F,B*B	5	0.8385	0.4121	39.6548	40.9011

5-term

CO2 Capture Process - Fit Stepwise 2 - JMP Pro

Stepwise Fit for Sqrt(Yield @ Time t)

All Possible Models

Model	Number	RSquare	RMSE	AICc	BIC
A,B,E,A*B,A*(E--0.1429)	5	0.6402	0.6150	58.8712	60.1175
A,B,E,F,A*(E--0.1429)	5	0.6401	0.6151	58.8813	60.1277
A,B,C,A*B,B*B,B*C	6	0.9004	0.3329	32.6422	32.4667
A,B,C,F,A*B,B*B	6	0.8893	0.3511	35.1906	35.0150
A,B,C,H,A*B,B*B	6	0.8840	0.3593	36.3016	36.1261

6-term

CO2 Capture Process - Fit Stepwise 2 - JMP Pro

Stepwise Fit for Sqrt(Yield @ Time t)

All Possible Models

Model	Number	RSquare	RMSE	AICc	BIC
A,B,C,D,B*B,A*D	6	0.8348	0.4289	44.7940	44.6185
A,B,E,F,A*B,B*B	6	0.8347	0.4290	44.8087	44.6331
A,B,C,G,A*B,B*B,B*(G-0.14286)	7	0.9239	0.3000	31.4479	29.1933
A,B,C,E,B*B,A*(E--0.1429),B*(E--0.1429)	7	0.9145	0.3180	34.2381	31.9835
A,B,C,F,A*B,B*B,B*C	7	0.9129	0.3209	34.6833	32.4287

7-term

ALL ANALYSES RANK FACTORS A, B & C AS TOP 3

FACTOR F APPEARS TO BE MOST LIKELY FOURTH FACTOR

- Linear terms only – fourth factor is F
- Linear + Squared terms – fourth factor is D
- Stepwise with min AICc stopping rule – fourth factor is F
- Stepwise with max K-Fold R-Square stopping rule – fourth factor is F
- Stepwise with max Validation R-Square as stopping rule – fourth factor is F
- All possible models – fourth factor is G

- When D & F are in same 5-factor (with A, B, & C) stepwise model, D drops out
- When G & F are in same 5-factor (with A, B, & C) stepwise model, G drops out
- When D & G are in same 5-factor (with A, B, & C) stepwise model, both drop out

- There is an important difference between saying, *"Factor F has no effect."* and, *"Given the amount of data taken an effect for factor F was not detected."*

- Augmenting design to support 6-factor quadratic model in A, B, C, D, F & G will
  - help resolve the relative contributions of D, F & G
  - increase the power for all – but especially - the squared terms

IF MORE THAN A FEW FACTORS ARE SIGNIFICANT, THEN AUGMENT DESIGN TO SUPPORT 2ND ORDER MODEL

	A	B	C	D	F	G	Block	Yield @ Time t
14	0	0	0	0	0	0	1	7.49
15	1	1	-1	1	-1	1	1	0.98
16	1	1	1	-1	-1	0	1	0.86
17	-1	1	-1	-1	1	1	1	1.25
18	1	-1	1	1	-1	-1	1	1.03
19	1	1	0	-1	1	-1	1	1.07
20	0	0	0	0	0	0	1	7.33
21	1	-1	-1	0	1	-1	1	2.61
22	-1	-1	0	1	-1	1	1	11.39
23	-1	0	1	-1	1	1	1	12.96
24	1	1	-1	1	1	1	1	1.18
25	1	0	1	1	-1	1	2	•
26	1	-1	0	1	1	0	2	•
27	1	-1	-1	1	0	1	2	•
28	1	-1	0	-1	0	-1	2	•
29	1	0	-1	-1	1	0	2	•
30	1	1	0	-1	0	1	2	•
31	1	0	1	0	1	-1	2	•
32	-1	-1	0	0	1	1	2	•
33	0	0	1	1	-1	-1	2	•
34	-1	-1	1	0	0	0	2	•
35	0	1	1	0	1	0	2	•
36	0	1	-1	1	1	-1	2	•

NOTE: First 13 rows of original design are not shown.

These 12 trials added onto original 24 trials to support full quadratic model in 6 most important factors plus a block effect between original and augmented trials

POWER FOR SQUARED TERMS IN 2ND ORDER MODEL IS INCREASED TO NEAR THAT OF 6-FACTOR RSM DESIGNS

Power Analysis

Significance Level 0.05

Anticipated RMSE 1

Parameter	Anticipated Coefficients	Power
Intercept	1	0.273
Block	1	0.983
A	1	0.965
B	-1	0.966
C	1	0.976
D	-1	0.969
F	1	0.975
G	-1	0.961
A*B	1	0.887
A*C	-1	0.881
A*D	1	0.825
A*F	-1	0.915
A*G	1	0.732
B*C	-1	0.728
B*D	1	0.853
B*F	-1	0.859
B*G	1	0.724
C*D	-1	0.872
C*F	1	0.838
C*G	-1	0.778
D*F	1	0.847
D*G	-1	0.838
F*G	1	0.86
A*A	1	0.299
B*B	-1	0.361
C*C	1	0.362
D*D	-1	0.309
F*F	1	0.384
G*G	-1	0.347

Power Analysis

Significance Level 0.05

Anticipated RMSE 1

Parameter	Anticipated Coefficients	Power
Intercept	1	0.364
A	1	0.998
B	-1	0.998
C	1	0.998
D	-1	0.998
F	1	0.998
G	-1	0.998
A*A	1	0.527
B*B	-1	0.599
C*C	1	0.582
D*D	-1	0.541
F*F	1	0.573
G*G	-1	0.568

	A	B	C	D	F	G	Block	Yield @ Time t
14	0	0	0	0	0	0	1	7.49
15	1	1	-1	1	-1	1	1	0.98
16	1	1	1	-1	-1	0	1	0.86
17	-1	1	-1	-1	1	1	1	1.25
18	1	-1	1	1	-1	-1	1	1.03
19	1	1	0	-1	1	-1	1	1.07
20	0	0	0	0	0	0	1	7.33
21	1	-1	-1	0	1	-1	1	2.61
22	-1	-1	0	1	-1	1	1	11.39
23	-1	0	1	-1	1	1	1	12.96
24	1	1	-1	1	1	1	1	1.18
25	1	0	1	1	-1	1	2	•
26	1	-1	0	1	1	0	2	•
27	1	-1	-1	1	0	1	2	•
28	1	-1	0	-1	0	-1	2	•
29	1	0	-1	-1	1	0	2	•
30	1	1	0	-1	0	1	2	•
31	1	0	1	0	1	-1	2	•
32	-1	-1	0	0	1	1	2	•
33	0	0	1	1	-1	-1	2	•
34	-1	-1	1	0	0	0	2	•
35	0	1	1	0	1	0	2	•
36	0	1	-1	1	1	-1	2	•

COMPARE AUGMENTED DESIGNS

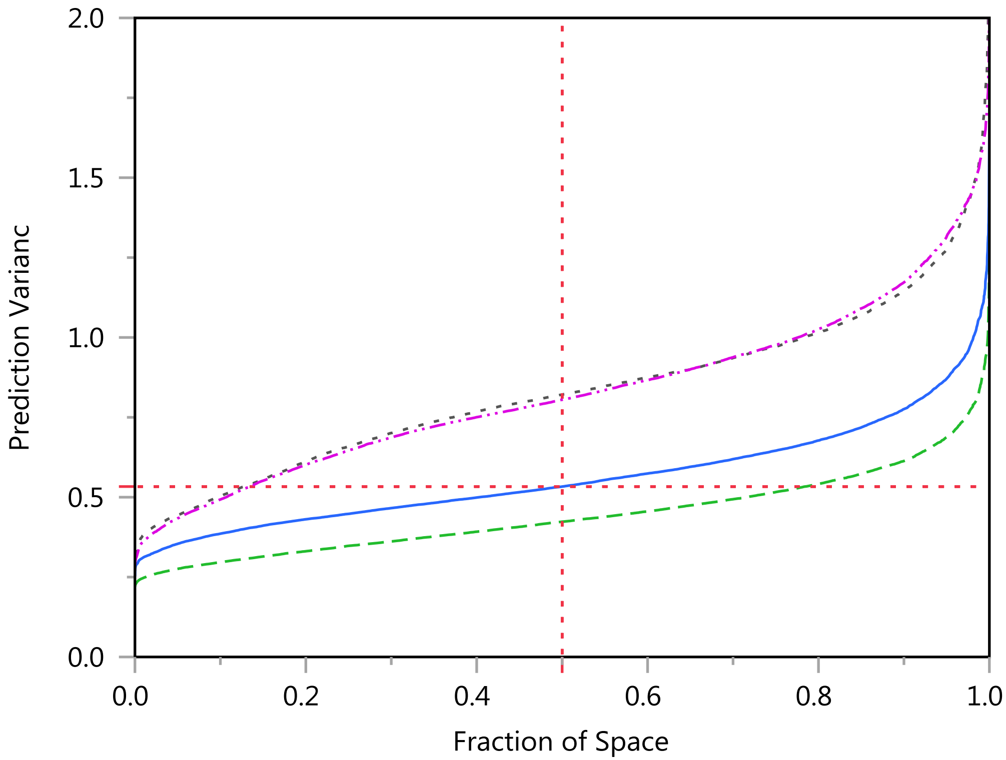
TOP: 10-FACTOR FRACTIONAL FACTORIAL + C.P. AUGMENTED TO SUPPORT FULL QUADRATIC MODEL IN 6 FACTORS
33 + 9 = 42 TOTAL TRIALS

UPPER MIDDLE: 10-FACTOR PLACKET-BURMAN + C.P. AUGMENTED TO SUPPORT FULL QUADRATIC MODEL IN 6 FACTORS
25 + 11 = 36 TOTAL TRIALS

LOWER MIDDLE: 10-FACTOR DEFINITIVE SCREENING AUGMENTED TO SUPPORT FULL QUADRATIC MODEL IN 6 FACTORS
21 + 15 = 36 TOTAL TRIALS

BOTTOM: 6-FACTOR CUSTOM DOE FOR FULL RSM MODEL
34 TOTAL TRIALS

Fraction of Design Space Plot



Design Diagnostics

I Optimal Design	
D Efficiency	40.729
G Efficiency	56.09719
A Efficiency	12.41717
Average Variance of Prediction	0.82307
Design Creation Time (seconds)	0.05

Design Diagnostics

I Optimal Design	
D Efficiency	38.46605
G Efficiency	54.33992
A Efficiency	14.61968
Average Variance of Prediction	0.833744
Design Creation Time (seconds)	0.05

Design Diagnostics

I Optimal Design	
D Efficiency	42.15506
G Efficiency	69.61262
A Efficiency	22.27027
Average Variance of Prediction	0.563765
Design Creation Time (seconds)	0.066667

Design Diagnostics

I Optimal Design	
D Efficiency	42.94028
G Efficiency	75.52931
A Efficiency	27.20305
Average Variance of Prediction	0.44424
Design Creation Time (seconds)	0.066667

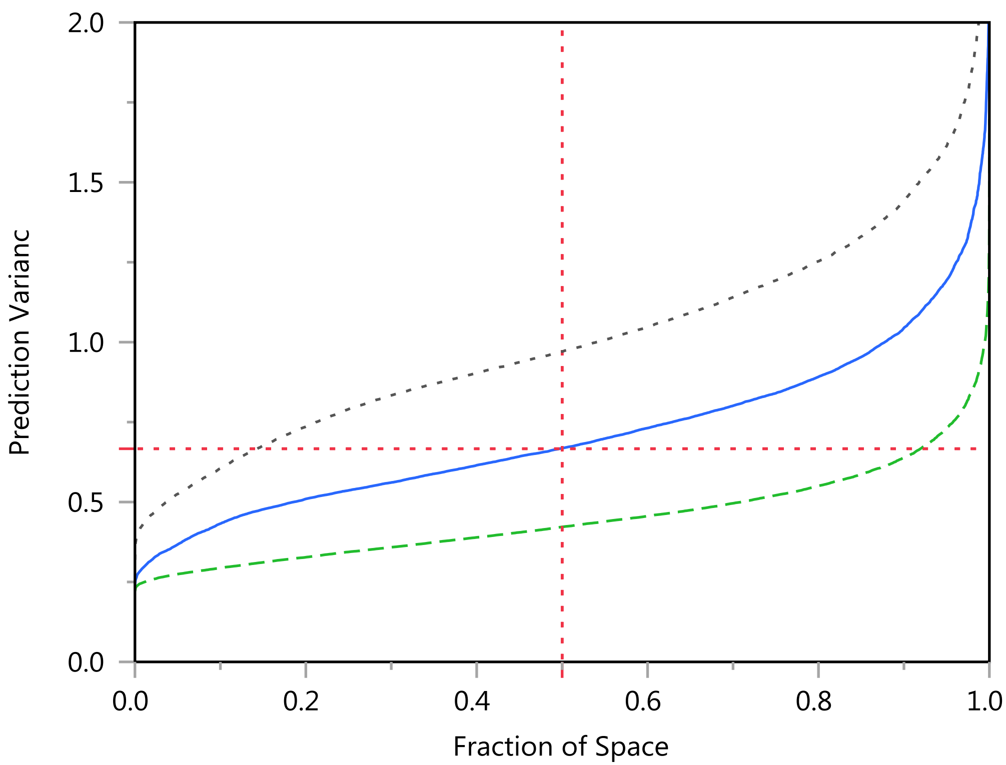
COMPARE AUGMENTED DESIGNS

TOP: 14-FACTOR FRACTIONAL FACTORIAL + C.P. AUGMENTED TO SUPPORT FULL QUADRATIC MODEL IN 7 FACTORS
33 + 13 = 46 TOTAL TRIALS

MIDDLE: 14-FACTOR DEFINITIVE SCREENING AUGMENTED TO SUPPORT FULL QUADRATIC MODEL IN 7 FACTORS
29 + 17 = 46 TOTAL TRIALS

BOTTOM: 7-FACTOR CUSTOM DOE FOR FULL RSM MODEL
42 TOTAL TRIALS

Fraction of Design Space Plot



Design Diagnostics

I Optimal Design	
D Efficiency	37.352
G Efficiency	48.68453
A Efficiency	11.13939
Average Variance of Prediction	1.006709
Design Creation Time (seconds)	0.133333

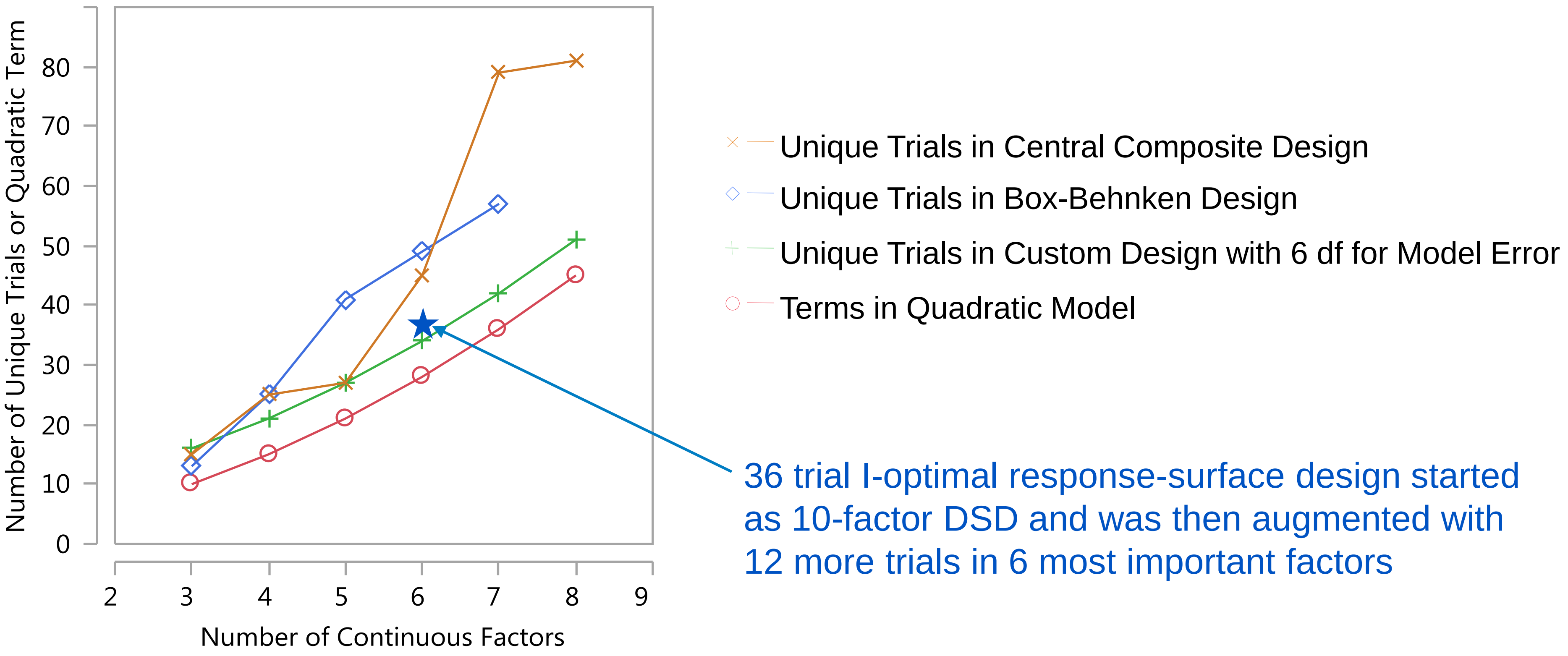
Design Diagnostics

I Optimal Design	
D Efficiency	36.69963
G Efficiency	58.39688
A Efficiency	15.61337
Average Variance of Prediction	0.714178
Design Creation Time (seconds)	0.133333

Design Diagnostics

I Optimal Design	
D Efficiency	41.03495
G Efficiency	71.04153
A Efficiency	27.70772
Average Variance of Prediction	0.449918
Design Creation Time (seconds)	0.216667

NUMBER OF UNIQUE TRIALS FOR 3 RESPONSE-SURFACE DESIGNS AND NUMBER OF QUADRATIC MODEL TERMS VS. NUMBER OF CONTINUOUS FACTORS



If generally running 3, 4 or 5-factor fractional-factorial designs…

1. How many interactions are you not investigating?
2. How many more trials needed to fit curvature?
3. Consider two stages: Definitive Screening + Augmentation

- ***Definitive Screening Designs***
  - Efficiently estimate main and quadratic effects for no more and **often fewer trials than traditional designs**
  - If only a few factors are important the design may collapse into a **"one-shot"** design that supports a response-surface model
  - If many factors are important the design can be **augmented** to support a response-surface model
  - Case study for a **10-variable process** shows that it can be **optimized in just 23 unique trials**

Thanks.
Questions or comments?

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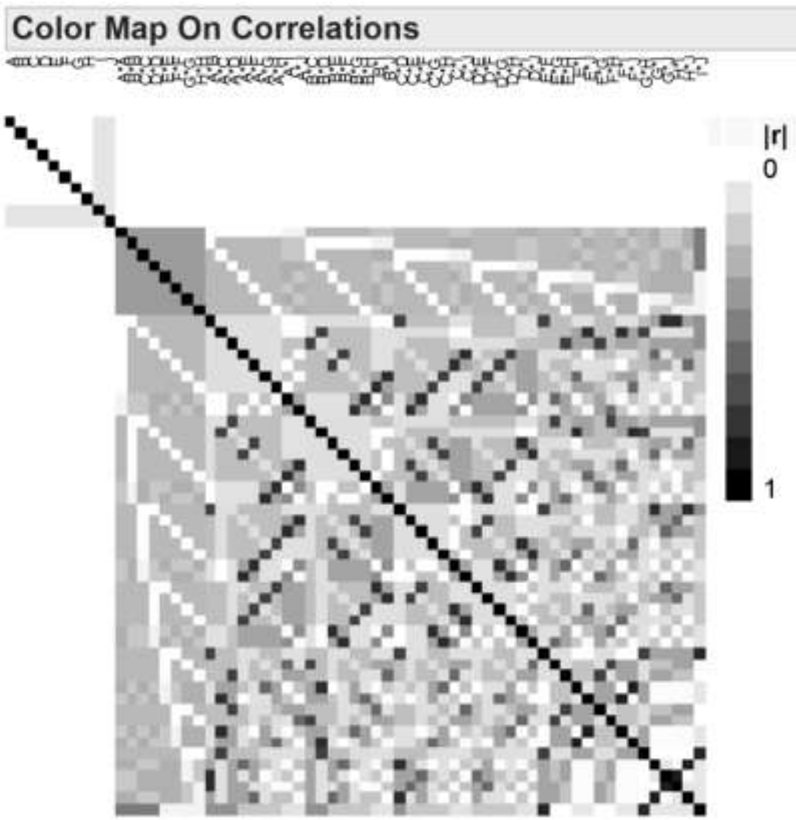
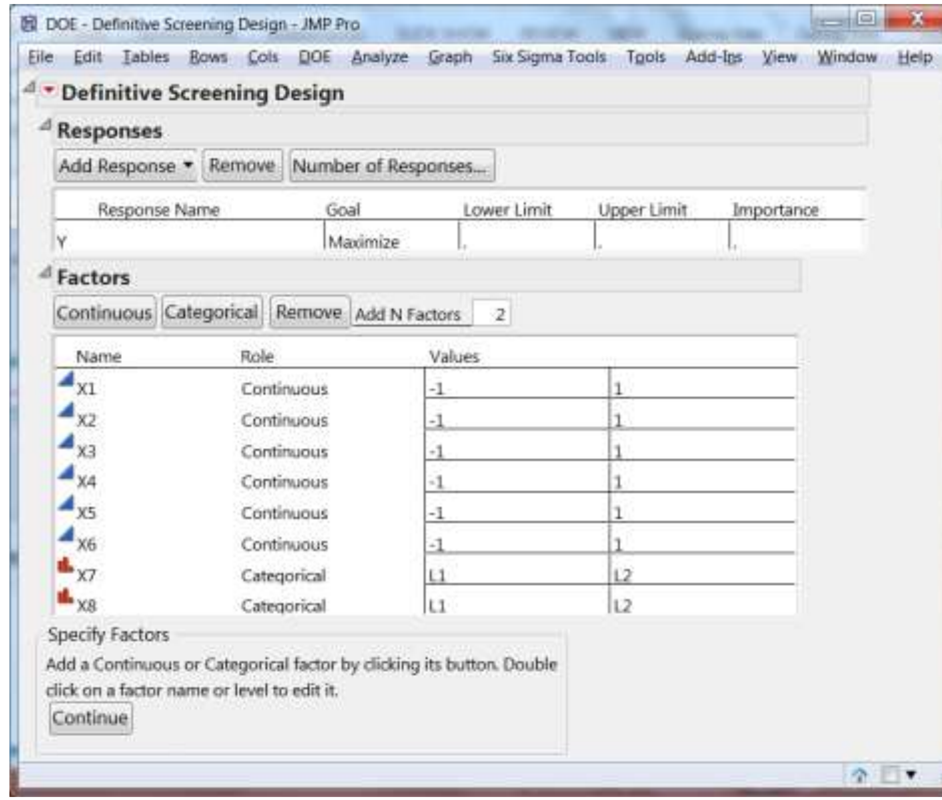
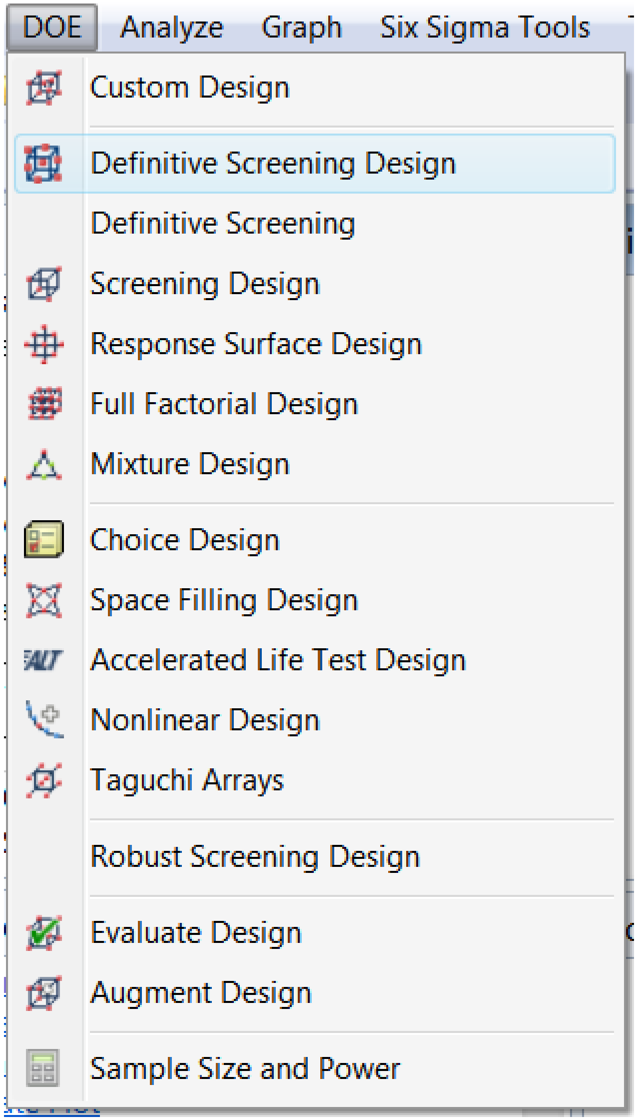
JMP 11 DEFINITIVE SCREENING DESIGN COLOR MAPS FOR 8-CONTINUOUS, 2-CATEGORICAL FACTOR

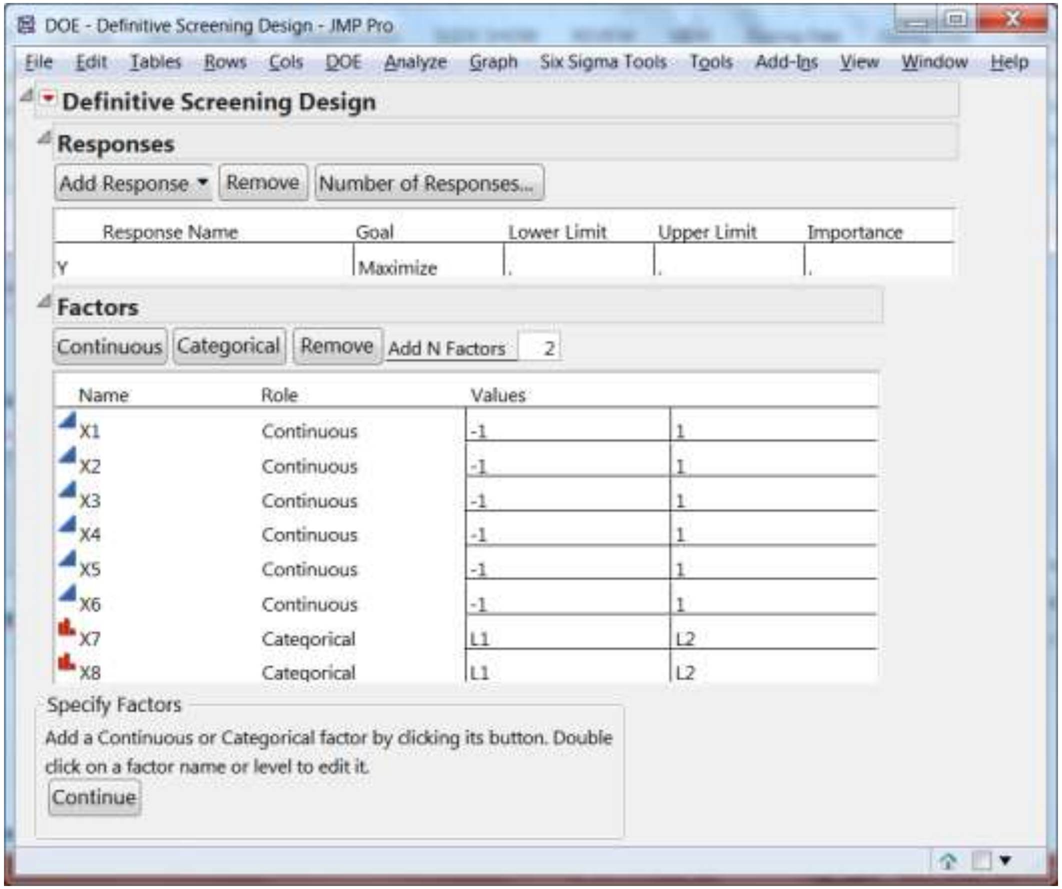
De-alias 2-f Interactions and Categorical Factors





WITH JMP 11 USE DEFINITIVE SCREENING ON DOE MENU



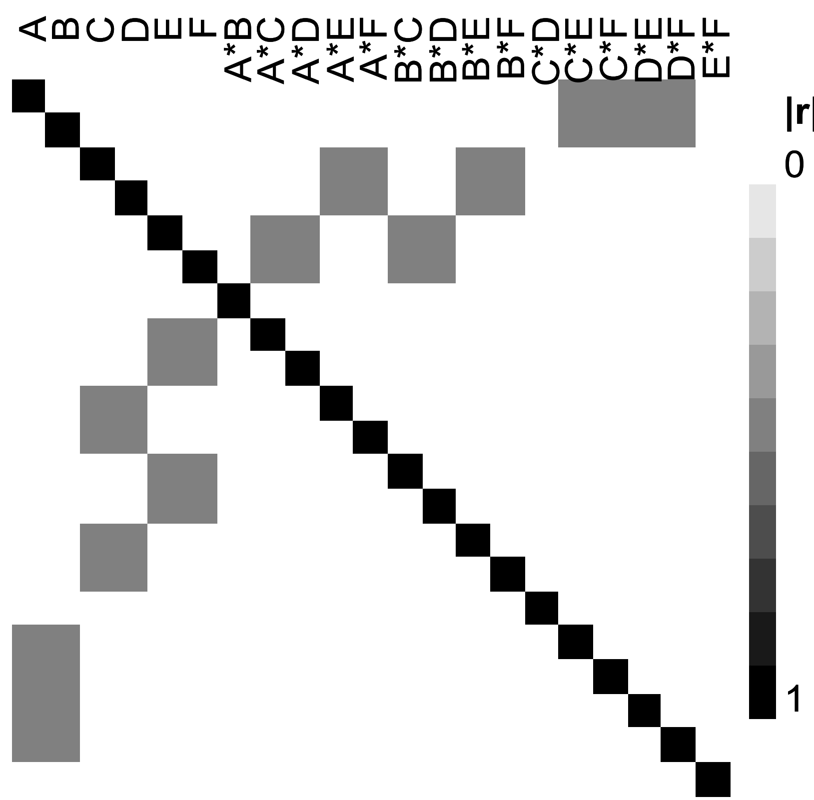


6-FACTOR, 16-TRIAL, NON-REGULAR FRACTIONAL FACTORIAL (“NO CONFOUNDING” DESIGN)

Jones, B. and Montgomery, D., (2010) “Alternatives to Resolution IV Screening Designs in 16 Runs.” *International Journal of Experimental Design and Process Optimization*, 2010; Vol. 1 No. 4: 285-295.

	A	B	C	D	E	F
1	1	1	1	1	1	1
2	1	1	-1	-1	-1	-1
3	-1	-1	1	1	-1	-1
4	-1	-1	-1	-1	1	1
5	1	1	1	-1	1	-1
6	1	1	-1	1	-1	1
7	-1	-1	1	-1	-1	1
8	-1	-1	-1	1	1	-1
9	1	-1	1	1	1	-1
10	1	-1	-1	-1	-1	1
11	-1	1	1	1	-1	1
12	-1	1	-1	-1	1	-1
13	1	-1	1	-1	-1	-1
14	1	-1	-1	1	1	1
15	-1	1	1	-1	1	1
16	-1	1	-1	1	-1	-1

Color Map On Correlations



MORE CONSERVATIVE ANALYSIS STRATEGIES THAN STEPWISE REGRESSION METHOD

- Fit just main effects to rank factors
- Fit main effects and squared effects together to not only identify dominant factors but look for curvature in factors
- Assuming **Factor Sparsity** and **Effect Heredity** principles* hold true - add interactions among dominant factors
  - If three or fewer factors have main effects, fit the full quadratic model for these factors with standard least squares regression.
  - If four or more factors have main effects, fit the full quadratic for these factors using stepwise regression

*Factor Sparsity states only a few variables will be active in a factorial DOE
Effect Heredity states significant interactions will only occur if at least one parent is active
Pg. 112 , Wu & Hamada, "*Experiments, Planning, Analysis and Parameter Design Optimization*"