

Suppose that you need to determine which of six factors affect the yield of an extraction process. The factors and ranges are as follows:

Methanol, 0-10 Ethanol, 0-10 Propanol, 0-10 Butanol, 0-10 pH, 6-9 Time, 1-2

- 1. Use Easy DOE, Definitive Screening Design, or Custom Design to create a design. Consider the benefits of any of these methods. Why might you choose one over another?
- 2. Using the Extraction Data table linked from the course journal, resulting from a DSD, analyze the results in order to determine the active factors. Because this is a DSD, you can determine the active main effects AND possibly identify curvature and 2-way interactions.

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Suppose that you need to determine which of six factors affect the yield of an extraction process. The factors and ranges are as follows:

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- 1. Use Easy DOE, Definitive Screening Design, or Custom Design to create a design. Consider the benefits of any of these methods. Why might you choose one over another?
  - a. Using Easy DOE:
    - 1) Select **DOE** > **Easy DOE**.
    - 2) In the Number of Factors box, enter 6, then click Add Factor.
    - 3) Enter the names and ranges of the factors as specified above.

•			untitled 3		
Guided Mode	Flexible Mode				
fine Model D	esign Data Entry Analyze Predic	t Report			
Responses					
Factors					
	Choices				
Role					
The factor	can take any numeric value betwee         Show Hint         takes numeric values set by user-d         How many levels do you have?         Show Hint         takes values from a set of categoric         How many levels do you have?         Show Hint         Show Hint	n a low and efined levels 2 s, groups, o 2	high level. (Continuous) s. (Discrete Numeric) or kinds. (Categorical)		
			Factor Table		
Add Factor	Number of Factors 1	Re	move Selected		
Name	Role	Changes	Values		Units
Methanol	Continuous	Easy	0	10	
Ethanol	Continuous	Easy	0	10	
Propanol	Continuous	Easy	0	10	
Butanol	Continuous	Easy	0	10	
⊿рН	Continuous	Easy	6	9	
Time	Continuous	Easy	1	2	
invitation controls					
avigation controls					

4) Click the forward navigation control button.

5) Choose the model of interest. Choose only Main Effects if your primary concern is a low budget for runs. Choose Main Effects with some Two-Factor Interactions to add just a few more runs but gain the possibility of testing for interactions and curvature from the screening experiment. Choose All Main Effects and Two-Factor Interactions if you want to estimate all main effects and all 2-way interactions from the initial screening experiment. Choose All Main Effects, Two-Factor Interactions, and Quadratics to create a response surface design that also allows curvature for any factor.

Here we show the choice of Main Effects with some Two-Factor Interactions for comparison with the DSD created through the Definitive Screening Design platform.

Guide	d Mode	Flexible	Mode							
efine	Model	Design	Data Entry	Analyze	Predict I	Report				
•								Design		
6/0 C	ols 💌							-		
17/0	-	Methanol	Ethanol	Propanol	Butanol	pН	Time			
	1	10	10	0	10	6	1			
	2	0	0	10	10	7.5	1			
	3	10	5	10	10	6	2			
	4	10	0	0	5	9	2			
	5	5	10	10	10	9	2			
	6	0	10	10	5	6	1			
	7	5	5	5	5	7.5	1.5			
	8	10	0	10	0	6	1.5			
	9	0	0	0	10	6	2			
	10	0	0	10	0	9	2			
	11	10	0	5	10	9	1			
	12	10	10	10	0	9	1			
	13	10	10	0	0	7.5	2			
	14	0	10	0	10	9	1.5			
	15	0	5	0	0	9	1			
	16	0	10	5	0	6	2			
	17	5	0	0	0	6	1			
Export	Data									
Navigatio	on contro	ols								

- b. Using Definitive Screening Design:
  - 1) Select **DOE** > **Definitive Screening** > **Definitive Screening Design**.
  - 2) In the Add N Factors box, enter 6, then click Continuous.
  - 3) Enter the names and ranges of the factors as specified above.
  - 4) Click Continue.

Add Response 🔻	Remove Number	of Responses					
Response Na	ime Goal	Lower Limit	Upper Limit	Importance	Lower Detection Limit	Upper Detection Limit	Units
Y	Maxim	ize .					
Continuous	Categorical Remove	Add N Factors 1		Linite			
Methanol	Continuous	values	10	Units			
4Ethanol	Continuous	0	10				
	Continuous	0	10				
	Continuous	0	10				
Butanol	Continuous	6	9				
▲Butanol ▲pH		1	2				
▲Butanol ▲pH ▲Time	Continuous		1-				
Butanol  pH Time  scify Factors	Continuous						
Butanol pH Time ecify Factors	Continuous	aliaking ita					

5) Click Make Design.

Dofin	itivo Cor	oonin~	Deciar	ve ooreening	Design 2	
Jenr	nuve SCr	eening	Design			
Desig	gn Methen - l	Ethon-I	Drenon-I	Butonel		Time
Run	wethanol	Etnanol 10	Propanol 10	Butanol 10	рн	Time
2	5	0	0	0	6	2
3	10	5	10	10	6	2
4	0	5	0	0	9	1
5	10	0	5	10	9	1
6	0	10	5	0	6	2
7	10	0	0	5	9	2
8	10	10	10	5	75	1
10	0	0	10	10	7.5	2
11	10	0	10	0	6	1.5
12	0	10	0	10	9	1.5
13	10	10	0	10	6	1
14	0	0	10	0	9	2
15	10	10	10	0	9	1
10	5	5	0	10	75	15
Desid	on Evalua	ation	0	Ŭ	1.0	1.0
		alveie				
		alysis Varian	a a Drafil			
	realction	varian		e		
▶ Fra	ction of	Design	Space P	lot		
►P	rediction	Varian	ce Surfa	се		
▶ Est	imation	Efficien	су			
▶ Alia	as Matrix					
► <b>C</b>	olor Map	o on Co	rrelation	S		
▶ Des	sign Diag	nostics	5			
output Op	otions					
Run O	rder: Rando	mize				
Mak	e Table					
Bac	ĸ					

6) Click Make Table.

- c. Using Custom Design:
  - 1) Select **DOE > Custom Design**.
  - 2) In the Add N Factors box, enter 6, then click Add Factor > Continuous.
  - 3) Enter the names and ranges of the factors as specified above.
  - 4) Click Continue.

Model		
Main Effects	Interactions •	RSM Cross Powers  Remove Term
Name	2nd	Estimability
Intercept	3rd	Necessary
Methanol	4th	Necessary
Ethanol	5th	Necessary
Propanol		Necessary
Butanol		Necessary
pH		Necessary
Time		Necessary

- 5) In the **Model**, select the **Interactions** drop-down and choose **2**<sup>nd</sup>. This model is equivalent to the *All Main Effects and Two-Factor Interactions* option from **Easy DOE**.
- 6) Select all of the 2-way interaction terms and click on **Necessary** next to one of these terms. Change **Necessary** to **If Possible** for all 2-way interactions. The Default **Number of Runs** changes from 28 to 12. Now it matches the Easy DOE option to estimate only *Main Effects*.

V	Model	
	Main Effects Interactions   RSM	Cross Powers   Remove Term
	Name	Estimability
	Butanol	Necessary
	pH	Necessary
	Time	Necessary
	Methanol*Ethanol	Necessary
	Methanol*Propanol	Nece
	Methanol*Butanol	Nece
	Methanol*pH	Nece If Possible
	Methanol*Time	Necessary

- 7) Click the **Design Explorer** button.
- 8) In the All Combinations box, enter 17 for Runs and 1 for Center Points.
- Select the Alias Optimality options in addition to the D-Optimality option which is selected by default.

<b>Design Explor</b>	er			
Design Explor	er Options			
Select options for a of specified options Single Design	single design, or :	all combinatio	All Combinations	
Criterion	D-Optimality	$\bigcirc$	Criterion	✓ D-Optimality A-Optimality I-Optimality ✓ Alias Optimality
Runs Center Points		12	Center Points	✓ Locked 1
Replicates		0	Replicates	
Random Starts Make Design		5	Generate All Designs	5

10) Click Generate All Designs.

• •				Rep	ort: Design E	xplorer 2				
Design Explo	orer									
Design Explo	orer O	ptions								
Select options for	a single	design, or all con	mbinations							
of specified option	18.									
Single Design				All Combinations	s					
Criterion	D-0	ptimality 🔇	)	Criterion		🗹 D-Optimali	ty 🗌 A-Optima	lity 🗌 I-Optim	ality 🗹 Alias Op	otimality
Runs		1	2	Runs		🗸 Locked	17			
Center Points			0	Center Poir	nts	Locked	1			
Replicates			0	Replicates		Locked	0			
Random Starts	3		5	Random St	arts	5				
Make Design				Generate	All Designs					
Results										
Use the check boy	k to set	the reference des	ign. Rows							
are selectable usin	ng the C	ontrol key.								
Reference			Center		Random	Relative D-	Relative I-	Relative G-	Relative A-	Average Varianc
Design	Runs	Criterion	Points	Replicates	Starts	efficiency	efficiency	efficiency	efficiency	of Prediction
10	17	D-Optimality		1 0	5	1.000	1.000	1.000	1.000	0.1
2	17	Alias Optimality		10	5	0.957	0.920	0.926	0.901	0.2
Evaluate Selected	d Designs	s Compare Se	lected Desig	ns Make Se	elected Tables	Remove D	esigns Ma	ke Enhanced Ta	ble	
	-									

11) Select both resulting designs. Click **Compare Selected Designs**. Explore the comparison report to identify benefits and drawbacks of each design. For example, in the randomly generated designs compared below, the Alias-Optimal design has lower power to detect an effect for Time than the D-Optimal design has.

•								Report: Design Explorer 2
Design E:	cplore	er						
Compare	Desi	gns						
• Referen	ce De	esign:	17 R	un D-	Opti	malit	ty 1 C	CPs 0 Replicates
• Desig	n Eva	luatio	n					
▼ <b>■</b> Pc	wer	Analvs	is					
Signif Antici	icance pated F	_evel (	0.05					
Term	A	nticipate oefficier	d 1 nt CP:	7 Run I s 0 Rep	D-Opti licate:	mality s Pow	1 er 1 C	17 Run Alias Optimality Ps 0 Replicates Power
Interc	ept		1			0.9	59	0.959
Meth	anol		1			0.94	49	0.931
Ethar	ol		1			0.94	49	0.931
Propa	anol		1			0.9	36	0.931
Bular			1			0.9	49 36	0.931
Time			1			0.0	19	0.848
Good	wer l	0.40 0.20 Plot	Bad					
	10							Design
	1.0							17 Bun D-Optimality 1 CPs 0 Benlicates
	0.8-						h	17 Run Alias Optimality 1 CPs 0 Replicates
	0.6							
ewo								
ď	0.4 -							
	0.2 -							
	0-							
		Methanol	Ethanol	Propanol	Butanol	H	Time	
		~						

The D-Optimal design is slightly more efficient (with tighter confidence intervals on estimates) than the Alias-Optimal design.

•			Report: Desi	gn Explore										
Design Expl	orer													
Compare De	esigns													
Reference	Design: 17 Run D-Optin	nality 1 Cl	Ps 0 Replica	ates										
Design E	Evaluation													
▼ <b>▼</b> Rela	✓ Relative Estimation Efficiency													
	Term Relative to 17 Run D-Optimality 1 CPs 0 Replicates													
Term														
Intercept Methanol Ethanol Propanol Butanol pH Time			1.000 1.044 1.044 1.011 1.044 1.011 1.206											
Bood ■	tive Std Error of Estimat	es												
Alias	Matrix Summary													
Term	Root Mean Squared Values 17 D-Optimality 1 CPs 0 Replice	Run Root N ates Alias O	lean Squared V ntimality 1 CPs	alues 17 Ru 0 Replicate										
Intercept	0.0	608	punnanty i ei e	0.135										
Methanol Ethanol	0.2	2327 2661		0.000										
Propanol	0.2	2459		0.000										
Butanol	0.2	2327		0.000										
Time	0.2	2661		0.000										
Total	0.2	313		0.051										
Good	10 0.30 0.50 0.70 Bad													
▼ <b>■Absc</b>	olute Correlations													
Model x	Madal	Average	Number of	Number of Pairs										
17 Run D	-Optimality 1 CPs 0 Replicates	0.017	Contoundings 0	or Pairs 15										
17 Run A	lias Optimality 1 CPs 0 Replicates	0.083	Ő	15										
Model x	Alias	Average Correlation	Number of Confoundings	Number of Pairs										
17 Run D	-Optimality 1 CPs 0 Replicates	0.134	0	90										
	nas optimality i ons o neplicates	Average	Number of	Number										
Alias x A	lias	Correlation	Confoundings	of Pairs										
17 Run D 17 Run A	-Optimality 1 CPs 0 Replicates lias Optimality 1 CPs 0 Replicates	0.110 0.187	0 3	105 105										

The Alias-Optimal design has 3 completely confounded pairs of effects, but all interactions are uncorrelated with the main effects. The D-Optimal design has some correlation between interactions and main effects, so their estimation cannot be completely independent.



12) Select your preferred design in the **Results** report list and click **Make Selected Tables**.

d. Consider the benefits of any of these methods. Why might you choose one over another?

For this simple example of a single continuous response and six continuous factors, with no constraints or complications, the Definitive Screening Design is an excellent choice. It has the benefits of extracting maximum information, especially about 2-way interactions and curvature, from a minimum number of runs. The DSD allows estimation of the main effects independent of any model form that might include higher-order effects, which allows the two-stage ability to first find active effects and then build the response surface model to those effects.

The DSD will be fit, in this case, from Easy DOE, so either platform can produce this design.

The Custom platform is the most flexible (and often the only choice) for more complex situations, but in this case the designs it produces will not be as efficient as the straightforward DSD.

- 2. Using the Extraction Data table linked from the course journal, resulting from a DSD, analyze the results in order to determine the active factors. Because this is a DSD, you can determine the active main effects AND possibly identify curvature and 2-way interactions.
  - a. Select Extraction Data from the Homework section of the journal.

Homework
Suppose that you need to determine which of six factors affect the yield of an extraction process.
<ul> <li>1. Use Easy DOE, Definitive Screening Design, or Custom Design to create a design. Consider the benefits of any of these methods. Why might you choose one over another?</li> <li>2. Using the "Extraction Data.jmp" table, resulting from a DSD, analyze the results in order to determine the active factors. Because this is a DSD, you can determine the active main effects</li> </ul>
AND possibly identify curvature and 2-way interactions.
Solution for Creating the Design Extraction Data
Next

b. Click the green play button next to the Fit Definitive Screening script in the table panel.

Extraction Data		
Design Definitive Screening Design		Met
Notes These fictional data were insp	1	
<ul> <li>Fit Definitive Screening</li> <li>Evaluate Design</li> </ul>	2	
DOE Dialog	3	
Model for Stepwise	4	
	5	



In Stage 1, Methanol and Time are identified as the only active factors. In Stage 2, these factors are added, along with their interaction and their quadratic effects. Stage 2 shows a statistically significant effect for Methanol, but non-significant effects for all others. A followup experiment, or augmentation to this experiment, may add power to further investigate the non-significant effects.

c. Click the Run Model button to produce additional output for this Stage 2 model.



**d.** From the red triangle by **Response Yield**, select **Factor Profiling > Surface Profiler**. Click in the plot to rotate and explore.

