

STA305/1004-Class 17

March 16, 2017

Today's Class

- ▶ Factorial designs at two levels
- ▶ Cube plots
- ▶ Calculation of factorial effects

Difference between ANOVA and Factorial Designs

In ANOVA the objective is to compare the individual experimental conditions with each other. In a factorial experiment the objective is generally to compare combinations of experimental conditions.

Let's consider the food diary study above. What is the effect of keeping a food diary?

Expt condition	Keep food diary	Increase physical activity	Home visit	weight loss
1	No	No	No	y_1
2	No	No	Yes	y_2
3	No	Yes	No	y_3
4	No	Yes	Yes	y_4
5	Yes	No	No	y_5
6	Yes	No	Yes	y_6
7	Yes	Yes	No	y_7
8	Yes	Yes	Yes	y_8

We can estimate the effect of food diary by comparing the mean of all conditions where food diary is set to NO (conditions 1-4) and mean of all conditions where food diary set to YES (conditions 5-8). This is also called the **main effect** of food diary, the adjective *main* being a reminder that this average is taken over the levels of the other factors.

Difference between ANOVA and Factorial Designs

Expt condition	Keep food diary	Increase physical activity	Home visit	weight loss
1	No	No	No	y_1
2	No	No	Yes	y_2
3	No	Yes	No	y_3
4	No	Yes	Yes	y_4
5	Yes	No	No	y_5
6	Yes	No	Yes	y_6
7	Yes	Yes	No	y_7
8	Yes	Yes	Yes	y_8

The main effect of food diary is:

$$\frac{y_1 + y_2 + y_3 + y_4}{4} - \frac{y_5 + y_6 + y_7 + y_8}{4}.$$

The main effect of physical activity is:

$$\frac{y_1 + y_2 + y_5 + y_6}{4} - \frac{y_3 + y_4 + y_7 + y_8}{4}.$$

The main effect of home visit is:

$$\frac{y_1 + y_3 + y_5 + y_7}{4} - \frac{y_2 + y_4 + y_6 + y_8}{4}.$$

Question

A chemical reaction experiment was carried out with the objective of comparing if a new catalyst B would give higher yields than the old catalyst A. The experiment was run on six different batches of raw material which were known to be quite different from one another.

This is an example of a factorial design.



Respond at **PollEv.com/nathantaback**



Text **NATHANTABACK** to **37607** once to join, then **A or B**

True

A

False

B

Total Results: 0

Figure 1:

Factorial designs at two levels

To perform a factorial design:

1. Select a fixed number of levels of each factor.
2. Run experiments in all possible combinations.

Pilot plant investigation - example of factorial design

A pilot plant investigation employed a 2^3 factorial design (Box, Hunter, and Hunter (2005)) with

Factors	level 1	level 2
Temperature	160C° (-1)	180C° (+1)
Concentration	20% (-1)	40% (+1)
Catalyst	A (-1)	B (+1)

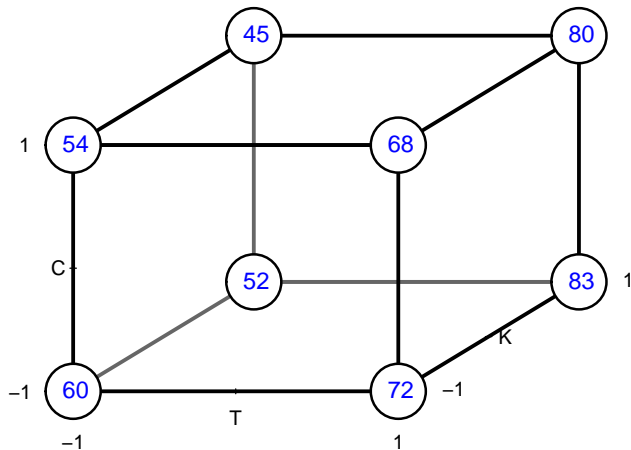
run	T	C	K	y
1	-1	-1	-1	60
2	1	-1	-1	72
3	-1	1	-1	54
4	1	1	-1	68
5	-1	-1	1	52
6	1	-1	1	83
7	-1	1	1	45
8	1	1	1	80

- Each data value recorded is for the response yield y averaged over two duplicate runs.

Cube plots

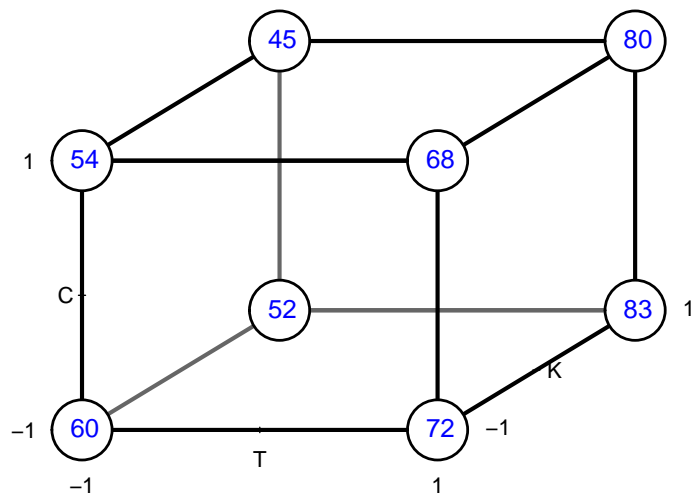
```
library("FrF2")  
bhh54 <- lm(y~T*C*K,data=tab0502)  
cubePlot(bhh54,"T","K","C",main="Cube Plot for Pilot Plant Investigation")
```

Cube Plot for Pilot Plant Investigation



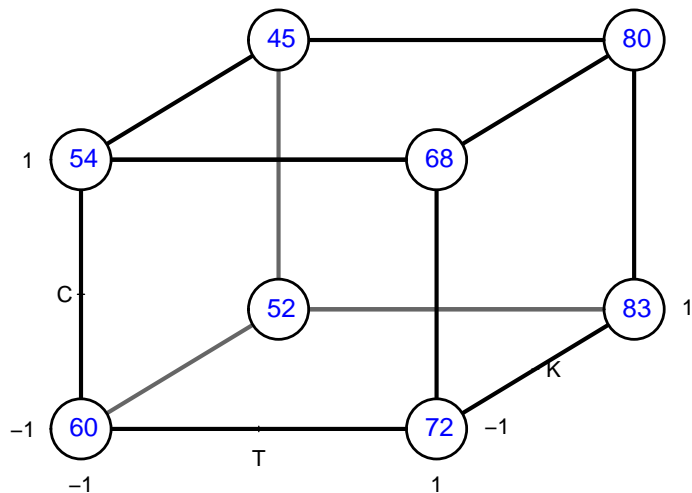
modeled = TRUE

Cube plots



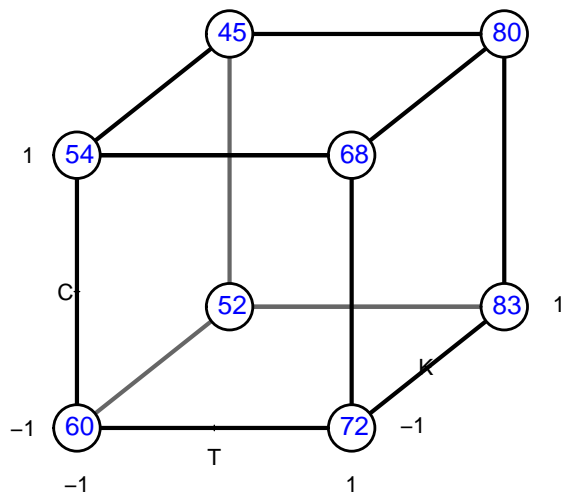
modeled = TRUE

Cube plots



modeled = TRUE

Cube plots



modeled = TRUE

Cube plots

- ▶ 8 run design produces 12 comparisons
- ▶ Each edge of cube only one factor changed while other 2 held constant.
- ▶ Therefore experimenter that believes in only changing one factor at a time is satisfied.

Cube plots

Using the cube plot below the main effects for T, C, K (respectively)
are approximately:

Respond at [PollEv.com/nathantaback](https://poll-ev.com/nathantaback)

Text **NATHANTABACK** to 37607 once to join, then **A, B, or C**

T=2.88; C=3.63; K=0.38

A

T=5.75; C=7.25; K=0.75

B

T=11.5; C=14.5; K=1.5

C

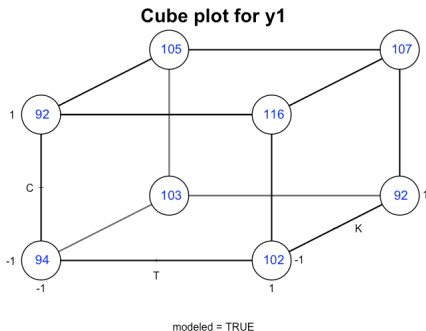


Figure 2:

Interaction effects - two factor interactions

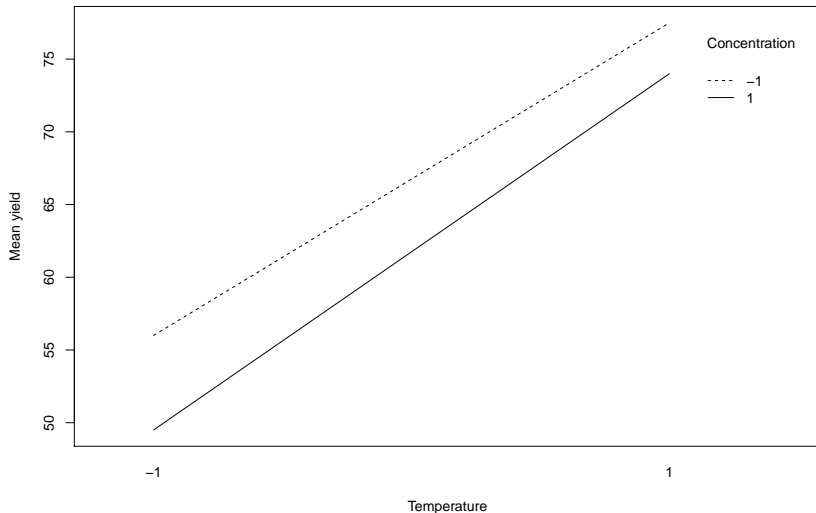
run	T	C	K	y
1	-1	-1	-1	60
2	1	-1	-1	72
3	-1	1	-1	54
4	1	1	-1	68
5	-1	-1	1	52
6	1	-1	1	83
7	-1	1	1	45
8	1	1	1	80

- ▶ When the catalyst K is A the temperature effect is: $\frac{68+72}{2} - \frac{60+54}{2} = 70 - 57 = 13$.
- ▶ When the catalyst K is B the temperature effect is: $\frac{83+80}{2} - \frac{52+45}{2} = 81.5 - 48.5 = 33$.
- ▶ The average difference between these two average differences is called the **interaction** between temperature and catalyst denoted by TK. This is the interaction between the two factors temperature and catalyst - the two factor interaction between temperature and catalyst.

$$TK = \frac{33 - 13}{2} = 10$$

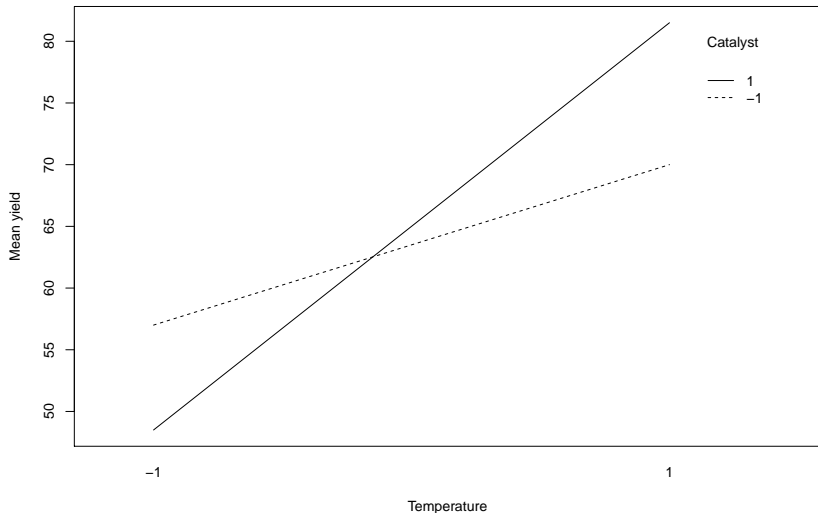
Interaction plots - Concentration by temperature

```
interaction.plot(tab0502$T,tab0502$C,tab0502$y, type="l",  
                xlab="Temperature",trace.label="Concentration",  
                ylab="Mean yield")
```



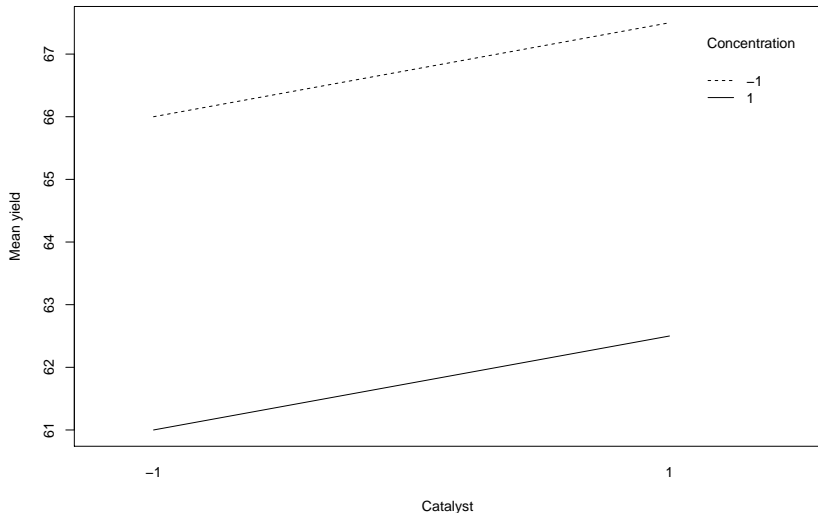
Interaction plots - Temperature by catalyst

```
interaction.plot(tab0502$T,tab0502$K,tab0502$y, type="l",  
                xlab="Temperature",trace.label="Catalyst",  
                ylab="Mean yield")
```



Interaction plots - Concentration by catalyst

```
interaction.plot(tab0502$K,tab0502$C,tab0502$y, type="l",  
                xlab="Catalyst",trace.label="Concentration",  
                ylab="Mean yield")
```



Three factor interactions

run	T	C	K	y
1	-1	-1	-1	60
2	1	-1	-1	72
3	-1	1	-1	54
4	1	1	-1	68
5	-1	-1	1	52
6	1	-1	1	83
7	-1	1	1	45
8	1	1	1	80

The temperature by concentration interaction when the catalyst is B (at it's +1 level) is:

$$\text{Interaction TC} = \frac{(y_8 - y_7) - (y_6 - y_5)}{2} = \frac{(80 - 45) - (83 - 52)}{2} = 2.$$

The temperature by concentration interaction when the catalyst is A (at it's -1 level) is:

$$\text{Interaction TC} = \frac{(y_4 - y_3) - (y_2 - y_1)}{2} = \frac{(68 - 54) - (72 - 60)}{2} = 1.$$

$$\text{TCK} = \frac{2 - 1}{2} = \frac{1}{2}.$$

Three factor interaction

- ▶ Interactions are symmetric in all factors.
- ▶ It could have been defined as half the difference between the temperature-by-catalyst interactions at each of the two concentrations.
- ▶ Mostly rely on statistical software such as R.

Replicate runs

- ▶ Each of the 8 responses in the table is the average of two (genuinely) replicated runs.
- ▶ Genuinely replicated run means that variation between runs made at same experimental conditions is a reflection of the total run-to-run variability.

run	T	C	K	y
1	-1	-1	-1	60
2	1	-1	-1	72
3	-1	1	-1	54
4	1	1	-1	68
5	-1	-1	1	52
6	1	-1	1	83
7	-1	1	1	45
8	1	1	1	80

Replicate runs

- ▶ Randomization of the run order for all 16 runs ensures the replication is genuine.
- ▶ `run1` is order of the first run and `run2` is order of the second run.

run1	run2	T	C	K	y1	y2	diff
6	13	-1	-1	-1	59	61	-2
2	4	1	-1	-1	74	70	4
1	16	-1	1	-1	50	58	-8
5	10	1	1	-1	69	67	2
8	12	-1	-1	1	50	54	-4
9	14	1	-1	1	81	85	-4
3	11	-1	1	1	46	44	2
7	15	1	1	1	79	81	-2

Replicate runs

- ▶ Replication not always feasible or easy.
- ▶ For the pilot plant experiment a run involved: cleaning the reactor; inserting the appropriate catalyst charge; and running the apparatus at a given concentration for 3 hours, and sampling output every 15 minutes.
- ▶ A genuine run involved taking all of these steps all over again!

Replicate runs

- ▶ There are usually better ways to employ 16 independent runs than by fully replicating a 2^3 factorial.
- ▶ Other designs can study four or five factors with a 16 run two-level design.

Estimate of error variance of the effects from replicated runs

run1	run2	T	C	K	y1	y2	diff
6	13	-1	-1	-1	59	61	-2
2	4	1	-1	-1	74	70	4
1	16	-1	1	-1	50	58	-8
5	10	1	1	-1	69	67	2
8	12	-1	-1	1	50	54	-4
9	14	1	-1	1	81	85	-4
3	11	-1	1	1	46	44	2
7	15	1	1	1	79	81	-2

$$s_i^2 = \frac{(y_{i1} - y_{i2})^2}{2},$$

- ▶ y_{i1} is the first outcome from i th run.
- ▶ $\text{diff}_i = (y_{i1} - y_{i2})$.
- ▶ A pooled estimate of σ^2 is

$$s^2 = \frac{\sum_{i=1}^8 s_i^2}{8} = \frac{64}{8} = 8.$$

- ▶ The variance of an effect is:

$$\text{Var}(\text{effect}) = \left(\frac{1}{8} + \frac{1}{8} \right) s^2 = 8/4 = 2$$

Interpretation of results

- ▶ Which effects are real and which can be explained by chance?
- ▶ A rough rule of thumb: any effect that is 2-3 times their standard error are not easily explained by chance alone.

Interpretation of results

- Assume that the observations are independent and normally distributed then

$$\text{effect}/\text{se}(\text{effect}) \sim t_8.$$

- A 95% confidence interval can be calculated as:

$$\text{effect} \pm t_{8,.05/2} \times \text{se}(\text{effect}).$$

where $t_{8,.05/2}$ is the 97.5th percentile of the t_8 . This is obtained in R via the `qt()` function.

```
qt(p = 1-.025,df = 8)
```

```
## [1] 2.306004
```

- In the pilot plant study

$$\text{effect} \pm 2.3 \times 1.4 = \text{effect} \pm 3.2.$$

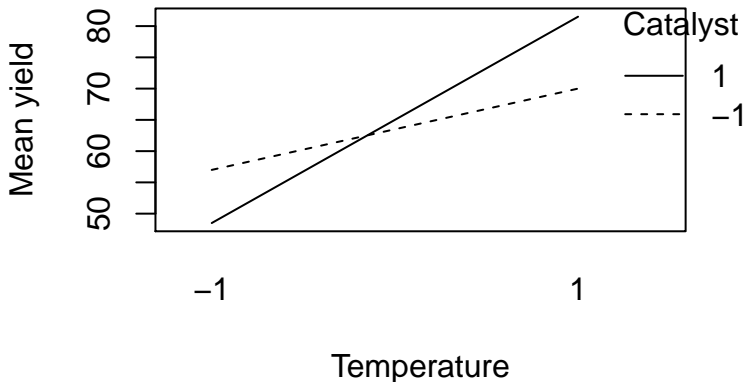
Interpretation of results

- ▶ The main effect of a factor should be individually interpreted only if there is no evidence that the factor interacts with other factors.
- ▶ Which effects should be considered jointly and which independently?

Effects	95% Confidence Interval
T	(19.8, 26.2)
C	(-8.2, -1.8)
K	(-1.7, 4.7)
TC	(-1.7, 4.7)
TK	(6.8, 13.2)
CK	(-3.2, 3.2)
TCK	(-2.7, 3.7)

Interpretation of results

- ▶ The effect of changing concentration over the ranges studied is to reduce yield by about 5 units. This is irrespective of the tested level of other variables.
- ▶ The effects of temperature and catalyst cannot be interpreted separately because of the large TK interaction. With catalyst A the temperature effect is 13 units and with catalyst B it is 33 units.



Linear model for factorial design

Let y_i be the yield from the i^{th} run,

$$x_{i1} = \begin{cases} +1 & \text{if } T = 180 \\ -1 & \text{if } T = 160 \end{cases}$$

$$x_{i2} = \begin{cases} +1 & \text{if } C = 40 \\ -1 & \text{if } C = 20 \end{cases}$$

$$x_{i3} = \begin{cases} +1 & \text{if } K = B \\ -1 & \text{if } K = A \end{cases}$$

A linear model for a 2^3 factorial design is:

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \beta_4 x_{i1} x_{i2} + \beta_5 x_{i1} x_{i3} + \beta_6 x_{i2} x_{i3} + \beta_7 x_{i1} x_{i2} x_{i3} + \epsilon_i.$$

The variables $x_{i1}x_{i2}$ is the interaction between temperature and concentration, $x_{i1}x_{i3}$ is the interaction between temperature and catalyst, etc.

Linear model for factorial design

The table of contrasts for a 2^3 design is the design matrix X from the linear model above.

Mean	T	K	C	T:K	T:C	K:C	T:K:C	yield average
1	-1	-1	-1	1	1	1	-1	60
1	1	-1	-1	-1	-1	1	1	72
1	-1	-1	1	1	-1	-1	1	54
1	1	-1	1	-1	1	-1	-1	68
1	-1	1	-1	-1	1	-1	1	52
1	1	1	-1	1	-1	-1	-1	83
1	-1	1	1	-1	-1	1	-1	45
1	1	1	1	1	1	1	1	80

- ▶ All factorial effects can be calculated from this table.
- ▶ Signs for interaction contrasts obtained by multiplying signs of their respective factors.
- ▶ Each column perfectly balanced with respect to other columns.
- ▶ Balanced (orthogonal) design ensures each estimated effect is unaffected by magnitude and signs of other effects.
- ▶ Table of signs obtained similarly for any 2^k factorial design.

Linear model for factorial design

What is the table of contrasts for a 2^4 factorial design?

Linear model for factorial design - calculating factorial effects from parameter estimates

The parameter estimates are obtained via the `lm()` function in R.

- ▶ Estimated least squares coefficients are one-half the factorial estimates.
- ▶ Therefore, the factorial estimates are twice the least squares coefficients.

$$\hat{\beta}_1 = 11.50 \Rightarrow T = 2 \times 11.50 = 23.26$$

$$\hat{\beta}_2 = 0.75 \Rightarrow K = 2 \times 0.75 = 1.5$$

$$\hat{\beta}_4 = 5.00 \Rightarrow TK = 2 \times 5.00 = 10.00$$

```
fact.mod <-lm(y~T*K*C,data=tab0502)
round(summary(fact.mod)$coefficients,2)
```

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	64.25	NaN	NaN	NaN
T	11.50	NaN	NaN	NaN
K	0.75	NaN	NaN	NaN
C	-2.50	NaN	NaN	NaN
T:K	5.00	NaN	NaN	NaN
T:C	0.75	NaN	NaN	NaN
K:C	0.00	NaN	NaN	NaN
T:K:C	0.25	NaN	NaN	NaN

Linear model for factorial design - significance testing

- ▶ When there are replicated runs we also obtain p-values and confidence intervals for the factorial effects from the regression model.
- ▶ For example, the p-value for β_1 corresponds to the factorial effect for temperature

$$H_0 : \beta_1 = 0 \text{ vs. } H_1 : \beta_1 \neq 0.$$

If the null hypothesis is true then $\beta_1 = 0 \Rightarrow T = 0 \Rightarrow \mu_{T+} - \mu_{T-} = 0 \Rightarrow \mu_{T+} = \mu_{T-}$.

- ▶ μ_{T+} is the mean yield when the temperature is set at 180° and μ_{T-} is the mean yield when the temperature is set to 160° .

Linear model for factorial design - significance testing

To obtain 95% confidence intervals for the factorial effects we multiply the 95% confidence intervals for the regression parameters by 2. This is easily done in R using the function `confint.lm()`.

```
fact.mod <-lm(y~T*K*C,data=tab0503)
round(2*confint.lm(fact.mod),2)
```

	2.5 %	97.5 %
(Intercept)	125.24	131.76
T	19.74	26.26
K	-1.76	4.76
C	-8.26	-1.74
T:K	6.74	13.26
T:C	-1.76	4.76
K:C	-3.26	3.26
T:K:C	-2.76	3.76

Advantages of factorial designs over one-factor-at-a-time designs

- ▶ Suppose that one factor at a time was investigated. For example, temperature is investigated while holding concentration at 20% (-1) and catalyst at B (+1).
- ▶ In order for the effect to have more general relevance it would be necessary for the effect to be the same at all the other levels of concentration and catalyst.
- ▶ In other words there is no interaction between factors (e.g., temperature and catalyst).
- ▶ If the effect is the same then a factorial design is more efficient since the estimates of the effects require fewer observations to achieve the same precision.
- ▶ If the effect is different at other levels of concentration and catalyst then the factorial can detect and estimate interactions.