AGENDA

• Why do we use Design of Experiments (DOE)?
• Review of Classic DOE
• Custom DOE is all about *Making Designs Fit the Problem – NOT Making Problems Fit the Designs!*  
• However, use Definitive Screening Designs (DSDs) – when possible!
• Quick example of creating and fitting a DSD.
• What are DSDs?
• How do we fit models for DSDs?
• When results are ambiguous, it is easy to augment DSD to RSM.
• Examples:
  • Extraction 3 Data.jmp : continuous with a blocking factor, & 4 extra runs
  • CO2_Process.jmp : all continuous factors, no extra runs
  • Peanut Data.jmp : continuous & categorical factors, & 4 extra runs
WHY USE DOE?

QUICKER ANSWERS, LOWER COSTS, SOLVE BIGGER PROBLEMS

- More rapidly answer “what if?” questions
- Do sensitivity and trade-space analysis
- Optimize across multiple responses
- By running efficient subsets of all possible combinations, one can – for the same resources and constraints – solve bigger problems
- By running sequences of designs one can be as cost effective as possible and run no more trials than needed to get a useful answer
Prediction Profiler

5.505435
Speed [5.43099, 5.57988]

0.689583
Contrast [0.66789, 0.71128]

0.362327
Cost [0.32333, 0.40133]

Desirability 0.00544

70 Sensitizer 1 70 Sensitizer 2 250 Dye 150 Reaction Time Desirability

Remembered Settings

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SHARE RESULTS ON JMP PUBLIC OR JMP LIVE

View optimizations on your phone. Scan the QR code to launch browser, then use finger to interact with the Prediction Profiler and to “Apply” saved settings.

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CLASSIC RESPONSE-SURFACE DOE IN A NUTSHELL

Fit requires data from all 3 blocks
Can fit data from blocks 1, 2 or 3
Fit requires data from blocks 1 & 2
Fit requires data from all 3 blocks

Lack-of-fit

Block 1

Block 2

Block 3
POLYNOMIAL MODELS USED TO CALCULATE SURFACES

Block 1

\[ y = a_0 + a_1 x_1 + a_2 x_2 + a_3 x_3 \]

Run this block 1st to:
(i) estimate the main effects*
(ii) use center point to check for curvature.

Block 2

\[ y = a_0 + a_1 x_1 + a_2 x_2 + a_3 x_3 + a_{12} x_1 x_2 + a_{13} x_1 x_3 + a_{23} x_2 x_3 \]

Run this block 2nd to:
(i) repeat main effects estimate,
(ii) check if process has shifted
(iii) add interaction effects to model if needed.

Block 3

\[ y = a_0 + a_1 x_1 + a_2 x_2 + a_3 x_3 + a_{12} x_1 x_2 + a_{13} x_1 x_3 + a_{23} x_2 x_3 + a_{11} x_1^2 + a_{22} x_2^2 + a_{33} x_3^2 \]

Run this block 3rd to:
(i) repeat main effects estimate,
(ii) check if process has shifted
(iii) add curvature effects to model if needed.
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?
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

36 trial I-optimal response-surface design started as 10-factor DSD and was then augmented with 12 more trials in 6 most important factors
CLASSIC DEFINITION OF DOE

Purposeful control of the inputs (factors) in such a way as to deduce their relationships (if any) with the output (responses).
**ALTERNATIVE DEFINITION OF DOE**  
A DOE is the specific collection of trials run to support a proposed model.

- If proposed model is *simple*, e.g. just main effects or *1st order* effects ($x_1$, $x_2$, $x_3$, etc.), the design is called a *screening* DOE  
  » Goals include *rank factor importance* or *find a “winner” quickly*  
  » Used with many (> 6?) factors at start of process characterization

- If the proposed model is *more complex*, e.g. the model is *2nd order* so that it includes two-way interaction terms ($x_1x_2$, $x_1x_3$, $x_2x_3$, etc.) and in the case of continuous factors, squared terms ($x_1^2$, $x_2^2$, $x_3^2$, etc.), the design is called a *response-surface* DOE  
  » Goal is generally to develop a *predictive model* of the process  
  » Used with a few (< 6?) factors after a screening DOE
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  » Used with a few (< 6?) factors after a screening DOE

**Definitive Screening Designs** allow the fitting of second order terms – ALL squared and potentially SOME interaction terms – for no more work than classic screening designs.
REAL-WORLD DESIGN ISSUES

How many experimenters have any of these issues? Most of these are NOT well treated by classic DOE

• Work with these different kinds of control variables/factors:
  » **Continuous/quantitative?** (Finely adjustable like *temperature, speed, force*)
  » **Categorical/qualitative?** (Comes in types, like material = *rubber, polycarbonate, steel* with mixed # of levels; 3 chemical agents, 4 decontaminants, 8 coupon materials…)
  » **Mixture/formulation?** (Blend different amounts of *ingredients* and the process performance is dependent on the *proportions* more than on the amounts)
  » **Blocking?** (e.g. “lots” of the same raw materials, multiple “same” machines, samples get processed in “groups” – like “eight in a tray,” run tests over multiple days – i.e. variables for which there *shouldn’t* be a causal effect)

• Work with **combinations of these four kinds** of variables?
• Certain **combinations cannot be run?** (too costly, unsafe, breaks the process)
• Certain factors are **hard-to-change** (temperature takes a day to stabilize)
• Would like to **add onto existing trials?** (really expensive/time consuming to run)
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Many of these issues prevent the use of Definitive Screening Designs. BUT, if your factors are **continuous**, **2-level categorical**, and/or **blocking** then consider doing a DSD first.
• Uses 6 continuous factors plus blocking at 2 levels
• Add 4 extra runs DSD
• Analyze with Fit Definitive Screening (p. 276 of DOE Guide)
• Factors and Ranges shown below

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SUMMARY OF MODERN SCREENING DOE

- **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 (RSM).
  - If many factors are important (so RSM can’t be fit) the design can be augmented to support an RSM.
  - Case study for a 10-variable process shows that it can be optimized in just 23 unique trials
    - Visually “model” factors
    - Fit Definitive Screening
    - Fit All Possible Models
    - Augment design with subset of original factors
WHAT IS THE MINIMUM # FACTORS “COLLAPSE” TO RSM

• For 6 through at least 30 factors, it is possible to estimate the parameters of any **full quadratic model** involving 3 or fewer factors with high precision.

• For 18 factors or more, they can fit full quadratic models in any 4 factors.

• For 24 factors or more, they can fit full quadratic models in any 5 factors.

• Due to factor sparsity, one can often fit response-surface models with more factors than these minimums.
REFERENCES

Original Research on Definitive Screening Designs


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The $D$-efficiency is 92.3%, higher than 89.8% for the design given in Jones and Nachtsheim (2011).
**CONFERENCE MATRIX METHOD IN 2012 JQT PAPER**  
**DESIGN SIZE IS 2M + 3 FOR ODD M**  
**DESIGN SIZE IS 2M + 1 FOR EVEN M**

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Both designs are orthogonal in linear and squared terms. Factor H will become a hidden Fake Factor in DSD Analysis.
DEFINITIVE SCREENING DESIGNS HAVE DESIRABLE PROPERTIES

• Main effects are not confounded with 2\textsuperscript{nd} order effects
• Number of trials for even numbers of factors is \((2m + 1)\)
  and for odd numbers of factors it is \((2m + 3)\)
  which is equal to or smaller than a Plackett-Burman (Res III) or Fractional
  Factorial (Res IV) design plus center point
• There are mid-levels for each factor allowing estimation of
curvature individually - not just globally as with a PB or FF
designs plus center point
• If drop a factor, the design retains all its properties
• If a subset of factors are significant there is a good chance that
  interaction terms may also be fit

The screening design may even collapse into a response-surface
design supporting a 2\textsuperscript{nd} order model in a subset of factors with which
one can optimize the process
6-FACTOR, 13-TRIAL, DEFINITIVE SCREENING DESIGN

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**Color Map On Correlations**

![Color map on correlations](image-url)
### 6-FACTOR, 12-TRIAL, PLACKETT-BURMAN DESIGN

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**Color Map On Correlations**

![Color Map On Correlations](image)
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

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### Color Map On Correlations

A, B, C, D, E, F

$|r|$ values range from 0 to 1.
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**

Or, add 4 extra rows to DSD to improve robustness of Fitting Models
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% (comparing just ME)
  ▪ Power for squared terms is “low”
    • Still better than power for single center point test for curvature
    • Power is same as larger Central Composite Design supporting full quadratic model
    • Power increases as fewer curvature terms are evaluated – drop least important terms (Factor Sparsity is our friend!)

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 designs testing mature systems
## PB12+CP

### Estimation Efficiency

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### Power Analysis

- Significance Level: 0.05
- Anticipated RMSE: 1
- Power for X1, X2, X3, X4, X5, X6: 0.821

## FF16+CP

### Estimation Efficiency

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### Power Analysis

- Significance Level: 0.05
- Anticipated RMSE: 1
- Power for X1, X2, X3, X4, X5, X6: 0.949

## DSD13

### Estimation Efficiency

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### Power Analysis

- Significance Level: 0.05
- Anticipated RMSE: 1
- Power for X1, X2, X3, X4, X5, X6: 0.75

## DSD17

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### Power Analysis

- Significance Level: 0.05
- Anticipated RMSE: 1
- Power for X1, X2, X3, X4, X5, X6: 0.92
## QUADRATIC TERM POWER FOR TEN 6-FACTOR DESIGNS – SCREENING & RSM

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### DSD13
- **AUGMENT DSD17 TO I-OPT34**
- **0.10**
- **0.21**
- **0.26**
- **0.49**
- **0.58**

### DSD17
- **0.12**
- **0.14**
- **0.32**
- **0.61**
- **0.63**

### DSD21
- **CCD45**
- **FF16+CP**
- **PB12+CP**
- **BB49**
- **I-OPT34**

### Power Parameters
- Intercept
- X1, X2, X3, X4, X5, X6
- X1*X1, X2*X2, X3*X3, X4*X4, X5*X5, X6*X6

### Power Calculation
- Power = \( \sum (\text{Coefficients} \times \text{Power}) \)

### Significance Level
- 0.05

### Anticipated RMSE
- 1
### Power for 6 Main Effects & 6 Quadratic Terms

**For All Terms vs. One Quad Term at a Time**

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#### Anticipated Parameter Coefficients

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#### Power Analysis

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<tbody>
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#### Anticipated Parameter Coefficients

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Secretary Chu Announces Six Projects to Convert Captured CO2 Emissions from Industrial Sources into Useful Products

$106 Million Recovery Act Investment will Reduce CO2 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 (CO2) 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 CO2 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."
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
DISTRIBUTIONS WITH “GOOD” AND “BAD” BEHAVIOR SELECTED
Y VS X PLOTS OF DATA FOR EACH X
SQRT(Y) VS X
PLOTS OF DATA FOR EACH X
ACTUAL BY PREDICTED PLOT FOR FINAL 3-FACTOR MODEL FOR THE 24 DESIGN TRIALS
PREDICTING WITH BEST 3-FACTOR AND 4-FACTOR MODELS
SETTINGS OF BEST OBSERVATION OF YIELD = 12.96

Prediction at settings of best observation

Prediction at best settings – run this checkpoint
ACTUAL BY PREDICTED PLOT FOR FINAL 3-FACTOR MODEL
FOR THE 24 DESIGN TRIALS AND 4 VERIFICATION TRIALS

Actual by Predicted Plot

Verification Trials (*)
Not Used in Fitting Model

Yield @ Time t
P<.0001 \(R^2=0.90\)
• 2017 JMP Discovery Summit presentation by Brad Jones on
  ▪ Simulating Responses and Fitting Definitive Screening Designs - JMP User Community
- Treat factors D and I as the dummy factors to be used for error estimates in Definitive Screening Fit
DSD FIT OUTPUT
WITH FACTORS D & I
USED FOR ERROR

NEW DEFINITIVE SCREENING ANALYSIS METHOD

Stage 1 - Main Effect Estimates

| Term | Estimate | Std Error | t Ratio | Prob>|t| |
|------|----------|-----------|---------|------|
| A    | -2.05    | 0.2228    | -9.2    | < 0.0001* |
| B    | -2.015   | 0.2228    | -9.043  | < 0.0001* |
| C    | -0.855   | 0.2228    | -3.839  | 0.0050* |
| F    | -0.427   | 0.2228    | -1.916  | 0.0917 |

Statistic Value

| RMSE | 0.9839 |
| DF   | 8      |

Stage 2 - Even Order Effect Estimates

| Term  | Estimate | Std Error | t Ratio | Prob>|t| |
|-------|----------|-----------|---------|------|
| A*B   | 8.6319   | 0.6421    | 13.442  | < 0.0001* |
| B*C   | 0.9481   | 0.3085    | 3.1232  | 0.0188* |
| B*D   | 0.5687   | 0.3056    | 1.8733  | 0.1052 |
| C*D   | 0.9163   | 0.3213    | 2.8517  | 0.0436* |
| B*B   | -4.755   | 0.7043    | -6.753  | 0.0003* |

Statistic Value

| RMSE | 1.2435 |
| DF   | 7      |

Combined Model Parameter Estimates

| Term  | Estimate | Std Error | t Ratio | Prob>|t| |
|-------|----------|-----------|---------|------|
| Intercept | 8.6319 | 0.5947 | 14.514 | < 0.0001* |
| A      | -2.05    | 0.2608   | -7.86   | < 0.0001* |
| B      | -2.015   | 0.2608   | -7.726  | < 0.0001* |
| C      | -0.855   | 0.2608   | -3.279  | 0.0055* |
| F      | -0.427   | 0.2608   | -1.637  | 0.1299 |
| A*B    | 1.2645   | 0.2749   | 4.6006  | 0.0004* |
| B*C    | 0.9481   | 0.2812   | 3.3722  | 0.0460* |
| B*D    | 0.5687   | 0.2812   | 2.0227  | 0.0620 |
| C*D    | 0.9163   | 0.2976   | 3.0791  | 0.0062* |
| B*B    | -4.755   | 0.6523   | -7.292  | < 0.0001* |

Statistic Value

| RMSE | 1.1516 |
| DF   | 14     |

Make Model | Run Model
FIT OF RAW YIELD

Actual by Predicted Plot

Yield @ Time t: Predicted RMSE = 1.1516, RSq = 0.95
PValue < .0001

Box-Cox Transformations

SSE

Best λ = 0.463

Prediction Profiler

Yield @ Time t: Predicted RMSE = 17.62586, RSq = 0.96
PValue < .0001

FIT OF SQRT YIELD

Actual by Predicted Plot

Yield @ Time t: Predicted RMSE = 0.2263, RSq = 0.96
PValue < .0001

Box-Cox Transformations

SSE

Best λ = 0.934

Prediction Profiler

Yield @ Time t: Predicted RMSE = 17.62586, RSq = 0.96
PValue < .0001
ANALYSIS STRATEGIES FOR WHEN YOU DON’T HAVE THE NEW DEFINITIVE SCREENING ANALYSIS METHOD

• Conservative – start by treating designs like traditional screening
  ▪ Fit main effects only – DSD is orthogonal in main effects
  ▪ Then fit ME + squared effects – DSD is orthogonal in squared terms too
  ▪ *Use factor sparsity and effect heredity principles to propose final models
  ▪ Use transformation to make error more uniform
    » square-root identified in plot of SSE vs. \( \lambda \) for Box-Cox transformation (i.e. \( \lambda \approx 0.5 \))

• Aggressive – use stepwise regression to pick “best” subsets of terms
  ▪ 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

*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
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
### 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

The graph depicts the Box-Cox transformations for different values of $\lambda$. The $SS$ is plotted against $\lambda$ ranging from -2.0 to 2.0.
TRANSFORMATIONS
SQRT, LOG, & NONE

**Actual by Predicted Plot**

Yield @ Time t Predicted
P<.0001 RSq=0.83
RMSE=0.4163

Yield @ Time t Predicted
P<.0001 RSq=0.82
RMSE=0.4509

Yield @ Time t Predicted
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 Wgts) 24

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

RSquare 0.789957
RSquare Adj 0.745738
Root Mean Square Error 1.938688
Mean of Response 4.72375
Observations (or Sum Wgts) 24
Model fit was reduced quadratic in A, B & C:

\[ \text{Yield} = \text{Intercept} + A + B + C + B*B + A*B + B*C \]
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  |

### PredictionProfiler

- **Term**: A
  - **Estimate**: -0.496169
  - **Std Error**: 0.080197
  - **t Ratio**: -6.19
  - **Prob>|t|**: <.0001 *

- **Term**: B
  - **Estimate**: -0.481867
  - **Std Error**: 0.080197
  - **t Ratio**: -6.01
  - **Prob>|t|**: <.0001 *

- **Term**: B*A
  - **Estimate**: 0.2339616
  - **Std Error**: 0.087698
  - **t Ratio**: 2.67
  - **Prob>|t|**: 0.0184 *

### Actual by Predicted Plot

- **Yield @ Time t**
  - **P>|t|**: <.0001
  - **R^2**: 0.90
  - **Yield @ Time t**
  - **P>|t|**: <.0001
  - **R^2**: 0.91
STEPWISE MODELS:
4-FACTOR (12 TERMS), 5-FACTOR (13 TERMS), 6-FACTOR (15 TERMS)
• 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
USE MIN AIC OR BIC CRITERION AS STOPPING RULE

21 TERMS, ME + SQ

TRANSFORMED VALUES USED

**的实际与预测图**

**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**

Yield @ Time t Predicted

P<.0001 RSq=0.83
RMSE=0.4163
USE MIN AIC OR BIC CRITERION AS STOPPING RULE

66 TERM QUADRATIC

RAW RESPONSE VALUES USED

Actual by Predicted Plot

Criterion History

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

Yield @ Time t Predicted
P<.0001 RSq=0.89
RMSE=1.4757

Actual vs 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

Yield vs Time
12.70336
[10.92203, 14.48469]

A -1
B -0.333
C -1
USE MIN AIC OR BIC CRITERION AS STOPPING RULE

66 TERM QUADRATIC

TRANSFORMED VALUES USED

Actual by Predicted Plot

Criterion History

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

Yield @ Time t Predicted

P<.0001 RSq=0.95 RMSE=0.2519
USE MAX K-FOLD R-SQUARE AS STOPPING RULE

66 TERM QUADRATIC TRANSFORMED VALUES USED

Actual by Predicted Plot

Yield @ Time t Predicted
P < .0001 RSq = 0.98
RMSE = 0.1839

RSquare History

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

Yield @ Time t Predicted
17.02979 [15.4468, 18.69]
USE MAX VALIDATION R-SQUARE FOR 4 CHECKPOINTS AS STOPPING RULE

66 TERM QUADRATIC TRANSFORMED VALUES USED

Actual by Predicted Plot

Yield @ Time t Actua

Yield @ Time t Predicted

P < .0001 RSq = 0.91
RMSE = 0.3209

RSquare History

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

Yield @ Time t

16.53064 [15.0175, 18.1164]
USE AIC CRITERION AS STOPPING RULE

66 TERM QUADRATIC

POISSON DISTRIBUTION USED WITH GENERALIZED REGRESSION

Solution Path

Prediction Profiler

Actual by Predicted Plot

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<th>Yield @ Time t</th>
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<tr>
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<td>[11.9342, 21.617]</td>
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AICc

RMSE = 0.3209

P < .0001 R^2 = 0.91
FIT ALL POSSIBLE MODELS UP TO 8 TERMS

Factors A & B  Rsquare = 0.77
Factors A, B & C  Rsquare = 0.90
Factors A, B, C & G Rsquare = 0.95
WISDOM FROM BOB

Although your model can fit the data, it may NOT fit the process from which the data come!

How do I know if my model fits?
   “ is right?
   “ adequate?
   “ accurate?

For me, nothing beats checkpoints!
   Do they fall within prediction limits?
   What does a plot of actual vs. prediction look like?

Continue to check model predictions over time.
   tools wear
   seasons change
   suppliers and operators change
ALL ANALYSES

RANK FACTORS
A, B & C AS TOP 3

• 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

FACTOR F APPEARS TO BE MOST LIKELY FOURTH FACTOR
IF MORE THAN A FEW FACTORS ARE SIGNIFICANT, THEN AUGMENT DESIGN TO SUPPORT 2\textsuperscript{ND} ORDER MODEL

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.

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<th>B</th>
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NOTE: First 13 rows of original design are not shown.
POWER FOR SQUARED TERMS IN 2\textsuperscript{ND} ORDER MODEL IS INCREASED TO NEAR THAT OF 6-FACTOR RSM 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
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
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

36 trial I-optimal response-surface design started as 10-factor DSD and was then augmented with 12 more trials in 6 most important factors.

NUMBER OF UNIQUE TRIALS
- Unique Trials in Central Composite Design
- Unique Trials in Box-Behnken Design
- Unique Trials in Custom Design with 6 df for Model Error
- Terms in Quadratic Model

Number of Unique Trials or Quadratic Terms

Number of Continuous Factors

0 10 20 30 40 50 60 70 80 90

2 3 4 5 6 7 8 9
• **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?

TOM.DONNELLY@JMP.COM
De-alias 2-f Interactions and Categorical Factors
### 6-FACTOR, 16-TRIAL, NON-REGULAR FRACTIONAL FACTORIAL ("NO CONFOUNDING" DESIGN)


#### Color Map On Correlations

![Color Map On Correlations](image)

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WITH JMP 11 USE DEFINITIVE SCREENING ON DOE MENU
ANALYSIS STRATEGIES

- **Visual Tools:**
  - **Distribution** – click on “good” and “bad” response values to see correlations with factor settings
  - **Graph Builder** – Y vs. X graphs – all data, summarized data, fit line, smoother
    - Drop factors side by side or alternatively (for coded factors) stack factors then replot
    - Use Overlay field to look at possible interactions between two factors

- **Analytic Tools:**
  - **Conservative**: Main Effects fit – look at Scaled estimates
    - Consider adding interactions among significant factors using Effects Heredity and Sparsity
  - **Aggressive**: Strepwise with various stopping criteria
    - AICc, BIC, K-fold, Excluded checkpoints,
    - Fit All Possible Models

- **Analytic Output:**
  - Stepwise Histories – Criterion or Rsquare
  - Actual vs. Predicted with Graph Builder – Col Switch different models
  - Create All Possible Models Table – Plot four metrics using Overlap Plot
COLOR MAP FOR 20-TRIAL PLACKETT-BURMAN DESIGN WITH 19 CONTINUOUS FACTORS
COLOR MAP FOR 40-TRIAL FOLD-OVER PLACKETT-BURMAN DESIGN WITH 19 CONTINUOUS FACTORS AND 20TH BLOCK FACTOR
COLOR MAP FOR A 42-TRIAL DEFINITIVE SCREENING DESIGN WITH 19 CONTINUOUS FACTORS AND 1 TWO-LEVEL CATEGORICAL FACTOR
COLOR MAP FOR 21-TRIAL HALF OF 42-TRIAL DSD WITH 19 CONTINUOUS FACTORS SPLIT ON 20TH CATEGORICAL FACTOR
COLOR MAP FOR 20-TRIAL PLACKETT-BURMAN DESIGN (LEFT) AND 21-TRIAL HALF OF 42-TRIAL DSD (RIGHT) BOTH WITH 19 CONTINUOUS FACTORS
COLOR MAP FOR A 40-TRIAL FOLD-OVER PLACKET-BURMAN DESIGN (LEFT) AND A 42-TRIAL DEFINITIVE SCREENING DESIGN (RIGHT) WITH 19 CONTINUOUS AND 1 TWO-LEVEL BLOCK/CATEGORICAL FACTOR
For designs containing only continuous factors, compare these properties of definitive screening designs versus standard screening designs:

- **Main effects are orthogonal to two-factor interactions.**
  - Definitive Screening Designs: Always
  - Standard Screening Designs: Only for Resolution IV or higher

- **No two-factor interaction is completely confounded with any other two-factor interaction.**
  - Definitive Screening Designs: Always
  - Standard Screening Designs: Only for Resolution V or higher

- **All quadratic effects* are estimable in models containing only main and quadratic effects.**
  - Definitive Screening Designs: Always
  - Standard Screening Designs: Never

* When quadratic effects are mentioned, the standard screening designs are assumed to have center points.