

## Tutorial 0: Excel Use

Provide an Excel workbook file and its PDF version.

Provided: The present statement, and a PDF version of the Excel workbook solution

EPFL-MD-2018

With the help of PDF Excel workbook solution, redo and produce your own Excel workbook:

- Use one Excel sheet per exercise (solutions in light green)
- By convention, gray cells are values typed and entered... Except text, all the remainder in worksheet is Excel formula cells
- By convention, when using use Naming of cells (typically kinetic parameters or constants, use yellow color)

Note: One Excel Sheet per exercise!

### 0.1 Redo this tutorial Excel System of Linear Equations (2)

<http://www.excel-easy.com/examples/system-of-linear-equations.html>.

Finally provide the equation system solution table like:

			x	y	z	
		(Known)	4	2	3	Check
$5x + 1y + 8z = 46$		46	5	1	8	46
$4x - 2y = 12$		12	4	-2	0	12
$6x + 7y + 4z = 50$		50	6	7	4	50

Using Excel formula: =TRANSPOSE(MMULT(MINVERSE(N28:P30);Q28:Q30))

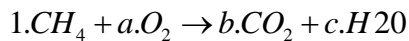
Hint: Excel Matrix formula French equivalent:

English	French
MMULT( )	PRODUIT.MAT( )
MINVERSE( )	INVERSEMAT( )
SLOPE( )	PENTE( )
INTERCEP( )	ORDONNEE.ORIGINE( )
RSQ( )	COEFFICIENT.DETERMINATION( )

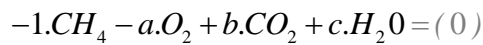
### 0.2 Use this solving method to solve CH4 combustion reaction (2)

Considering the combustion or catabolic reaction from methane .

Primary equation:



or



To solve this reaction equation, considering the atomic (C, H and O) balances, it becomes a 3 unknowns equation system:

$$\text{C Balance: } 0.a + 1.b + 0.c = 1$$

$$\text{H Balance: } 0.a + 0.b + 2.c = 4$$

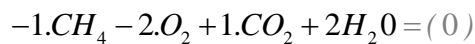
$$\text{O Balance: } 2.a + 2.b + 1.c = 0$$

Use Excel solve the equation system with  $X = A^{-1}B$ , like:

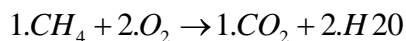
	CH4		O2	CO2	H2O	
	-1	-(Known)	-2	1	2	Check
C Balance	1	1	0	1	0	1
H Balance	4	4	0	0	2	4
O Balance	0	0	2	2	1	0

By using this formula: =TRANSPOSE(MMULT(MINVERSE(C30:E32);F30:F32)), to compute a, b and c (green cells)

Thus, get the solved catabolic ultimate reaction equation:



or



### **0.3 Use of Excel for Linear Functions of Formula and Excel Solver (2+2+2)**

From this data set provided, you will use 3:

- a) **You will first use Excel SLOPE (.) and INTERCEPT (.) functions for a linear estimation of Yobs vs X**

Then produce data of estimated values of Y, YCalc:

From this, you will produce a plot of this date according the one from PDF solution (same in details of the one in the PDF Excel workbook solution).

- b) **Then you will provide a linear estimation of Yobs vs X using the very useful Excel SOLVER Add-In**

First, you will have to install in Excel (from OPTIONS Tab of FILE menu, choose ADD-INS Tab, and then choose “**Solver Add-in**”). Then you can use it, from the DATA menu, **Analyse** sub-menu, **Solver**...

Build a table, with observed Y values and calculates Y based on 2 parameter cells (standing for slope an intercept guesses), and compute the sum of the square errors between observed and calculated Y. Then, you will use the Excel Solver to minimize the value of the Sum of the Square errors cell, by manipulating the 2 slope an intercept guess cells with the Solver.

Use the PDF Excel workbook Solution to build the computation of the linear estimation of this data set, by the minimization of the sum of the square errors of calculated Y (from X) calculated from a linear function  $Y = A \cdot X + B$  cell, using other two cells, standing respectively, for A and B.

**c) Plot comparison of this 2 linear estimation (Excel Linear Functions and Excel Solver ( 2 Y scatter plot of the square errors**

Then as a training for Excel plot use, you will provide a plot (like in details of the one in the PDF Excel workbook solution), which shows on a double Y scatter plot, the 2 linear estimations calculated Ycalc and square errors of the two Ycalc estimation fo YObs

X	Yobs
[hr <sup>-1</sup> ]	[mol/L] <sup>-1</sup> ]
1.6667	10.0000
1.1111	5.0000
0.5556	3.3333
0.4348	2.5000
0.4000	2.0000
0.3704	1.0000
0.3571	0.5000
0.3448	0.3333
0.3413	0.2500
0.3373	0.2500
0.3401	0.2000
0.3390	0.1667
0.3378	0.1429
0.3378	0.1250

**0.4 Ordinary Least Square estimation using Excel Matrix formula regression (2)**

On the same data set, you will build a linear estimation of Yobs vs X, using the matrix formulation to obtaine an Ordinary Least Square estimation by:

$$y = X\beta + u$$

$$\hat{\beta} = (X^T X)^{-1} X^T y$$

[https://en.wikipedia.org/wiki/Ordinary\\_least\\_squares](https://en.wikipedia.org/wiki/Ordinary_least_squares)

Using PDF Excel workbook Solution, build this estimation using Excel matrix functions with CTRL+SHIFT+ENTER.

**0.5 Use of Excel Multilinear Regression Tool (2)**

First, you will have installed (in Excel from OPTIONS Tab of FILE menu, choose ADD-INS Tab, and then choose “**Analysis Tool Pak**”). Then you can use it, from the DATA menu, **Analyse** sub-menu, **Data Analysis**...

Use this Multilinear regression tool, to perform a linear regression on the (X, Yobs) proposed dataset.

**0.6 Comparison of the 4 linear estimations (3)**

Then with this 4 linear estimations, providing 4 slopes and 4 intercepts from the same data set, you will provide the comparison of this estimation by comparing them to their average.

Use the PDF Excel workbook solution.

You will also provide a plot for this comparison (same as the one of the PDF solution).

Your comment?