# **Probability Distribution**

1. In scenario 2, the particle size distribution from the mill is:

	Counts
<10 mm	50
11-20 mm	125
21-30 mm	350
31-40 mm	275
41-50 mm	250
51-60 mm	200
61-70 mm	40
71-80 mm	10
>81 mm	5

Use JMP to perform the following:

- (1) Distribution of Counts Vs Size
- (2) % Distribution Vs Size

(3) Mean

(4) Variance

Solution:

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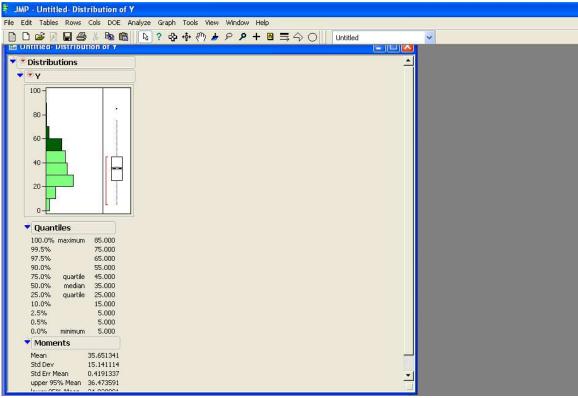
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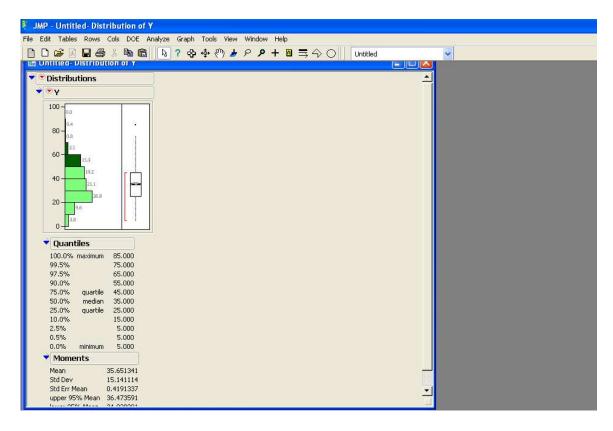
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## Click "OK".



To Show the percentage of each bar, click the hot spot left to "Y" and choose "Show Percents" in "Histogram Options":

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The mean and variance could be easily found in the output "Moments" below the graph. Here the Mean is 35.651341. The variance 15.141114.

2. In scenario 2, the Percent Dissolution of tablets as a function of time is as the following:

Time	% Dissolution
0	0
15	35
30	55
45	70
60	83
75	92
90	97
105	98
120	99

Use JMP to plot the Distribution and calculate the time at which 85% of the tablet has been dissolved.

Solution:

Input the data:											
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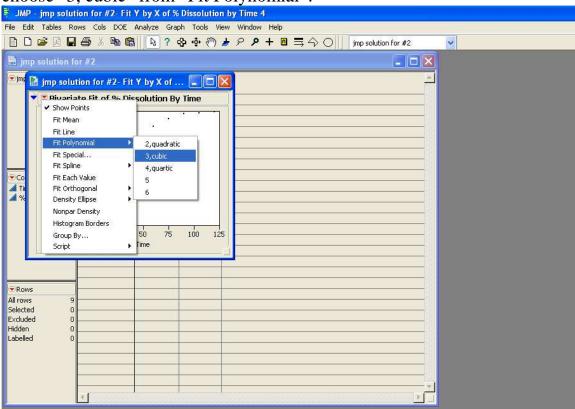
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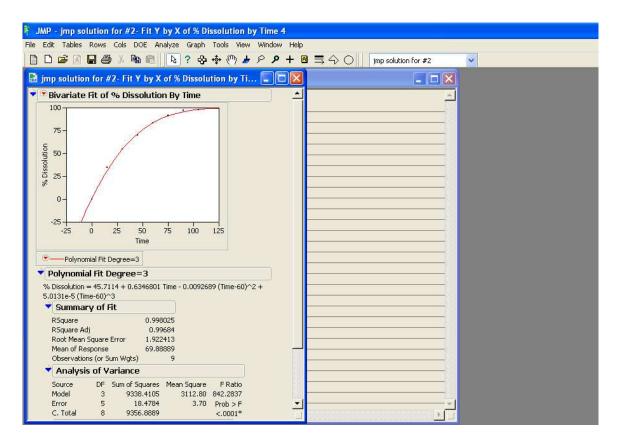
Choose % Dissolution as "Y, Response", Time as "X, Factor":

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Click the hot spot left to "Bivariate Fit of % Dissolution By Time" and choose "3, cubic" from "Fit Polynomial":





From the polynomial function JMP offered, we could calculate the time when Dissolution is 85%:

x = 61.9584

# **Comparison Tests**

3. Two different catalysts are studied in the batch reactor. (Scenario 1) Differece runs are made with each catalyst and the yield of A measured after 1 hour. (all other factors held constant)

Catalyst C1	Catalyst C2
74	71
70	74
69	73
71	75
72	77

- (1) Determine the mean and variance of each catalyst.
- (2) Use the appropriate distribution to decide whether there is a difference at the 95% confidence level.
- (3) At what level is there a difference between the two catalyst (p value).
- (4) Use an F test to determine the level at which there is a difference between the variance of the yield between the catalysts.

Solution:

Input the data. Here Catalyst is the type of Catalyst and its data type is "Character":

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C2 5 74.0000 0.93274 71.849 76.151 Std Error uses a pooled estimate of error variance	
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Level Number Mean Std Dev Std Err Mean Lower 95% Upper 95%	
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C2 5 74.0000 2.23607 1.0000 71.224 76.776	
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Upper CL Dif 5.8537 Prob > [t] 0.0673	
Lower CL Dif -0.2537 Prob > t 0.0337*	
Confidence 0.95 Prob < t 0.9663 -4 -3 -2 -1 0 1 2 3 4	

(1) From the output, the mean and variance for C1 and C2 are 71.2,

1.92354 and 74, 2.23607.

(2)and (3). From the t test, there is a significant difference between the means and the p-value .0337.

(4) From "Analysis of Variance", the p-value for F test is .0665, which is not significant.

## **Regression Analysis**

4. Once the API is produced in a reactor described in Scenario 1, crystallization from solution is to separate the desired product  $C(t_f)$  from  $A(t_f)$  and  $B(t_f)$  once the impurity  $D(t_f)$  has been removed. In general for a pharmaceutical process crystallization may be used to achieve sufficient product purity, to minimize the filtration time or to achieve tablet stability when mixed with other crystals of other chemical species before forming a tablet. In this example we will dwell only on a single criterion filtration time In this example, based on the work of Togkalidou et al (2001), "Experimental Design and Inferential Modeling in Pharmaceutical Crystallization (AIChe Journal, Vo 27, No1), a pharmaceutical salt was crystallized in a baffled reactor, where the supersaturation was created by adding a less efficient solvent that was miscible in the original solvent. The details are not relevant for the example but the student is referred to the paper if more information about the crystallization process is required.

Experiment Number	Agitation(rpm)	Seed Amount (% of Batch)	Temperature (deg C)	Charge Time h	Filtration Time Min
1	2200	4	20	6	150
2	400	5	15	3	105
3	1300	3.5	15	9	165
4	2200	4	17.5	7.5	170
5	3100	3.5	17.5	7.5	90
6	2200	4	20	6	155
7	4000	5	20	6	50
8	400	3	20	6	280
9	1300	3.5	22.5	4.5	122
10	2200	4	22.5	4.5	100
11	3100	4.5	25	9	82
12	2200	4	20	6	145

The following data were collected:

Use Regression Analysis from JMP to determine a regression model and the conditions under which the filtration time is minimized.

### Solution:

# (1) Run a regression model with all four factors in the model using the steps as showed in the JMP tutorial S2E4 and S2E5:

▼ Summary	of Fi	t							
RSquare			0.700	772					
RSquare Adj			0.529	785					
Root Mean So	juare E	rror	40.42	272					
Mean of Resp	onse		13	4.5					
Observations	(or Su	m Wgts)		12					
▼ Analysis of Variance									
Source	DF S	5um of Sq	uares	Меа	n Square	F	Ratio		
Model	4	2678	7.025		6696.76	4	.0984		
Error	7	1143	7.975		1634.00	Pro	ob > F		
C. Total	11	3822	5.000			0.	0506		
Lack Of Fi	t								
Source	DF	Sum of	Square	s M	lean Squ	are	F Ra	itio	
Lack Of Fit	5	11	387.97	5	2277	60	91.10	)38	
Pure Error	2		50.00	0	25	.00	Prob 0	> F	
Total Error	- 7	11	437.97	5			0.010	)9*	
						I	Max R:	Sq	
							0.99	87	
▼Paramete	er Est	imates							
Term		Estimate	Std E	ror	t Ratio	Prob	> t		
Intercept	31	3.02873	164.7	935	1.90	0.09	993		
Agitation	-0	.032988	0.016	513	-1.99	0.08	374		
Seed Amount	-4	0.78237	25,80	307	-1.58	0.15	580		
Temperature	0.9	5069102	4,592	396	0.11	0.91	52		
Charge Time	6.3	7678051	8.777	356	0.77	0.46	559		
•									

(2) Remove the most insignificant term by comparing the p-values. Temperature is eliminated and the model is run again:

💙 Summary	of Fi	t						
RSquare			0.700	252				
RSquare Adj			0.587	846				
Root Mean So	quare E	rror	37.84	489				
Mean of Resp	onse		13	84.5				
Observations	(or Su	m Wgts)		12				
Analysis	of Va	riance						
Source	DF S	Sum of Sq	uares	Меа	n Square		F Rati	0
Model	3	2676	7.116		8922.37		6.229	7
Error	8	1145	7.884		1432.24	P	rob >	F
C. Total	11	3822	5.000			0	.0173	*
Lack Of F	it							
Source	DF	Sum of	Square	s M	lean Squa	are	FR	atio
Lack Of Fit	6	11	407.88	4	1901.		76.0	526
Pure Error	2		50.00	-	25.	00	Prob	> F
Total Error	8	11	457.88	4			0.01	30*
							Max P	٩Sq
							0.99	987
▼Paramete	er Est	imates						
Term	I	Estimate	Std E	rror	t Ratio	Pro	b> t	
Intercept	32	5.80338	109.8	334	2.97	0.0	)180*	
Agitation		.032151	0.013		-2.32		)487*	
Seed Amount		1.53415	23.3		-1.78		125	
Charge Time	6.5	5187692	7.941	494	0.82	0.4	355	

(3) Once again, remove the most insignificant term, Change Time. Run the model again:

Summary	OT HI						
RSquare			0.675	006			
RSquare Adj			0.602	785			
Root Mean Se	quare Er	ror	37.15	271			
Mean of Resp	onse		13	34.5			
Observations	(or Sum	i Wgts)		12			
Analysis	of Var	iance					
Source	DF S	um of Sq	juares	Mea	n Square	!	F Ratio
Model	2	2580	2.085		12901.0	I	9.3464
Error	9	1242	2.915		1380.3	P	rob > F
C. Total	11	3822	5.000			0	1.0064*
Lack Of F	it						
Source	DF	Sum of	Square	es M	lean Squ	are	F Ratio
Lack Of Fit	4	8	728.41	5	2182	10	2,9532
Pure Error	5	3	694.50	0	738.	90	Prob > F
Total Error	9	12	422.91	5			0.1330
							Max RSq
							0.9033
Paramete	er Esti	mates	;				
Term	E	stimate	Std E	rror	t Ratio	Pro	b> t
Intercept	390	.22516	75.43	199	5.17		)006*
Agitation	-0.	025807	0.01	127	-2.29	0.0	)478*
Seed Amount	-50	.70497	20.07	366	-2.53	0.0	)325*

Both the Agitation and Seed Amount are significant at .05 level. The result regression equation is:

Filtration Time= 390.22516 -.025807 Agitation - 50.70497 Seed Amount

By comparing the sign of the coefficient, the filtration time would be minimized when Agitation is set at its maximum value of 4000 and Seed Amount at 5. At these values the filtration time is 33.47231

5. A study was launched to determine the effect of several factors on the %Dissolution after 60 minutes of a new product from the Tabletting machine in Scenario 2. The following data were obtained:

Expt	Speed	Fill	Pressure	Blade	Punch	Powder	%
Number	(Rpm)	Weight	(Ton)	Speed	Distance	Flow	Diss
		(kg)		(rpm)	(mm)	(kg/hr)	
1	1000	100	1	2000	1	10	50
2	1205	110	.90	2010	.55	.99	77
3	770	115	.91	2020	.48	.98	38
4	750	118	.92	2030	1.85	.97	83
5	1210	120	.93	2040	2.05	.98	95
6	820	118	.94	2050	.5	.99	40
7	800	115	.95	2060	1.9	.95	80
8	1185	110	.96	2070	2.1	.98	97
9	1200	119	1.1	2080	.54	.99	75
10	990	105	.97	1995	1.01	10.1	55
11	1185	95	1.4	1990	.52	10.2	75
12	760	85	1.5	1980	2.0	10.3	69
13	777	88	1.6	1970	1.95	10.2	75
14	1190	81	1.5	1960	.48	10.5	80
15	1205	105	1.3	1950	2.1	10.1	98
16	775	107	.95	1940	.52	10.6	35
17	810	75	1.2	1930	2.06	10.2	60
18	740	77	.97	1920	.47	10.1	30
19	1010	95	1.03	2010	.97	9.9	48

(1) Determine the extent of correlation between the various factors.

(2) Build a regression model relating the %Dissolution to the factors.

i)Use Standard Regression

ii)Use Stepwise Regression

iii) Why are results in ii) different than in i)

Solution: (1)

(a) To acquire the correlation between the factors, choose "Multivariate" from "Multivariate Method" in "Analyze":

🕴 JMP - JMP soluti	ion for #5								
File Edit Tables Rov	ws Cols DOE	Analyze Grap	h Tools Vie	w Window	Help				
🖹 🗅 🚅 🗟 🔲	a X 🖻 🖻		<b>5. 46</b> + 400 ,	ц <sub>р</sub> р.	<b>+ ⋒ =</b> ∠		roblem3		<b>~</b>
							i obienio		
🛗 JMP solution fo	r #5								
▼problem3	<ul> <li>€</li> </ul>					Punch			A
· · · · · · · · · · · · · · · · · · ·	•	Speed	Fill Weight	Pressure	Blade Speed	Distance	Powder Flow	%Dissolution	
		1000	100	1	2000	1	10	50	
	2	1205	110	0.9	2010	0.55	0.99	77	
	3	770	115	0.91	2020	0.48	0.98	38	
	4	750	118	0.92	2030	1.85	0.97	83	
	5	1210	120	0.93	2040	2.05	0.98	95	
0.0.1 (210)		820	118	0.94	2050	0.5	0.99	40	
Columns (7/0)		800	115	0.95	2060	1.9	0.95	80	
🚄 Speed 🚄 Fill Weight	8	1185	110	0.96	2070	2.1	0.98	97	
Pressure	9	1200	119	1.1	2080	0.54	0.99	75	
A Blade Speed	10	990	105	0.97	1995	1.01	10.1	55	
A Punch Distance	11	1185	95	1.4	1990	0.52	10.2	75	
🚄 Powder Flow	12	760	85	1.5	1980	2	10.3	69	
🚄 %Dissolution	13	777	88	1.6	1970	1.95	10.2	75	
	14	1190	81	1.5	1960	0.48	10.5	80	
		1205	105	1.3	1950	2.1	10.1	98	
	16	775	107	0.95	1940	0.52	10.6	35	
	17	810	75	1.2	1930	2.06	10.2	60	
	18	740	77	0.97	1920	0.47	10.1	30	
	19	1010	95	1.03	2010	0.97	9.9	48	
■Rows									
All rows 19									
Selected 19									
Excluded 0									
Hidden 0									
Labelled 0									
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	4								

## (b) Choose all the factors in "Y, Columns":

🗟 Report: Multivariate and C	Correlation	s	
Pairwise and higher relationships amo Select Columns Speed Fill Weight Pressure Blade Speed Punch Distance Powder Flow %Dissolution	-	of columns d Columns into Roles Speed Fill Weight Pressure Blade Speed Punch Distance Powder Flow optional Numeric optional Numeric optional Numeric	Action OK Cancel Remove Recall Help

## (c) Click "OK":

🕈 🛡 Sc	atterplot N	/latrix				
1200 -		r=0.2027	r≖0.0761.	r=0.2714 .	r⊋-0.0715 💂	r⊫-0.1135 🖕
1000 -	Speed	··.	-	-	•	•
800 -		1.4.4	ą <sup>1</sup>	· · · ·	÷	!;
100 - 80 -	r=0.2027	Fill Weight	r=-0.6238	r=0.7851	r≕-0.0179	r≓-0.8001
1.3 1.3 1.1 0.9	r=0.0761	r=-0.6238	Pressure	r=-0:4207	r=0.2034	r=0.5899 :
2100 - 2050 - 2000 - 1950 -	r=0.2714	r=0.7851	r <del>⇒</del> 0.4207	Blade Speed	r=0.0645	r⊫-0.8285
2-	r <b>≠-</b> 0.0715	r=-0.0179	r <b>≕</b> D.2034	r=0.0645		r <b>⊨</b> -0.0463 ≀
1.5- 1- 0.5-			 	 	Punch Distance	
ے – 10	ra=-0.1 <b>1</b> 35 •	r=~9.8001	r <b>≕Q</b> .5899 • •	r <b>∞•0•6</b> 285	r≖-0.0463 ~	
6-						Powder Flow
2-			<b>_</b> .			
	8001000 130	080 100 120	.91.1 1.4 1.	71950 2050	.5 1 1.5 2	246810

Note the following pair of factors are highly correlated: Fill Weight and Blade Speed. Fill Weight and Powder Flow. Blade Speed and Powder Flow

Fill Weight and Pressure

(2)

#### i. Standard Regression:

ii Stand									
♥ Summai	ry of l	Fit							
RSquare		(	).920888						
RSquare Ac	dj 🛛	(	).881331						
Root Mean	Square	Error 7	7.411549						
Mean of Re	sponse	: 6	6.31579						
Observatio	ns (or S	ium Wgts)	19						
Analysi:	s of V	'ariance							
Source	DF	Sum of Squa	ares Mean	Square	F Ratio				
Model	6	7672.9	325 :	1278.82	23.2805				
Error	12	659.1	727	54.93	Prob > F				
C. Total	18	8332.1	053		<.0001*				
▼ Parameter Estimates									
Term		Estimate	Std Error	t Ratio	Prob> t				
Intercept		113.97311	142.6448	0.80	0.4398				
Speed		0.0626565	0.009696	6.46	<.0001*				
Fill Weight		0.2232583	0.231023	0.97	0.3529				
Pressure		38.856114	10.82738	3.59	0.0037*				
Blade Spee	d	-0.090549	0.075411	-1.20	0.2530				
Punch Dista	ance	17.220037	2.584938	6.66	<.0001*				
Powder Flo	W	-2.188226	0.794755	-2.75	0.0175*				

Based on the analysis, Fill Weight and Blade Speed are unimportant. This is not surprising since they are correlated with Powder Flow in Part (1).

Problem3         Fk Y by X         Matched Pairs           Problem3         Fk Model         Punch         Punch         Distance         Powder Flow         %Dissolution           * Columns (7/0)         75         118         0.9         2030         1.85         0.99         77           * Columns (7/0)         75         118         0.92         2030         1.85         0.97         83           * Columns (7/0)         76         820         118         0.94         2050         0.5         0.99         40           * Speed         820         118         0.94         2050         0.5         0.99         40           * Fill Weight         9         1200         119         1.1         2080         0.5         0.99         40           * Pressure         1185         110         0.96         2070         2.1         0.98         97           * Pressure         1185         110         0.96         2070         2.1         0.98         97           * Powder Flow         9         1200         119         1.1         2080         0.54         0.99         75           * Powder Flow         113         777 <td< th=""><th>) 🗅 😅 🖪 🗐 🎒 👗 🛙</th><th>🚡 🛒 📴 Distribution</th><th></th><th>0.</th><th>+ 🛛 ≒ 4</th><th></th><th>oroblem3</th><th>~</th><th></th></td<>	) 🗅 😅 🖪 🗐 🎒 👗 🛙	🚡 🛒 📴 Distribution		0.	+ 🛛 ≒ 4		oroblem3	~	
Problem3         Price         Fit Model         Punch Modeling Multivariate Methods survival and Reliability         Punch Distance         Powder Flow         %Dissolution           * Columns (7/0)         1         10         50         1         100         50           * Columns (7/0)         3         750         118         0.92         2030         1.65         0.97         83           * Columns (7/0)         5         6         20         118         0.94         2050         0.5         0.99         40           * Speed Pli Weight Pressure Blade Speed         1185         110         0.96         2070         2.1         0.98         97           * Blade Speed         1185         110         0.96         2070         2.1         0.98         97           * Blade Speed         1185         110         0.96         2070         2.1         0.98         97           * Punch Distance Powder Flow         1185         119         0.97         1.99         1.01         10.1         55           * Powder Flow         13         777         88         1.6         1970         1.95         10.2         75           * Powder Flow         17         10.7							<u>.</u>	and the second se	
Columns (7/0)         Modeling Multivariate Methods Survival and Reliability         net (1)         Distance 2000         Powder Flow         %Dissolution           • Columns (7/0)         1         10         50           • Columns (7/0)         5         1210         120         0.93         22030         1.85         0.99         77           • Columns (7/0)         6         820         118         0.92         2030         1.85         0.97         83           • Fill Weight Pressure Blade Speed         7         800         115         0.94         2050         0.5         0.99         40           • Pressure Blade Speed         1185         110         0.96         2070         2.1         0.98         97           • Pressure Blade Speed         11         1185         95         1.1         2080         0.54         0.99         75           • Pressure Powder Flow         10         990         105         0.97         1995         1.01         10.1         55           • Powder Flow         11         1185         95         1.4         1990         0.52         10.2         75           • Powder Flow         11         1185         95         1.4	problem3	🔜 🔛 Matched Pairs	5						
Columns (7/0)         Modeling         Modeling         Multivariate Methods         Mu	problem3	🔽 💷 Fit Model				Punch	15.16		
Multivariate Methods         1         1         2000         1         10         50           Survival and Reliability         0,9         2010         0.055         0.99         77           0,91         2020         0.48         0.99         38           1         750         118         0.92         2030         1.85         0.99         38           1         750         118         0.92         2030         1.85         0.99         38           5         1210         120         0.93         2040         2.05         0.98         95           6         820         118         0.94         2050         0.5         0.99         40           Speed         8         1185         110         0.96         2070         2.1         0.98         97           Pressure         9         1200         119         1.1         2080         0.54         0.99         75           Pressure         10         990         105         0.97         1995         1.01         10.1         55           Powder Filower         11         118         95         1.5         1980         2         10.3		Modeling		ure	Blade Speed	Distance	Powder Flow	%Dissolution	
Columns (7/0)         3         Survival and Reliability         0.99         2010         0.055         0.99         77           • Columns (7/0)         4         750         118         0.92         2030         1.85         0.97         83           • Columns (7/0)         6         820         118         0.94         2050         0.5         0.99         40           • Speed         6         820         118         0.95         2060         1.9         0.95         80           • Fill Weight         9         1200         119         1.1         2080         0.54         0.99         75           • Pressure         118         195         1.4         1990         0.52         10.2         75           • Powder flow         11         1185         95         1.4         1990         0.52         10.2         75           • Powder flow         12         760         85         1.5         1980         2         10.3         69           • * Dissolution         13         777         88         1.6         1970         1.95         10.2         75           • Powder flow         15         1205         10.3 <td></td> <td></td> <td></td> <td>1</td> <td>2000</td> <td></td> <td>10</td> <td></td> <td></td>				1	2000		10		
Columns (7/0)         Columns		- Z			2010	0.55	5 0.99	77	
Columns (7/0)         5         1210         120         0.93         2040         2.05         0.98         95           Speed         6         820         118         0.94         2050         0.5         0.99         40           Speed         7         800         115         0.95         2060         1.9         0.95         80           Fill Weight Pressure Blade Speed         91         200         119         1.1         2080         0.54         0.99         75           Punch Distance Powder Flow         990         105         0.97         1995         1.01         10.1         55           900         13         777         88         1.6         1970         1.95         10.2         75           900         13         777         88         1.6         1970         1.95         10.2         75           14         1190         81         1.5         1960         0.48         10.5         80           16         775         107         0.95         1940         0.52         10.6         35           17         810         75         1.2         1930         2.06         10.2						Territori -	- Christen	10000	
Columns (7/0)         6         820         118         0.94         2050         0.5         0.99         40           Speed Fill Weight Pressure Blade Speed Punch Distance Powder Flow         3         1185         110         0.96         2070         2.1         0.98         97           90         105         0.97         1995         1.01         10.1         55           90         105         0.97         1995         1.01         10.1         55           Powder Flow         12         760         85         1.5         1980         2         10.3         69           % Dissolution         13         777         88         1.6         1970         1.95         10.2         75           14         1190         81         1.5         1960         0.48         10.5         80           16         775         107         0.95         1940         0.52         10.6         35           17         810         75         1.2         1930         2.06         10.2         60           18         740         77         0.97         1.920         0.47         10.1         30           19			10.000						
* Columns (7/0)         7         800         115         0.95         2060         1.9         0.95         80           Speed Fill Weight Pressure Blade Speed Punch Distance Powder Flow %Dissolution         1105         110         0.96         2070         2.1         0.98         97           990         100         119         1.1         2080         0.54         0.99         75           Blade Speed Punch Distance Powder Flow         11         1185         95         1.4         1990         0.52         10.2         75           11         1185         95         1.4         1990         0.52         10.2         75           Ponch Distance Powder Flow         12         760         85         1.5         1980         2         10.3         69           114         1190         81         1.5         1960         0.48         10.5         80           116         775         107         0.95         1940         0.52         10.6         35           117         810         75         1.2         1930         2.06         10.2         60           19         1010         95         1.03         2010         0.97			in the second						
Speed         8         116         0.73         2000         1.19         0.73         600           Fill Weight Pressure Blade Speed Punch Distance Powder Flow %Dissolution         9         1200         119         1.1         2080         0.54         0.99         75           Pide Speed Punch Distance Powder Flow %Dissolution         1185         9100         0.97         1995         1.01         10.1         55           11         1185         95         1.4         1990         0.52         10.2         75           Powder Flow %Dissolution         13         777         88         1.6         1970         1.95         10.2         75           14         1190         81         1.5         1960         2.1         10.1         98           15         1205         105         1.3         1950         2.1         10.1         98           16         775         107         0.95         1940         0.52         10.6         35           19         1010         95         1.03         2010         0.97         9.9         48           * Rows         19         1010         95         1.03         2010         0.97	Columna (7/0)								
Fill Weight Pressure Blade Speed Punch Distance Powder Flow         9         1103         1103         0.796         2.21         0.790         977           Plack Distance Powder Flow         9         1200         119         1.11         2080         0.54         0.99         75           Powder Flow         11         1185         95         1.4         1990         0.52         10.2         75           Solissolution         12         760         85         1.5         1980         2         10.3         69           * Obissolution         13         777         88         1.6         1970         1.95         10.2         75           14         1190         81         1.5         1960         0.48         10.5         80           16         775         107         0.95         1940         0.52         10.6         35           17         810         75         1.2         1930         2.06         10.2         60           18         740         77         0.97         1920         0.47         10.1         30           19         1010         95         1.03         2010         0.97         9.9									
Pressure Blade Speed Punch Distance Powder Flow         1200         119         1.1         2080         0.054         0.099         75           Punch Distance Powder Flow         10         990         105         0.97         1995         1.01         10.1         55           Powder Flow         12         760         85         1.5         1980         2         10.3         69           13         777         88         1.6         1970         1.95         10.2         75           14         1190         81         1.5         1960         0.48         10.5         80           15         1205         105         1.3         1950         2.1         10.1         98           16         775         107         0.95         1940         0.52         10.6         35           17         810         75         1.2         1930         2.06         10.2         60           18         740         77         0.97         1.920         0.47         10.1         30           19         1010         95         1.03         2010         0.97         9.9         48           r Rows         <							in the second		
Blade Speed Princh Distance         10         990         105         0.97         1995         1.01         10.1         55           Powder Distance         11         1185         95         1.4         1990         0.52         10.2         75           Powder Tow         12         760         85         1.5         1980         2         10.3         69           *&Dissolution         13         777         88         1.6         1970         1.95         10.2         75           14         1190         81         1.5         1960         0.48         10.5         80           15         1205         105         1.3         1950         2.1         10.1         98           16         775         107         0.95         1940         0.52         10.6         35           17         810         75         1.2         1930         2.06         10.2         60           18         740         77         0.97         1920         0.47         10.1         30           19         1010         95         1.03         2010         0.97         9.9         48           If rows <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td>									
Powder Towards         12         760         85         1.5         1980         2         10.3         69           Powder Towards         13         777         88         1.6         1970         1.95         10.2         75           14         1190         81         1.5         1960         0.48         10.5         80           15         1205         105         1.3         1950         2.1         10.1         98           16         775         107         0.95         1940         0.52         10.6         35           17         810         75         1.2         1930         2.06         10.2         60           18         740         77         0.97         1920         0.47         10.1         30           19         1010         95         1.03         2010         0.97         9.9         48           * Rows					1				
*Abisolution         13         777         88         1.6         1970         1.95         1.0.2         75           *Abisolution         14         1190         81         1.5         1960         0.48         10.5         80           15         1205         105         1.3         1950         2.1         10.1         98           16         775         107         0.95         1940         0.52         10.6         35           17         810         75         1.2         1930         2.06         10.2         60           18         740         77         0.97         1920         0.47         10.1         30           19         1010         95         1.03         2010         0.97         9.9         48           * Rows		1997	1000						
Rows         Image: scale of the state									
Rows         Image: space sp	%Dissolution	2 2 2 C							
Rows         Image: Constraint of the system of the sy									]
17         810         75         1.2         1930         2.06         10.2         60           18         740         77         0.97         1920         0.47         10.1         30           19         1010         95         1.03         2010         0.97         9.9         48           * Rows									
18         740         77         0.97         1920         0.47         10.1         30           19         1010         95         1.03         2010         0.97         9.9         48           r Rows		100 C						tertaitet in	
19         1010         95         1.03         2010         0.97         9.9         48           FRows		2-7 C				S. S. S. S.		and the second sec	
Rows         Image: Constraint of the second se								(10.100 C	
II rows         19         III rows         10         10         10         10         10         10         10         10         10         10         10         10         10         10         10		19 1010	95	1.03	2010	0.97	9.9	48	
ielected 19	Rows								
Excluded 0									
iidden 0									
							-		
	Delled U						-		

# ii) Stepwise Regression(a) Choose "Fit Model" in "Analyze":

problem3					
🔝 Fit Model			Flow	%Dissolution	
Model Specificat	ion		10	50	
Select Columns	Pick Role Variables	onality: Standard Least Square		77	
Speed	Y required	Stepwise	55	38	
Fill Weight	optional	<ul> <li>Second and second</li> </ul>		83	
Pressure	Help	Manova		95	
Blade Speed	Weight optional Numeric	Loglinear Variance		40	
Punch Distance	Ren	Nominal Logistic		80	
M M Dissolution	Freq optional Numeric	Ordinal Logistic		97	
100 00 00 00 00 00 00 00 00 00 00 00 00	By optional	Orumai Eugistic		75	
		Proportional Hazard		55	
Or     Punch Distance     Popular Toptional Numeric       Sp     Powder Flow     Freq     optional Numeric       Frid     %Dissolution     By     optional       BL     Po     Construct Model Effects       Po     Add		Parametric Survival		75	
d	Add			69	
6		Generalized Linear Mo		75	
	Cross		10.5		
	Nest		10.1	98	
			10.6	35	
	Macros 🗸		10.2	60	
	Degree 2		10.1	30	
	Attributes 💌		9.9	48	
	Transform 🐨				
4	No Intercept		-		
en O					
en O			12		

## (b) Select "Stepwise" in "Personality":

## (c) Fit in the Response and Factors:

JRP	Fit Model		X
•	Model Specification	n	
	Select Columns	Pick Role Variables Personality: Stepwise	~
		Y A%Dissolution	
	Fill Weight		
	ABlade Speed	Weight optional Numeric Run Model	
	Punch Distance	Remove	
	A %Dissolution	Freq optional Numeric	
		By optional	
		Construct Model Effects	
		Add Speed	
		Fill Weight	
		Cross Pressure Blade Speed	
		Nest Punch Distance	
		Macros   Powder Flow	
		Degree 2	
		Attributes 💌	
	-	Transform 💌	
		No Intercept	

## (d) Hit "Run Model":

📓 problem3- Fit Stepwise									
👻 🗢 Stepwise Fit						-			
Response: %Dissolution									
Stepwise Regression Control									
Prob to Enter 0.250 Enter All Prob to Leave 0.100 Remove All									
Go Stop Step Make	e Model								
♥ Current Estimates									
SSE DFE	MSE RSquare	RSc	quare Adj	Ср	AIC				
8332.1053 18 462.8	39474 0.0000		0.0000	134.68294	117.5852				
Lock Entered Parameter	Estimate	nDF	SS	"F Ratio"	"Prob>F"				
🗹 🗹 Intercept	66.3157895	1	0	0.000	1.0000				
Speed	0	1	2975.048	9.441	0.0069				
🗌 🔲 🛛 Fill Weight	0	1	407.3309	0.874	0.3630				
Pressure	0	1	698.1432	1.555	0.2294				
🗌 🔲 🛛 Blade Speed	0	1	910.2736	2.085	0.1669				
Punch Distance	· –	1	3226.701		0.0044				
Powder Flow	0	1	635.8756	1.405	0.2523				
✓ Step History									

(e) Now we may choose either forward selection or backward selection.

To do forward selection, input .05 as the  $\alpha$  Entry level and Exit level. Pick "Forward" in "Direction". Hit "Go":

🔝 prob	lem3	- Fit Stepwise	9							×
🔶 🖻 Ste	epwis	se Fit								
Respons	se: %D	Dissolution								
🔷 🕈 Ste	Stepwise Regression Control									
	to En		Enter	All						
	to Lea		Remo							
Direc	tion: F	Forward 😽	Remo							
Go	Sto	p Step Mak	e Model	)						
🔶 Cui	rrent	Estimates								
	SSE	E DFE	MSE	RSquare	RS	quare Adj	Ср	AIC		
165	3.2307	7 16 103.	32692	0.8016	i	0.7768	17.096464	90.85491		
Lock E	Entere	d Parameter	E	stimate	nDF	SS	"F Ratio"	"Prob>F"		
Image: A start and a start	1	Intercept	-26.1	140878	1	0	0.000	1.0000		
	$\checkmark$	Speed	0.070	029302	1	3452.173	33.410	0.0000		
		Fill Weight		0	1	90.78878	0.872			
		Pressure		0	1	95.57831	0.920			
		Blade Speed		0	1	114.3366				
		Punch Distance	e 20.1	154033	1					
		Powder Flow		0	1	250.5261	2.679	0.1225		
🔷 🕈 Ste	ep His	story								
Step	р	Parameter	Action	"Sig Pi	rob"	Seq SS	RSquare	Ср	Р	
	1	Punch Distance	Entered	l 0.0	044	3226.701	0.3873	77.942	2	
:	2	Speed	Entered	l 0.0	000	3452.173	0.8016	17.096	3	

Punch Distance and Speed are kept in the final model.

(f) To do backward selection, input .05 as the  $\alpha$  Entry level and Exit level. Pick "Backward" in "Direction". Hit "Enter All" and "Go":

📓 problem3- Fit Stepwise								
👻 💌 Stepwise Fit								
Response: %Dissolution								
▼ Stepwise Regression Control								
Prob to Enter 0.050 Enter All								
Prob to Leave 0.050								
Direction: Backward 🗸 Remove All								
Go Stop Step Make Model								
Current Estimates								
SSE DFE MSE RSquare RSquare Adj Cp	AIC							
	95015							
	rob>F"							
	1.0000							
	0.0000							
	0.6033							
	0.0038							
Blade Speed 0 1 44.00445 0.805 (	0.3859							
	0.0000							
Powder Flow -1.8539565 1 803.1748 14.904 (	0.0017							
✓ Step History								
Step Parameter Action "Sig Prob" Seq SS RSquare C	рр							
1 Fill Weight Removed 0.3529 51.30044 0.9147 5.933	96							
2 Blade Speed Removed 0.3859 44.00445 0.9094 4.73	55							

Speed, Pressure, Punch Distance and Powder Flow are in the final model.

iii) However, the results are different because of the correlations among the factors.

## **Single Factor Experiments**

6. Completely Randomized Design

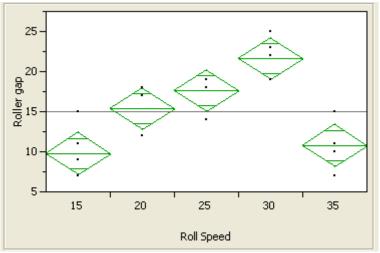
In a study to determine the effect of roller speed on roller gap in a roller compactor (Scenario 2), five replicates of the Roller Gap in mm were measured at five different values of roll speed (rpm) where the experiments were run in random order. The following data were obtained:

Roll Speed (rpm)	Roller gap (mm)					
15	7	7	15	11	9	
20	12	17	12	18	18	
25	14	18	18	19	19	
30	19	25	22	19	23	
35	7	10	11	15	11	

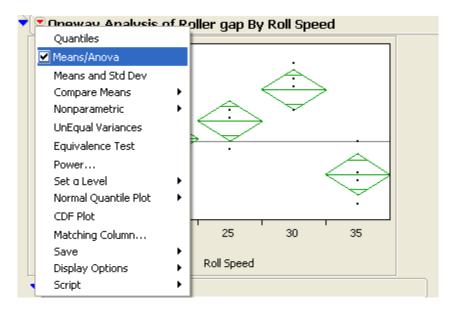
- (1)Does roller speed affect roller gap at the 95% confidence level? Perform an ANOVA.
- (2) Using a multiple range test at 95% confidence which levels are different from one another?
- (3) Find a suitable regression model between roller gap and roll speed if one exists.
- (4) Compare the results of (2) and (3).

Solution:

(1) Choose "Fit Y by X" in "analyze" with Roller gap as Y and Roll speed as X.



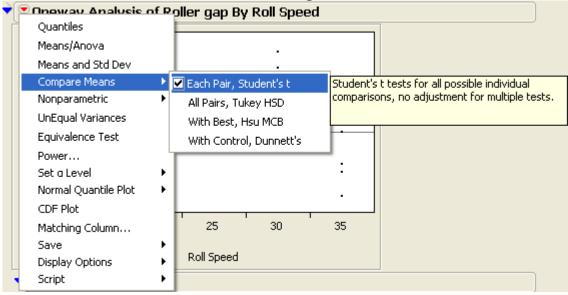
Choose "means/Anova" in hot spot aside "Oneway analysis of Roller gap by Roller speed":



▼ Analysis of Variance										
Source		DF Sum	of Squares	Mean Square	F Ratio	Prob > F				
Roll Spe	eed	4	475.76000	118.940	14.7568	<.0001*				
Error		20	161.20000	8.060						
C. Tota	C. Total 24 636.96000									
Means for Oneway Anova										
Level	Number	Mean	Std Error	Lower 95%	Upper 95%					
15	5	9.8000	1.2696	7.152	12.448					
20	5	15.4000	1.2696	12.752	18.048					
25	5	17.6000	1.2696	14.952	20.248					
30	5	21.6000	1.2696	18.952	24.248					
35	5	10.8000	1.2696	8.152	13.448					

Yes, roller speed affects roller gap at the 95% confidence level since the p value is <.0001.

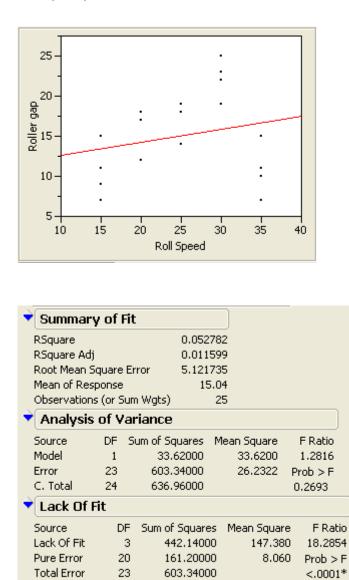
## (2) Choose "each Pair, Student's t" in "Compare Means":



ľ	<ul><li>C</li></ul>	omparis	sons for ea	ach pair u	ising Stud	lent's t	
		t	Alpha				
	2.0	8596	0.05				
	Abs(Di	if)-LSD					
		30	25	20	35	15	
	30	-3.7455	0.2545	2.4545	7.0545	8.0545	
	25	0.2545	-3.7455	-1.5455	3.0545	4.0545	
	20	2.4545	-1.5455	-3.7455	0.8545	1.8545	
	35	7.0545	3.0545	0.8545	-3.7455	-2.7455	
	15	8.0545	4.0545	1.8545	-2.7455	-3.7455	
		e values s	how pairs of i	means that a	are significan	itly differer	nt.
	Level		Mean				
	30	A	21.600000				
	25	В	17.600000				
	20	В	15.400000				
	35	C	10.800000				
	15	C	9.800000				
	Levels	not conne	ected by same	e letter are s	ignificantly d	lifferent.	
	Level	- Level	Difference	Lower CL	Upper CL	p-Value	
	30	15	11.80000	8.05455			
	30	35	10.80000	7.05455	14.54545		
	25	15	7.80000	4.05455	11.54545		
	25	35	6.80000	3.05455	10.54545		
	30	20	6.20000	2.45455		0.0025*	
	20	15	5.60000	1.85455		0.0054*	
	20	35	4.60000	0.85455		0.0186*	
	30	25	4.00000	0.25455		0.0375*	
	25	20	2.20000	-1.54545	5.94545		
	35	15	1.00000	-2.74545	4.74545	0.5838	

By the analysis, Level 30 in Group A is different from level 25 and 20 in group B. Level 25 and 20 in group B are different from 35 and 15 in group C.

(3) Firstly, fit a first order linear model: Let roll speed be X, roller gap be Y  $Y = \beta_0 + \beta_1 X + \epsilon$ 



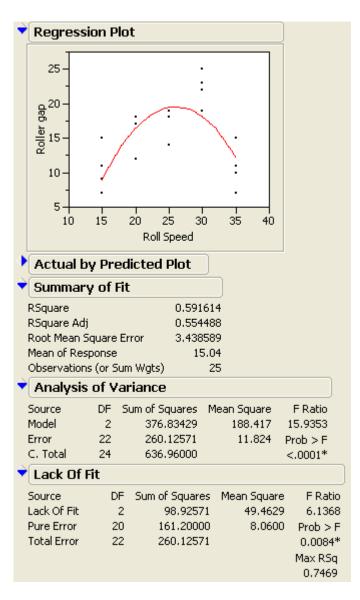
There is a significant lack of fit at the .05 level. Then try a second order model:

Max RSq 0.7469

Let roll speed be X, roller gap be Y

 $Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \epsilon$ 

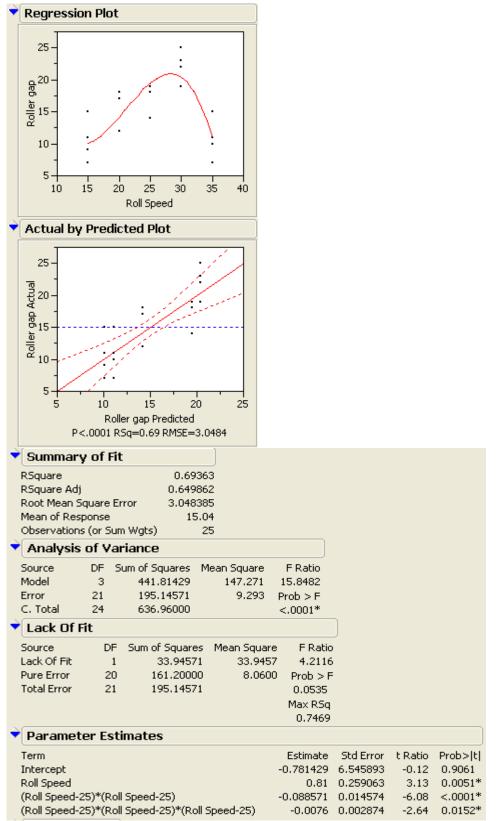
Choose "fit model" in "analyze". Then add Roll speed and Roll speed\*Roll speed as factors. (To add Roll speed\*Roll speed, click Roll speed in the added factor area, then click cross, then click Roll speed in the Select Columns.)



There is still a significant lack of fit. Then try a third order model. Let roll speed be X, roller gap be Y

 $\mathbf{Y} = \boldsymbol{\beta}_0 + \boldsymbol{\beta}_1 \mathbf{X} + \boldsymbol{\beta}_2 \mathbf{X}^2 + \boldsymbol{\beta}_3 \mathbf{X}^3 + \boldsymbol{\epsilon}$ 

The third order term, Roll speed\* Roll speed\* Roll speed is added the similar way as the second order term Roll speed\* Roll speed.



There is no significant lack of fit. We can conclude a cubic model is adequate to describe the data.

## **Randomized Block Design**

7. A study was conducted to determine effect of Roll Speed (rpm) on ribbon uniformity (dimensionless) in a roller compactor (Scenario 2).. Six different replicates were conducted on six batches of material from a blending operation. The order of selecting the samples was from the blenders were randomized as was the order of running the experiments. The data from this completely randomized block design is shown below:

	В	atch Numbe	er			
Roll	1	2	3	4	5	6
Speed (rpm)						
(rpm)						
10	.78	.80	.81	.75	.77	.78
16	.85	.85	.92	.86	.81	.83
23	.93	.92	.95	.89	.89	.83
31	1.14	.97	.98	.88	.86	.83
40	.97	.86	.78	.76	.76	.75

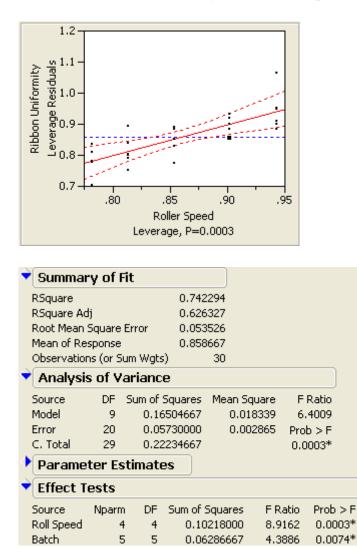
- (1) Does Roll Speed affect the ribbon uniformity? Is the between batch variation significant?
- (2) Determine the regression equation between roller uniformity and roll speed. Compare the results with a)
- (3) Are the residuals from this experiment normally distributed?

Solution:

(1) In JMP, double click the tab of "Roll speed" and choose the data type as "Character":

🔝 Roller Speed			
Roller Speed' in	Table 'problem5'		ОК
Column Name	Roller Speed	🗆 Lock	Cancel
Data Type	Character 🗸		Apply
Modeling Type	Nominal 💙		Help
Column Propertie	es 🗸		

Use "Fit model" in "Analyze" as in the previous problems:

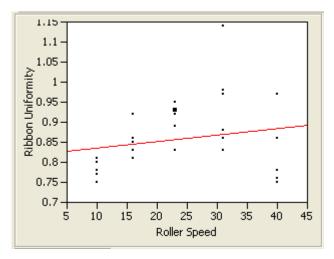


Roll Speed affects the ribbon uniformity at the .05 level since the p value is .0003. There is significant variation between the Batches at the .05 level since the p value is .0074.

(2) Double click the tab of "Roll speed" and choose the data type as "Numeric" and Modeling type as "Continuous":

🔝 Roll Speed		
'Roll Speed' in Table 'problem5'         Column Name       Roll Speed         Data Type       Numeric         Modeling Type       Continuous         Format       Best < Width 2	🗆 Lock	OK Cancel Apply Help

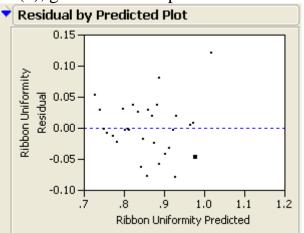
Use "Fit Y by X" in "Analyze" as in the previous problems:



Joannary	of Fit				
RSquare 0.042576				6	
RSquare Adj			0.00838	3	
Root Mean So	Root Mean Square Error 0.087194				
Mean of Resp	onse		0.85866	7	
Observations	(or Sum	n Wgts)	3	0	
Lack Of F	it				
Source	DF	Sum of	f Squares	Mean Squ	iare F Ratio
Lack Of Fit	3	0.0	09271330	0.030	904 6.4295
Pure Error	25	0.1	12016667	0.004	807 Prob > F
Total Error	28	0.2	21287997		0.0022*
					Max RSq
					Max RSq 0.4596
Analysis	of Var	iance	,		
Analysis     Source				lean Square	0.4596
<u> </u>		um of S		lean Squari 0.009463	0.4596 e F Ratio
Source	DF S	um of S 0.009	quares M		0.4596 e F Ratio 7 1.2451
Source Model	DF Si 1	um of 5 0.009 0.212	quares M 946670	0.00946	0.4596 e F Ratio 7 1.2451
Source Model Error	DF 50 1 28 29	um of 5 0.009 0.212 0.222	quares M 946670 287997 234667	0.00946	0.4596 e F Ratio 7 1.2451 3 Prob > F
Source Model Error C. Total	DF 50 1 28 29 <b>er Esti</b>	um of 5 0.009 0.212 0.222	quares M 946670 287997 234667	0.00946	0.4596 e F Ratio 7 1.2451 3 Prob > F
Source Model Error C. Total	DF 50 1 28 29 <b>er Esti</b> Es	um of S 0.009 0.212 0.222 <b>mate</b> s	quares M 946670 287997 234667 <b>S</b>	0.00946 0.00760 t Ratio	0.4596 e F Ratio 7 1.2451 3 Prob > F 0.2740

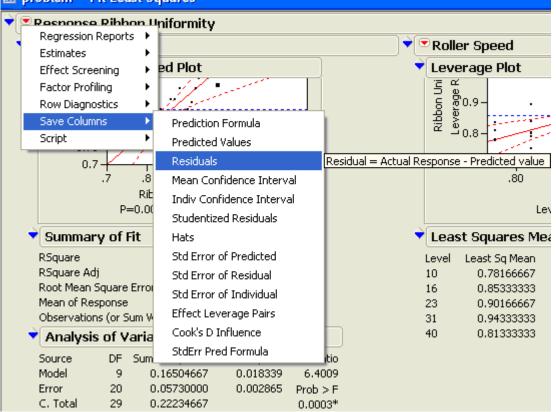
The Roll speed is not significant in this model which has a significant lack of fit in this linear regression model. Comparing the results with (a), the Batch effect has been lumped in with experimental error dramatically increasing its size and limiting the suitability of the regression analysis. It is necessary to remove the batch effect to get an effective model.

(3)



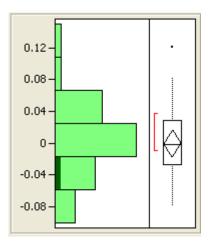
In (1), get the residual plot from the results:

To further check its normality, save the residual by choosing "Residuals" in "Save Columns" from the hot spot aside the Response Ribbon Uniformity: problem Fit Least Squares



Then we analyze it in "Distribution":

Report: Distribution						
The distribution of values in each c	The distribution of values in each column					
Select Columns	Cast Selected Columns into Roles	Action				
Roller Speed     Batch     Ribbon Uniformity     Residual Ribbon Uniformity	Y, Columns	OK Cancel				
	Weight optional Numeric	Remove				
	Freq optional Numeric By optional	Recall Help				



The residuals are normally distributed.

## **Optimization Problem.**

8. The product uniformity y from a continuous blender in scenario 2 is related to the tilt(deg) T by the relationship:

$$Y = 100-(20.5-T)2 + ε, if Y>0$$
  
0, if Y≤0

It is clear from the above relationship that the maximum uniformity is obtained at T=20.5

Show how (1) dichotomous search and (2) golden section search can be used to search out this optimum over the region  $0 \le T \le 50$  where the measurement error at any point is

 $\boldsymbol{\varepsilon} \sim N(0,.25)$ 

The smallest difference in T which can be detected is 2 degree.

(Hint: Program the relationship in Excel using the available random number generator)

Solution:

In excel, input  $Y = 100-(20.5-D2)^2+0.5*RAND()$  as the uniformity generator.

(1) Dichotomous search:

	Worki	ng	middle		
Step	interv	/al	point	Т	Y
1	0	50	25	24	88.13416
I	0	50	25	26	69.75396
2	0	26	13	12	27.75556
Ζ	0	26	13	14	57.95248
2	12	26	19	18	93.89717
3	12	26	19	20	100.2358
1	18	26	22	21	100.0315
4	18	26	22	23	94.03289

Note in step 1 since Y(26) < Y(24), the optimum cannot lie in the interval (26,50) which is dropped. The rest steps are similar.

Since the smallest detectable difference is 2, we find the maximum is close to (20, 21) as expected.

(2) Golden section method:

	Workin	g		
Step	interva	l	Т	Y
1	0	50	19.19	98.42316
I	0	50	30.9	0

2	0	30.9	11.824.34522
3	11.8	30.9	23.690.42856
4	11.8	23.6	16.382.70831
5	16.3	23.6	20.8100.2592

In step 1, by gold section ratio,  $50^{*}.618 = 30.9$ ,  $50^{*}.382 = 19.1$ . Since the uniformity is greater at 19.1 than at 30.9, the interval (30.9, 50) cannot contain the optimum. The next experiment is located at 11.8 symmetrically with the (0, 30.9) interval. ( $30.9^{*}.382 = 11.8$ )

Since only smallest detectable difference is 2, we find the maximum is close to 20.8 as expected.

Comparing these two methods, Dichotomous search requires 8 runs while Golden section only 6.

## **Factorial Experimentation**

9. A study is conducted to assess the effect of Pressure (Ton) and Punch Distance (mm) on percent dissolution of a new API after 80 minutes in a Tablet Press in Scenario 2. Three different replicates were taken at random at three pressures and two Punch Distances The data are as follows:

Pressure (Ton)					
Punch Distance	.75	1	1.5		
(mm)					
1	74,64,50	73,61,44	78,85,92		
2	92,86,68	98,73,88	66,45,85		

- (1)Build a mathematical model to describe the mathematical relationship between %Dissolution and (Pressure, Punch Distance).
- (2) Analyze the residuals from this experiment.

Solution:

(1) (a) The mathematical model for a 2\*3 full factorial experiment is:

 $Y=\beta_0+\beta_1P+\beta_2D+\beta_3PD+\beta_4P^2+\beta_5P^2D$ 

(b) Input the data in JMP:

▼ problem		Punch		
		Distance	Pressure	% Dissolution
	1	1	0.75	74
	2	1	0.75	64
	3	1	0.75	50
Columns (4/0)	4	1	1	73
Punch Distance	5	1	1	61
A Pressure	6	1	1	44
% Dissolution	7	1	1.5	78
🚄 Residual % Dissolution	8	1	1.5	85
	9	1	1.5	92
	10	2	0.75	92
	11	2	0.75	86
	12	2	0.75	68
▼Rows	13	2	1	98
All rows 18	14	2	1	73
Selected (	1 1 5	2	1	88
Excluded (	16	2	1.5	66
Hidden (	) 17	2	1.5	45
Labelled (	18	2	1.5	85
	•			►

(c) Use stepwise regression. Input the response and all the factors as in the mathematical model in (a).

JRP	Fit Model		
<b>(</b>	Model Specification	n	
	Select Columns	Pick Role Variables Personality: Stepwise	~
	Punch Distance	γ A% Dissolution	
	Pressure		
	Residual % Dissolution	Weight optional Numeric Run Model	
		Remove	
		Freq optional Numeric	
		By optional	
		Construct Model Effects	
		Add Pressure	
		Punch Distance	
		Cross Pressure*Pressure Punch Distance*Pressure	
		Nest Punch Distance*Pressure*Pressure	
		Macros 🗸	
		Degree 2	
		Attributes 💌	
L		Transform 💌	
		No Intercept	

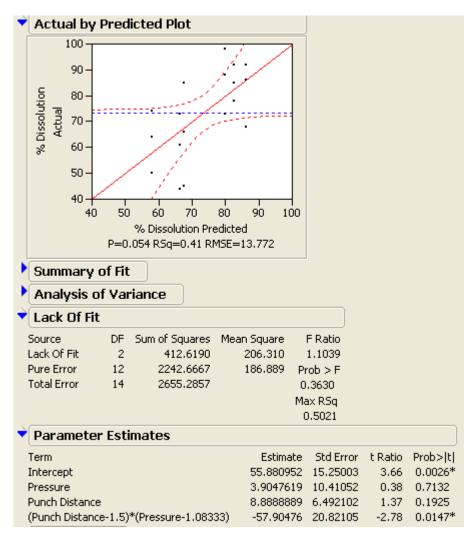
### (c) Hit "Run Model":

📓 problem7- Fit Stepwise		
👻 🗷 Stepwise Fit		
Response: % Dissolution		
Stepwise Regression Control		
Prob to Enter 0.250 Enter All Prob to Leave 0.100 Remove All Rules: Combine		
Go Stop Step Make Model		
Current Estimates		
SSE DFE MSE RSquare RSquare Adj Cp AIC 4504.4444 17 264.96732 0.0000 0.0000 8.1022592 101.4041		
Lock Entered Parameter SS	"F Ratio"	"Prob>F"
✓ ✓ Intercept 73.444444 1 0	0.000	1.0000
Pressure     0 1 26.68254	0.095	0.7615
Punch Distance     0 1 355.5556	1.371	0.2588
(Pressure-1.08333)*(Pressure-1.08333)         0         2         27.44444           (Punch Distance-1.5)*(Pressure-1.08333)         0         3         1849.159	0.046	0.9552
	3.250	0.0540
(Punch Distance-1.5)*(Pressure-1.08333)*(Pressure-1.08333)	2.420	0.0973
▼ Step History		

(d) Input .05 as Entry and Exit  $\alpha$  level. Choose "Backward" in "Direction". Hit "Enter All" and "Go":

🗟 Fit Stepwise	×
▼ Stepwise Fit	
Response: % Dissolution	
▼ Stepwise Regression Control	
Prob to Enter 0.050 Enter All Prob to Leave 0.050 Direction: Backward  Remove All	
Rules: Combine  Go Stop Step Make Model	
▼ Current Estimates	
SSE DFE MSE RSquare RSquare Adj Cp AIC 2655.2857 14 189.66327 0.4105 0.2842 4.2078308 97.89084	
Lock Entered Parameter SS "F Ratio" "Prob>	•F"
✓ ✓ Intercept 55,8809524 1 0 0.000 1.00	00
□ 🗹 Pressure 3.9047619 2 1493.603 3.938 0.04	40
□ 🗹 Punch Distance 8.88888889 2 1822.476 4.805 0.02	58
✓         Punch Distance         8.88888889         2         1822.476         4.805         0.02           □         (Pressure-1.08333)*(Pressure-1.08333)         0         1         0.761905         0.004         0.95           □         ✓         (Punch Distance-1.5)*(Pressure-1.08333)         -57.904762         1         1466.921         7.734         0.01	22
	47
Participant (Punch Distance-1.5)*(Pressure-1.08333)*(Pressure-1.08333)	30
▼ Step History	
Step Parameter Action "Sig Prob" Seq SS RSquare Cp p	
1 (Pressure-1.08333)*(Pressure-1.08333) Removed 0.3630 412.619 0.4105 4.2078 4	

Now since the interaction term is significant, for the sake of easy explanation, we keep both main effects from the interaction in the model.

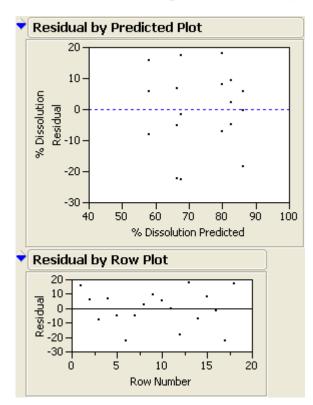


(e) Hit "Make Model" and run the model:

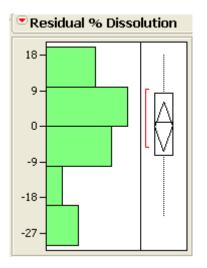
The final model is:

Y = 55.88 + 3.90P + 8.89D - 57.90PD

(2) Get the residual plots in the analysis in (1):



The residuals seem randomly scattered.



But its normality needs further test.

10. Design a full factorial experiment to determine the effect of Tilt, Speed, Load and Inlet powder flow on the uniformity and density in a series of batch runs in a continuous blender in scenario 2. Consider the following cases:

(a) All factors at two levels.

(b) All factors at three levels.

(c) Tilt at 2 levels, Speed at three levels, load at four levels and inlet powder flow at 2 levels.

(1) For each of these cases give the following:

i) the actual experiments that must be run.

ii) the mathematical model

(2) Describe the role of replication, randomization and blocking

Solution:

(1)

(a)

i) Use "Full Factorial Design" in "DOE", input the factors and levels. Hit "Make Table":

2x2x2x2 Factorial								
	● ●					Inlet		<b>▲</b>
Design 2x2x2x2 Factorial		Pattern	Tilt	Speed	Load	powder	Y	
▼Model	1		-1	-1	-1	-1	•	
	2	+	-1	-1	-1	1	•	
	3	+-	-1	-1	1	-1	•	
	4	++	-1	-1	1	1	•	
	5	-+	-1	1	-1	-1	•	
💌 Columns (6/0)	6	-+-+	-1	1	-1	1	•	
🆺 Pattern 🖉	7	-++-	-1	1	1	-1	•	
🔺 Tilt 🗶	8	-+++	-1	1	1	1	•	
🚄 Speed 苯 🚄 Load 苯	9	+	1	-1	-1	-1	•	
Inlet powder flow 🗶	10	++	1	-1	-1	1	•	
	11	+-+-	1	-1	1	-1	•	
	12	+-++	1	-1	1	1	•	
	13	++	1	1	-1	-1	•	
	14	++-+	1	1	-1	1	•	
	15	+++-	1	1	1	-1	•	
Rows	16	++++	1	1	1	1	•	
All rows 16	1							
Selected 0								
Excluded 0								
Hidden O								
Labelled 0								
	4							

The mathematical model is:

(Where T is for Tilt, S is for Speed, L is for Load, I is for Inlet powder flow)

$$\begin{split} Y = \mu + T + S + L + I + TS + TL + TI + SL + SI + LI + TSL + TSI + TLI \\ + SLI + TSLI + \epsilon \end{split}$$

(b) Use the same method as in (a)(The table is copied from JMP):

				IIIIet
				Powder
Pattern	Tilt	Speed	Load	Flow
1111	1	1	1	1
1112	1	1	1	2
1113	1	1	1	3
1121	1	1	2	1
1122	1	1	2	2

Inlet

.

The mathematical model is:

(Where T is for Tilt, S is for Speed, L is for Load, I is for Inlet powder flow)

$$\begin{split} Y &= \mu + T + S + L + I + TS + TL + TI + SL + SI + LI + TSL + TSI + TLI \\ &+ SLI + TSLI + T^2 + S^2 + L^2 + I^2 + T^2S + TS^2 + T^2S^2 + T^2L + TL^2 + T^2L^2 \\ &+ T^2I + TI^2 + T^2I^2 + S^2L + SL + SL^2 + S^2I + SI^2 + S^2I^2 + L^2I + LI^2 + L^2I^2 \\ &+ T^2SL + TS^2L + TSL^2 + T^2S^2L + T^2SL^2 + TS^2L^2 + T^2S^2L^2 + T^2SI + TS^2I \\ &+ TSI^2 + T^2S^2I + TS^2I^2 + T^2SI^2 + T^2S^2I^2 + T^2LI + TLI^2 + TLI^2 + T^2L^2I + \\ &+ T^2LI^2 + TL^2I^2 + T^2L^2I^2 + S^2LI + SLI^2 + S^2L^2I + S^2LI^2 + SL^2I^2 + \\ &+ S^2L^2I^2 + T^2SLI + TS^2LI + TSL^2I + TSLI^2 + T^2S^2LI + T^2SL^2I + T^2SLI^2 + \\ &+ TS^2L^2I + TS^2LI^2 + TSL^2I^2 + T^2S^2L^2I + T^2S^2LI^2 + T^2SL^2I + \\ &+ TS^2L^2I + TS^2LI^2 + TSL^2I^2 + T^2S^2L^2I + T^2S^2LI^2 + T^2SL^2I^2 + \\ &+ TS^2L^2I + TS^2LI^2 + TSL^2I^2 + T^2S^2L^2I + T^2S^2LI^2 + T^2SL^2I^2 + \\ &+ TS^2L^2I^2 + TS^2LI^2 + TSL^2I^2 + T^2S^2L^2I + T^2S^2LI^2 + \\ &+ TS^2L^2I^2 + TS^2LI^2 + TSL^2I^2 + T^2S^2L^2I + T^2S^2LI^2 + \\ &+ TS^2L^2I^2 + TS^2LI^2 + \\ &+ TS^2L^2I^2 + TS^2LI^2 + \\ &+ TS^2L^2I^2 + \\ &+ TS^2LI^2 + \\ &+ T$$

(c) Use the same method as in (a) (The table is copied from JMP):

Inlat

				Inlet
				Powder
Pattern	Tilt	Speed	Load	Flow
-11-	-1	1	1	-1
-11+	-1	1	1	1
-12-	-1	1	2	-1
-12+	-1	1	2	1
-13-	-1	1	3	-1
–13+	-1	1	3	1
-14-	-1	1	4	-1
-14+	-1	1	4	1
-21-	-1	2	1	-1
-21+	-1	2	1	1
-22-	-1	2	2	-1
-22+	-1	2	2	1
-23-	-1	2	3	-1
-23+	-1	2	3	1
-24-	-1	2	4	-1
-24+	-1	2	4	1
-31-	-1	3	1	-1
-31+	-1	3	1	1
-32-	-1	3	2	-1
-32+	-1	3	2	1

-33-	-1	3	3	-1
-33- -33+	-1	3	3	1
-34-	-1	3	4	-1
-34+	-1	3	4	1
-34- -34+ +11- +11+ +12- +12+ +13- +13+	-1 -1 -1 1 1	1	1	-1
+11+	1	1	1	1
+12–	1	1	2	-1
+12+	1	1	2	1
+13–	1 1	1	3	-1
+13+	1	1	3	1
+14- +14+ +21- +21+ +22-	1	1	4	-1
+14+	1 1	1	4	1
+21–		2	1	-1
+21+	1 1 1	2	1	1
+22–	1	2	2	-1
+22+	1	2	2	1
+22+ +23- +23+ +24- +24+ +31- +31+ +32-	1	2	3	-1
+23+	1	2	3	1
+24–	1 1 1	2	4	-1
+24+	1	2	4	1
+31–	1	3	1	-1
+31+	1 1	3	1	1
+32–	1	3	2	-1
+32+	1 1	3	2	1
+32+ +33–	1	3	3	-1
+33+	1	3 3 3 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2 3 3 3 3	3 3 4 4 1 1 2 2 3 3 4 4 4 1 2 2 3 3 4 4 4 1 2 2 3 3 4 4 4 1 1 2 2 3 3 4 4 4 1 1 2 2 3 3 4 4 4 1 1 2 2 3 3 4 4 4 1 1 2 2 3 3 4 4 4 1 1 2 2 3 3 4 4 4 1 1 2 2 3 3 4 4 4 1 1 2 2 3 3 4 4 4 1 1 2 2 3 3 4 4 4 1 1 2 2 3 3 4 4 4 1 1 2 2 3 3 4 4 4 1 1 2 2 3 3 4 4 4 1 1 2 2 3 3 4 4 4 1 1 2 2 3 3 4 4 4 1 2 3 3 4 4 4 1 1 2 2 3 3 3 4 4 4 1 1 2 2 3 3 4 4 4 1 2 3 3 3 4 4 4 1 2 3 3 3 4 4 4 3 3 3 4 4 4 3 3 3 4 4 4 3 3 3 4 4 3 3 3 4 4 4 3 3 3 3 4 4 3 3 3 3 4 4 3 3 3 3 3 4 4 3 3 3 3 3 4 4 3 3 3 3 3 3 3 4 4 3	-1 1 -1 1 -1 1 -1 1 -1 1 -1 1 -1 1 -1
+34–	1 1 1	3	4	-1
+33+ +34– +34+	1	3	4	1

The mathematical model is:

(Where T is for Tilt, S is for Speed, L is for Load, I is for Inlet powder flow)

$$\begin{split} Y &= \mu + T + S + L + I + TS + TL + TI + SL + SI + LI + TSL + TSI + TLI \\ &+ SLI + TSLI + S^2 + L^2 + L^3 + TS^2 + TL^2 + TL^3 + S^2L^2 + S^2L^3 + S^2I + L^2I \\ &+ L^3I + TS^2L + TSL^2 + TSL^3 + TS^2L^2 + TS^2L^3 + TS^2I + TL^2I + TL^3I + \\ S^2LI + SL^2I + SL^3I + S^2L^2I + S^2L^3I + TS^2LI + TSL^2I + TSL^3I + TS^2L^2I + \\ TSL^3I + \epsilon \end{split}$$

(2) Replication provides the estimate of pure error. Randomization is necessary for conclusions drawn from the experiment to be correct, unambiguous and defensible. Randomization eliminates the batch effects. Blocking may show the batch effects.

## **Fractional Factorial Experiments with two levels**

11. In the investigation of the conditions of filtration during the preparation of an API, the objective was to improve the quality of the product. Four factors were examined:

- A. Concentration of liquor when filtered (concentrated v. dilute)
- B. Effect of Liquor Storage (fresh vs old). The liquor was either filtered immediately or kept a week before filtration.
- C. Presence or absence of an anti-frothing agent.
- D. Temperature of Filtration (high vs low)

It was considered unlikely that large interactions would exist between these factors so that a  $\frac{1}{2}$  replicate of a 2<sup>4</sup> factorial was selected with defining contrast D=ABC. The purity of the product was recorded in the table below:

Run No	А	В	С	D	Purity
1	-1	-1	-1	-1	107
2	1	-1	-1	+1	114
3	-1	1	-1	1	122
4	+1	+1	-1	-1	130
5	-1	-1	1	1	106
6	1	-1	+1	-1	121
7	-1	+1	+1	-1	120
8	1	1	1	1	132

Determine:

- (1) The pattern of aliases for the experiment.
- (2) The main effects and interactions
- (3) If the error in the measurements is 2 units, which factors are significant?

Solution"

(1) A= BCD, B=ACD, C=ABD, D=ABC.

and

AB=CD, AC=BD, AD=BC

#### (2) Input the data in the JMP:

🛗 problem 11							×
♥problem 11	•						-
Design Custom Design		A	В	C	D	Purity	_
Criterion D Optimal	1	-1	-1	-1	-1	107	_
▼Model	2	1	-1	-1	+1	114	
	3	-1	1	-1	1	122	
💌 Columns (5/0)	4	1	1	-1	-1	130	
ња 🛪	5	-1	-1	1	1	106	
🔥 в 🗱	6	1	-1	1	-1	121	
<b>止</b> ∈ <b>*</b>	7	-1	1	1	-1	120	
<b>ii.</b> D <b>*</b>	8	1	1	1	1	132	
🚄 Purity 米							
Rows							
All rows 8 🔺							
Selected 0							
Excluded 0							- <b>-</b>
	•					•	

Run "Fit Model" in "Analyze" with main effects A, B, C and interactions AB, AC and ABC as factors:

ľ	▼Summar	y of I	Fit					
	RSquare			0.992	2991			
	RSquare Ad	lj		0.950	)935			
	Root Mean :	Square	Error	2.12	2132			
	Mean of Re:	sponse			119			
	Observation	ns (or S	ium Wgts)		8			
ľ	Analysis	s of V	ariance	1				
	Source	DF	Sum of S	quares	Mean 9	Square		F Ratio
	Model	6	637.	50000	10	6.250	2	3.6111
	Error	1	4.	50000		4.500	P	rob > F
	C. Total	- 7	642.	.00000			0	.1562
Ì	Parame	ter Es	stimate	5				
	Term		Estir	mate	Std Erro	r tRa	tio	Prob> t
	Intercept			119	0.75	5 158.0	67	0.0040*
	A[-1]		-	5.25	0.75	5 -7.0	00	0.0903
	B[-1]			-7	0.75	5 -9.3	33	0.0680
	⊂[-1]		-	0.75	0.75	5 -1.0	00	0.5000
	A[-1]*B[-1]		-	0.25	0.75	5 -0.3	33	0.7952
	A[-1]*⊂[-1]			1.5	0.75	5 2.0	00	0.2952
	A[-1]*B[-1]	*C[-1]		0.5	0.75	5 0.0	67	0.6257

(3) Calculate the Z statistic and check the Z value as:

Term	Estimate	error	Z statistic	Prob> Z			
А	-5.25	2	-2.625	0.0087			
В	-7	2	-3.5	0.0005			
С	-0.75	2	-0.375	0.7077			
AB	-0.25	2	-0.125	0.9005			
AC	1.5	2	0.75	0.4533			
ABC	0.5	2	0.25	0.8026			

Main effects A and B are significant at .05 level.

12. O.L. Davies. The following experiment was conducted in a batch reactor (Scenario 1) to investigate conditions affecting the yield of an API. Five factors were investigated with the following levels:

Factors	Le	vel
A A/B Feed ratio	Low	High
B Amount of Liquid Catalyst	Concentrated	Dilute
C Amount of Anti-foaming agent	None	Some
D Time of Reaction	Short	Fast
E Agitation	Slow	Fast

Setting the signs of D=-AE and C=+AB, the following Percent Yield data were obtained (the analysis for each run was repeated)

Run No	A	В	С	D	Е	Yield
1	-1	-1	+1	-1	-1	53.1,54.6
2	+1	-1	-1	+1	-1	49.3,48.4
3	-1	+1	-1	-1	-1	50.1,51.4
4	+1	+1	+1	+1	-1	68.3,67.4
5	-1	-1	+1	+1	+1	73.4,75.3
6	+1	-1	-1	-1	+1	79.7,78.0
7	-1	+1	-1	+1	+1	84.5,86.4
8	+1	+1	+1	-1	+1	81.3,80.4

Design of Experiment and Product Yield

(1) What are the defining contrasts?

(2) Determine the pattern of aliases.

(3) What are the significant main effects and interactions?

(4) Is there a significant lack of fit?

(5) Based on this data what is the optimal way to run the reaction?

Solution:

The defining contrasts are:

$$I = -ADE = ABC = -BCDE$$

$$(2) A = -DE = BC = -ABCDE$$
$$B = -ABDE = AC = -CDE$$
$$C = -ACDE = AB = -BDE$$
$$D = -AE = ABCD = -BCE$$
$$E = -AD = ABCE = -BCD$$
$$BD = -ABE = ACD = -CE$$
$$BE = -ABD = ACE = -CD$$

(3)

(a) Input the data in the JMP:

🛗 problem 12								
♥ problem 12	•							
Design Custom Design		A	В	С	D	E	Yield	_
Criterion D Optimal		-1	-1	1	-1	-1	53.1	_
▼Model	2	-1	-1	1	-1	-1	54.6	_
	3	1	-1	-1	1	-1	49.3	
	4	1	-1	-1	1	-1	48.4	
Columns (6/0)	5	-1	1	-1	-1	-1	50.1	
<b>L</b> A <b>*</b>	6	-1	1	-1	-1	-1	51.4	
🔥 в 🗱	7	1	1	1	1	-1	68.3	
<b>L</b> c*	8	1	1	1	1	-1	67.4	_
<b>ii.</b> D 🛠	9	-1	-1	1	1	1	73.4	_
<b>L E *</b>	10	-1	-1	1	1	1	75.3	_
🚄 Yield 苯	11	1	-1	-1	-1	1	79.7	-
	12	1	-1	-1	-1	1	78	-
Rows	13	-1	1	-1	1	1	84.5	-
All rows 16	14	-1	1	-1	1	1	86.4	
Selected 0	15	1	1	1	-1	1	81.3	
Excluded 0	16	1	1	1	-1	1	80.4	
Hidden 0								•
Labelled 0	•						Þ	

(b) Input the response and the factors:

🔝 Report: Fit Model				
▼ Model Specificatio	n			
Select Columns	Pick Role Variables          Y       Yield         optional       Optional         Weight       optional Numeric         Freq       optional Numeric         By       optional         Construct Model Effects       A         Add       A         Cross       D         Nest       E         B*D       B*E         Degree       2         Attributes       Transform	Personality: Emphasis: Help Remove	Standard Least Squa Effect Screening Run Model	ares V
	No Intercept			

#### (c) Run the model:

Summary of	f Fit						
RSquare		0.997	244				
RSquare Adj		0.994	833				
Root Mean Squar	re Error	1.014	889				
Mean of Respons	;e	6	7.6				
Observations (or	Sum Wgts	)	16				
Analysis of	Variance	e					
Source DF	Sum of S	5quares	Mea	an Squa	re	F Ra	atio
Model 7	298	31.8400		425.9	77	413.5	700
Error 8	}	8.2400		1.0	30	Prob	> F
C. Total 15	5 299	90.0800				<.00	D1*
Parameter I	Estimate	es					
Term	Estimate	Std Erro	or	t Ratio	Pr	ob> t	
Intercept	67.6	0.25372	22 3	266.43	<	.0001*	
A[-1]	-1.5	0.25372	22	-5.91	0	.0004*	
B[-1]	-3.625	0.25372	22	-14.29	<	.0001*	
⊂[-1]	-1.625	0.25372	22	-6.40	0	.0002*	
D[-1]	-1.525			-6.01		.0003*	
E[-1]	-12.275			-48.38		.0001*	
B[-1]*D[-1]	3.9			15.37		.0001*	
B[-1]*E[-1]	-0.35	0.25372	22	-1.38	0	.2051	

All the main effects are significant on the .05 level. BD interaction is also significant on the .05 level.

(4) Remove BE interaction, run the model again:

▼ Summary	y of Fit							
RSquare			0.996	589				
RSquare Adj			0.994	315				
Root Mean S		ror	1.064	581				
Mean of Res	•			57.6				
Observations	•	) Wats	) -	16				
Analysis								
Source	DF S	um of S	õquares	Mea	an Squa	re	F Rati	io
Model	6	297	79.8800		496.6	47 43	8.217	6
Error	9	1	0.2000		1.1	33 PI	rob >	F
C. Total	15	299	90.0800			<	.0001	*
Lack Of F	īt							
Source	DF	Sumo	of Square	s M	Mean Sc	uare	FR	tatio
Lack Of Fit	1		1.96000	0	1.9	6000	1.9	9029
Pure Error	8		8.24000	0	1.0	3000	Prob	> F
Total Error	9	:	10.20000	0			0.20	)51
							Max I	RSq
							0.9	972
Paramet	er Esti	mate	es					
Term	Est	imate	Std Err	or	t Ratio	Prob:	>ltl	
Intercept		67.6	0.26614	<del>1</del> 5 2	254.00	<.00		
A[-1]		-1.5	0.26614	<del>1</del> 5	-5.64	0.00	03*	
B[-1]	-:	3.625	0.26614	<del>1</del> 5	-13.62	<.00	01*	
⊂[-1]	-	1.625	0.26614	<del>1</del> 5	-6.11	0.00	02*	
D[-1]	-	1.525	0.26614	<del>1</del> 5	-5.73	0.00	03*	
E[-1]	-13	2.275	0.26614	<del>1</del> 5	-46.12	<.00	01*	
B[-1]*D[-1]		3.9	0.26614	<del>1</del> 5	14.65	<.00	01*	

There is no significant lack of fit on the .05 level.

(5) To maximize the yield, all the main effects should be run on the low level.

13. In the batch reaction API yield study described in scenario 1, it was decided to make a series of runs including temperate as well as the other five factors. Based on their previous success they were allowed to conduct 16 runs.

(1) Design a fractional factorial experiment which is a <sup>1</sup>/<sub>4</sub> fraction of a  $2^6$  full factorial experiment which maximizes the probability of testing for the significant of main effect and two factor interactions.

(2) What are the defining contrasts and pattern of aliases for this design.

(3) List the considerations in deciding which fraction to run.

Solution:

Run	А	В	С	D	E=ABC	F=BCD
1	-	-	-	-	-	-
2	+		_		+	
3	-	+	_		+	+
4	+	+	_			+
5	-	-	+		+	+
6	+		+		_	+
7	_	+	+		_	
8	+	+	+		+	_
9		т		-		-
	-	-	-	+	-	+
10	+	-	-	+	+	+
11	-	+	-	+	+	-
12	+	+	-	+	-	-
13	-	-	+	+	+	-
14	+	-	+	+	-	-
15	-	+	+	+	-	+
16	+	+	+	+	+	+

#### (2) Generators:

E = ABC and F = BCD

The defining contrasts are:

I = ABCE = BCDF = ADEF

The aliases pattern are:

A = BCE = DEF = ABCDF
B = ACE = CDF = ABDEF
C = ABE = BDF = ACDEF
D = BCF = AEF = ABCDE
E = ABC = ADF = BCDEF
F = BCD = ADE = ABCEF
AB = CE = ACDF = BDEF
AC = BE = ABDF = CDEF
AD = EF = BCDE = ABCF
AE = BC = DF = ABCDEF
AF = DE = BCEF = ABCD
BD = CF = ACDE = ABEF
BF = CD = ACEF = ABDE
ABD = CDE = ACF = BEF
ACD = BDE = ABF = CEF

(3) All fractions have the same extent of confounding between main effects and interactions. Frequently several experiments are already available and it is wise to select for the fraction in which the greatest number of existing experiments has been run. Another consideration is the actual level of the experiments. Run the easiest ones. For example, the run with all the factors at their highest level might be difficult. Carefully go over the potential difficulties before selecting the fraction.

## **Response Surface Modeling and Optimization**

14. An experiment was run in a batch reactor to determine the effect of temperature and reaction time on the yield of the API. These factors are coded as x1= (temperature -300deg)/50deg and x2=(time-10hrs)/5 hours. The following coded data was obtained where the yield is in percent

Run No	X1	X2	Yield (%)
1	-1	0	78.03
2	1	0	80.4
3	0	0	80.1
4	0	0	80.95
5	0	-1	80.3
6	0	1	80.08
7	0	0	80.97
8	-1.4142	-1.4142	74.38
9	-1.4142	1.4142	74.87
10	1.4142	-1.4142	75.68
11	1.4142	1.4142	78.13
12	0	0	80.44

(1) Fit a response surface model to the data. Is the model adequate to describe the data?

(2) Plot the yield response curve. What recommendations would you make about the operating conditions for the reactor?

Solution

(1)

(a) Input the data:

🛗 problem 14					
▼problem 14	• •				<u> </u>
Design Central Composite (	j 💿 🦳	X1	X2	Yield	
▼Model	1	-1	0	78.03	
	2	1	0	80.4	
	3	0	0	80.1	
Columns (3/0)	4	0	0	80.95	
X1 *	5	0	-1	80.3	
▲ X2 ★	6	0	1	80.08	
Vield \star	7	0	0	80.97	
	8	-1.4142	-1.4142	74.38	
	9	-1.4142	1.4142	74.87	
	10	1.4142	-1.4142	75.68	
Rows	11	1.4142	1.4142	78.13	
All rows 12	12	0	0	80.44	
Selected ( Excluded (					
Labelled (					

## (b) Run script in "Model":

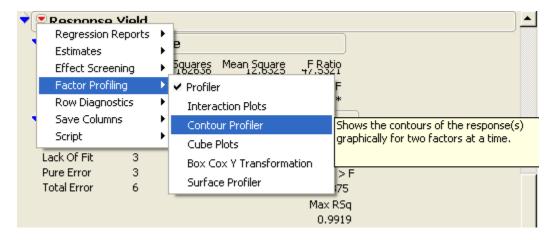
🔡 Report: Fit Model		
Model Specification	n	
Select Columns	Pick Role Variables	Personality: Standard Least Squares 💙
▲ X1 ▲ X2	Y Vield	Emphasis: Effect Screening 🗸
Vield	optionar	
	Weight optional Numeric	Help Run Model
	Freq optional Numeric	
	By optional	Remove
	Construct Model Effects	
	Add X1& RS X2& RS	
	Cross X1*X2	
	Nest V2*V2	
	Macros V	
	Degree 2 Attributes 💌	
	Transform 💌	
	No Intercept	

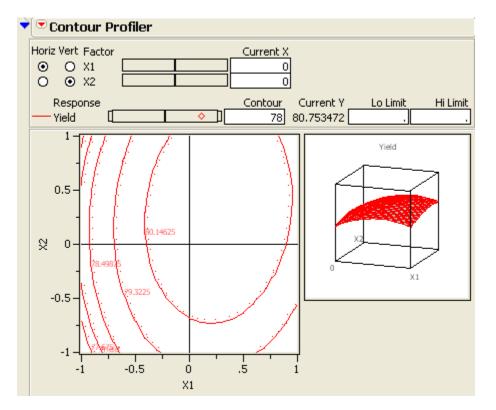
#### (3) Run model:

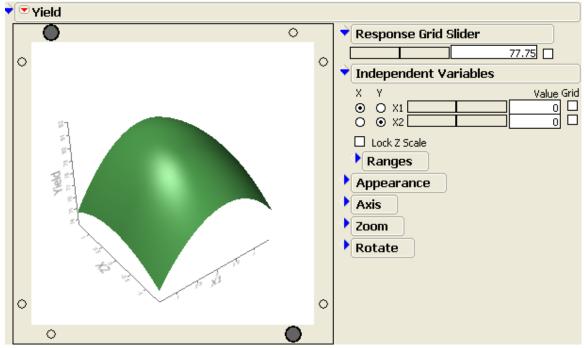
Summary	y of Fit	t						
RSquare			0.975	376				
RSquare Adj			0.954	855				
Root Mean S	quare Ei	rror	0.519	592				
Mean of Resp	ponse		78.69	417				
Observations	s (or Sur	n Wç	gts)	12				
Analysis	of Va	riar	nce					
Source	DF S	ium c	of Squares	Меа	n Sqi	uare	FF	Ratio
Model	5	6			12.8	3325 ·	47.5	5321
	6				0.2	•		) > F
C. Total	11	6	5.782492			•	<.00	001*
Lack Of F	īt							
Source	DF	Su	m of Square	s M	lean	Square		F Ratio
	3			•				2.0329
	-			-	0.3	178033	P	rob > F
Total Error	6		1.619855	7			0	.2875
								ax RSq
							_ (	0.9919
Paramet	er Est	ima	tes					
Term	Estin	nate	Std Error	tΡ	atio	Prob>	t	
Intercept	80.753	472	0.210074	384	1.41	<.000	1*	
<1	0.8818	887	0.164311	5	5.37	0.0013	7*	
				-				
X2*X2	-0.748	102	0.274376	-2	2.73	0.0343	3*	
	RSquare RSquare Adj Root Mean S Mean of Res Observations Analysis Source Model Error C. Total Lack Of Fit Pure Error Total Error	RSquare RSquare Adj Root Mean Square E Mean of Response Observations (or Sur Analysis of Va Source DF S Model 5 Error 6 C. Total 11 Lack Of Fit 3 Pure Error 3 Total Error 6 Parameter Estin Intercept 80.753 X1 0.8818 X2 0.3937 X1*X2 0.2450 X1*X1 -1.723	RSquare Adj Root Mean Square Error Mean of Response Observations (or Sum Wo Analysis of Variar Source DF Sum of Model 5 6 Error 6 C. Total 11 6 Lack Of Fit Source DF Sum Lack Of Fit 3 Pure Error 3 Total Error 6 Parameter Estimate Intercept 80.753472 X1 0.8818887 X2 0.3937808 X1*X2 0.2450047 X1*X1 -1.723102	RSquare         0.9753           RSquare Adj         0.9543           Root Mean Square Error         0.5193           Mean of Response         78.694           Observations (or Sum Wgts)         Analysis of Variance           Source         DF         Sum of Squares           Model         5         64.162636           Error         6         1.619856           C. Total         11         65.782492           Lack Of Fit         3         1.085755           Pure Error         3         0.534100           Total Error         6         1.619855           Parameter Estimates         Intercept         80.753472           Term         Estimate         Std Error           Intercept         80.753472         0.210074           X1         0.8818887         0.164311           X2         0.3937808         0.164311           X1*X1         -1.723102         0.274376	RSquare       0.975376         RSquare Adj       0.954855         Root Mean Square Error       0.519592         Mean of Response       78.69417         Observations (or Sum Wgts)       12         Analysis of Variance         Source       DF         Model       5         6       1.619856         C. Total       11         6       1.619856         C. Total       11         Ack Of Fit       3         Source       DF         Source       DF	RSquare         0.975376           RSquare Adj         0.954855           Root Mean Square Error         0.519592           Mean of Response         78.69417           Observations (or Sum Wgts)         12           Analysis of Variance           Source         DF           Model         5           6         1.619856           C. Total         11           65.782492           Lack Of Fit         3           Source         DF           Sum of Squar	RSquare       0.975376         RSquare Adj       0.954855         Root Mean Square Error       0.519592         Mean of Response       78.69417         Observations (or Sum Wgts)       12         Analysis of Variance         Source       DF         Source       DF	RSquare       0.975376         RSquare Adj       0.954855         Root Mean Square Error       0.519592         Mean of Response       78.69417         Observations (or Sum Wgts)       12         Analysis of Variance         Source       DF Sum of Squares Mean Square         Model       5       64.162636       12.8325         Fror       6       1.619856       0.2700       Prote         C. Total       11       65.782492       <.00

Since the p-value of lack of fit test is large than .05, the model is adequate.

(2) Choose "Contour Profiler" and "Surface Profiler" in "Factor Profiling" by clicking the hot spot aside the "Response Yield":







Response Surface								
Coef								
		X1	X2	Yield				
X1	-1.723	8102	0.2450047	0.8818887				
X2			-0.748102	0.3937808				
⇒ s	▼ Solution							
Va	riable	Criti	cal Value					
×1		0.	2778471					
X2		0.	3086843					
Solution is a Maximum								
Predicted Value at Solution 80.936764								

The solution is a maximum. The maximum will be reached at:

X1=.278, X2 =.309

15. Design a Central Composite Design, a Three Level Factorial Design and a Box Behnken design for generating a response surface for yield in a batch reactor system(Scenario 1) where the effect of temperature, termination time and agitation rate are to be investigated. Compare the features of the three designs in terms of the number of runs required.

Solution

Let X1 = Temperature, X2 = Termination time, X3 = Agitation rate and Y = Yield:

(1) CCD. Choose "Response Surface Design" in "DOE".

OE- Response Surface I	Design			
Response Surface De	sign			
Responses				
Add Response 💉 Remove	e N Responses			
Response Name	Goal	Lower Limit	Upper Limit	Importance
Y	Maximize			
optional item				
Factors				
Add Continuous				
Remove Selected				
Name R	tole	Values		
		-1	1	
<u>⊿</u> X2 (	Iontinuous	-1	1	
sponce Surface Design				
sponse Surface Design Specify Factors				
Specify Factors	rs. Double click on a facto	r name or setting		
	rs. Double click on a facto	r name or setting		
Specify Factors becify desired number of facto	rs. Double click on a facto	r name or setting		
	Response Surface De         Responses         Add Response V         Response Name         Y         optional item         Factors         Add         Continuous         Remove Selected         Name       R         X1       Continuous	Add Response       Remove       N Responses         Response Name       Goal         Y       Maximize         optional item       Goal         Factors       Goal         Add       Continuous         Remove Selected       Name         Name       Role         X1       Continuous	Response Surface Design         Responses         Add Response ♥ Remove       N Responses         Response Name       Goal       Lower Limit         Y       Maximize       .         optional item       Factors       Second       Second         Remove Selected       Role       Values         Name       Role       Values         Image: Name       Role       Values	Response Surface Design         Responses         Add Response       Remove       N Responses         Response Name       Goal       Lower Limit       Upper Limit         Y       Maximize       .       .         optional item       Selected       Values       .         Name       Role       Values       .         X1       Continuous       .       .

Input factors and continue. Choose CCD-Orthogonal:

<b>B</b> D	OE- Resp	ponse Sur	face Design			
Ŷ	Respon	nse Surfa	ce Design			
÷	Respon	ises				
	Add Respo	onse 🖌 🖡	Remove N Responses			
		ponse Name	Goal	Lower Limit	Upper Limit	Importance
	Y		Maximize			
	optional iti	em				
- 🔶	Factors	;				
	Name		Role	Values		
	<b>/</b> X1		Continuous	-1	1	
	<b>4</b> X2		Continuous	-1	1	
	⊿ ХЗ		Continuous	-1	1	
Dev	l spopso Sur	face Design				
	actors	race besign				
	Choose a D	Design				
1	Number Bl	lock Center				
<u> </u>	Of Runs Si	ize Points	Design Type			
	15	3	Box-Behnken			
	16	2	Central Composite Design			
11 -	20	6	CCD-Uniform Precision			
11 -	206 23	6 9	CCD-Orthogonal Blocks			
18 -	23 optional itei	-	CCD-Orthogonal			
	<i>урнопа</i> лсы					
Ĩ	Continue					
	_					
	Back					

Continue. Make the table:

🖩 Central Composite Design								
💌 Central Composite Desig	<ul> <li>▼</li> <li>▼</li> </ul>						<b>▲</b>	
Design Central Composite D		Pattern	X1	X2	Х3	Y		
▼Model	1	000	0	0	0	•		
	2	-++	-1	1	1	•		
	3	+++	1	1	1	•		
	4	000	0	0	0	•		
	5	+	-1	-1	1	•		
	6	0a0	0	-1.6680318	0	•		
Columns (5/0)	7	A00	1.66803177	0	0	•		
🆺 Pattern 🖉	8	000	0	0	0	•		
🔺 X1 🗶	9	0A0	0	1.66803177	0	•		
⊿ x2 <b>米</b> ⊿ x3 <b>米</b>	10	000	0	0	0	•		
⊿ x3 <b>≭</b> ⊿ y <b>≭</b>	11	-+-	-1	1	-1	•		
<b>4</b>   T	12	000	0	0	0	•		
	13	a00	-1.6680318	0	0	•		
	14	+-+	1	-1	1	•		
	15		-1	-1	-1	•		
	16	++-	1	1	-1	•		
Rows	17	000	0	0	0	•		
All rows 23	18	00a	0	0	-1.6680318	•		
Selected 0	19	+	1	-1	-1	•		
Excluded 0	20	000	0	0	0	•		
Hidden 0	21	000	0	0	0	•		
Labelled 0	22	000	0	0	0	•		
	23	00A	0	0	1.66803177	•		
							<b>_</b>	
	4							

# (2) 3 level factorial design

Choose "Full Factorial Design" in "DOE":

	OE- Full Factorial Desi	gn									
<b>)</b>	Full Factorial Design										
- 🔶	Responses										
	Add Response 🖌 Remov	e N Responses									
	Response Name Goal Lower Limit Upper Limit Importance										
	Y optional item	Maximize			<u>.</u>						
	Factors										
	Continuous 🗸 Categoric	al 🗸 Remove									
	Name	Role	Values								
	l Factorial Design										
	Specify Factors										
	dd a Continuous or Categoria n a factor name or level to ea		tton, Double click								
	Continue										

腸 3x3x3 Factorial							
Sx3x3 Factorial	• •						A
Design 3x3x3 Factorial		Pattern	X1	X2	XЗ	Y	
▼Model	1	122	1	2	2	•	
	2	312	3	1	2	•	
	3	113	1	1	3	•	
	4	321	3	2	1	•	
	5	111	1	1	1	•	
	6	133	1	3	3	•	
	7	222	2	2	2	•	
Columns (5/0)	8	332	3	3	2	•	
III. Pattern 🖉	9	333	3	3	3	•	
🖌 X1 🗱	10	212	2	1	2	•	
⊿ X2 苯	11	311	3	1	1	•	
🚄 X3 苯	12	213	2	1	3	•	
🚄 Y 🗶	13	331	3	3	1	•	
	14	323	3	2	3	•	
	15	121	1	2	1	•	
	16	231	2	3	1	•	
	17	223	2	2	3	•	
	18	211	2	1	1	•	
	19	123	1	2	3	•	
Rows	20	233	2	3	3	•	
All rows 27	21	313	3	1	3	•	
Selected 0	22	132	1	3	2	•	
Excluded 0	23	131	1	3	1	•	
Hidden 0	24	221	2	2	1	•	
Labelled 0	25	232	2	3	2	•	
	26	112	1	1	2	•	
	27	322	3	2	2	•	
	•						

### (3) Box- Behnken Design:

🛗 Box-Behnken							
💌 Box-Behnken	• •						
Design Box-Behnken		Pattern	X1	X2	X3	Y	
Model	1	0	-1	-1	0	•	
	2	-+0	-1	1	0	•	
	3	+-0	1	-1	0	•	
	4	++0	1	1	0	•	
	5	0	0	-1	-1	•	
Columns (5/0)	6	0-+	0	-1	1	•	
🆺 Pattern 🖉	7	0+-	0	1	-1	•	
▲ X1 ★	8	0++	0	1	1	•	
⊿ x2 ¥ ⊿ x3 ¥	9	-0-	-1	0	-1	•	
⊿ ∧ 3 ≁ ⊿ Y <b>≭</b>	10	+0-	1	0	-1	•	
- 1 m	11	-0+	-1	0	1	•	
	12	+0+	1	0	1	•	
	13	000	0	0	0	•	
	14	000	0	0	0	•	
	15	000	0	0	0	•	

Compare these three designs, the Box-Behnken has the minimum runs.