Chemical Product Experimentation

Half-Fraction of 2^4 with 4 center points

A	B	C	D=ABC	Purity, Y_1	Yield, Y_2
1.00 (—)	1.0 (—)	1.00 (—)	2.0 (—)	62.1	35.1
2.50 (+)	1.0 (—)	1.00 (—)	5.0 (+)	92.2	45.9
1.00 (—)	1.8 (+)	1.00 (—)	5.0 (+)	7.0	4.0
2.50 (+)	1.8 (+)	1.00 (—)	2.0 (—)	84.0	46.0
1.00 (—)	1.0 (—)	2.50 (+)	5.0 (+)	61.1	41.4
2.50 (+)	1.0 (—)	2.50 (+)	2.0 (—)	91.6	51.2
1.00 (—)	1.8 (+)	2.50 (+)	2.0 (—)	9.0	10.0
2.50 (+)	1.8 (+)	2.50 (+)	5.0 (+)	83.7	52.8
1.75 (0)	1.4 (0)	1.75 (0)	3.5 (0)	87.7	54.7
1.75 (0)	1.4 (0)	1.75 (0)	3.5 (0)	89.8	52.8
1.75 (0)	1.4 (0)	1.75 (0)	3.5 (0)	86.5	53.3
1.75 (0)	1.4 (0)	1.75 (0)	3.5 (0)	87.3	52.0

Yates' Algorithm for Yield, Y_2, first half-fraction.

Trmt. Comb.	Y_2	1	2	3	Estimated Effect	Effect Name
(1)	35.1	81.0	131.0	286.4	35.80	Mean=ABCD
ad	45.9	50.0	155.4	105.4	26.35	A=BCD
bd	4.0	92.6	52.8	–60.8	–15.20	B=ACD
ab	46.0	62.8	52.6	64.2	16.05	AB=CD
cd	41.4	10.8	–31.0	24.4	6.10	C=ABD
ac	51.2	42.0	–29.8	–0.2	–0.05	AC=BD
bc	10.0	9.8	31.2	1.2	0.30	BC=AD
abcd	52.8	42.8	33.0	1.8	0.45	ABC=D

Second Half-Fraction of 2^4

A	B	C	D=–ABC	Purity, Y_1	Yield, Y_2
1.00 (—)	1.0 (—)	1.00 (—)	5.0 (+)	64.0	35.3
2.50 (+)	1.0 (—)	1.00 (—)	2.0 (—)	91.9	47.2
1.00 (—)	1.8 (+)	1.00 (—)	2.0 (—)	6.5	3.9
2.50 (+)	1.8 (+)	1.00 (—)	5.0 (+)	86.4	45.9
1.00 (—)	1.0 (—)	2.50 (+)	2.0 (—)	63.9	39.5
2.50 (+)	1.0 (—)	2.50 (+)	5.0 (+)	93.1	51.6
1.00 (—)	1.8 (+)	2.50 (+)	5.0 (+)	6.8	9.2
2.50 (+)	1.8 (+)	2.50 (+)	2.0 (—)	84.6	54.3

Yates Algorithm for Yield, Y_2: Full Factorial

Trmt. Comb.		1	2	3	4	Estimated Effect	Effect Name
(1)	**35.1**	82.3	132.2	287.2	573.3	35.83125	Mean
a	47.2	49.9	155.0	286.1	216.5	27.0625	A
b	3.9	90.7	131.1	110.2	–121.1	–15.1375	B
ab	**46.0**	64.3	155.0	106.3	127.3	15.9125	AB
c	39.5	81.2	54.2	–58.8	46.7	5.8375	C
ac	**51.2**	49.9	56.0	–62.3	3.1	0.3875	AC
bc	**10.0**	93.0	52.5	62.6	6.3	0.7875	BC
abc	54.3	62.0	53.8	64.7	4.7	0.5875	ABC
d	35.3	12.1	–32.4	22.8	–1.1	–0.1375	D
ad	**45.9**	42.1	–26.4	23.9	–3.9	–0.4875	AD
bd	**4.0**	11.7	–31.3	1.8	–3.5	–0.4375	BD
abd	45.9	44.3	–31.0	1.3	2.1	0.2635	ABD
cd	**41.4**	10.6	30.0	6.0	1.1	0.1375	CD
acd	51.6	41.9	32.6	0.3	–0.5	–0.0625	ACD
bcd	9.2	10.2	31.3	2.6	–5.7	–0.7125	BCD
abcd	**52.8**	43.6	33.4	2.1	–0.5	–0.0625	ABCD

Third phase of experimentation

A	B	C	D=ABC	Purity, Y_1	Yield, Y_2
0.6895	1.4	1.75	3.5	20.8	13.0
2.8105	1.4	1.75	3.5	95.9	54.3
1.75	0.8344	1.75	3.5	99.9	62.4
1.75	1.9656	1.75	3.5	65.9	41.2
1.75	1.4	0.6895	3.5	64.4	32.7
1.75	1.4	2.8105	3.5	64.8	40.3
1.75	1.4	1.75	1.379	88.1	52.7
1.75	1.4	1.75	5.621	88.9	50.5

$$X_1 = \frac{(A-1.75)}{0.75} \qquad X_3 = \frac{(C-1.75)}{0.75}$$

$$X_2 = \frac{(B-1.4)}{0.4} \qquad X_4 = \frac{(D-3.5)}{1.5}$$

Regression Analysis

The prediction equation, using all 28 observations and only significant predictors is:

$$Y\hat{i}eld = 52.45 + 13.75X_1 - 7.55X_2 + 7.96X_1X_2 - 9.10X_1^2 + 2.87X_3 - 7.67X_3^2$$