

Download SIMCA software

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SIMCA 13.0.3 Product download included the installation instruction

Download the appropriate (32- or 64-bit version) file from our web page under column Older versions <http://umetrics.com/downloads/simca>

User Information:

Password to unzip the SIMCA 13.0.3 download: ExploreAnalyzeInterpret

Local Activation Key: IWRUL-OB1Z2-RYPD9-G0T84

Background information

Drying process after wet granulation

Data are from 13 batches

One quality attribute – Moisture as Y

6 parameters – time, bed temp, wet mass, added water, inlet temp, inlet air flowrate

Exp. No.	moisture content (%)	Time (sec)	Bed Temperature (degC)	wet Weight (g)	Added Water	Inlet temperature (degC)	Inlet flowrate (m3/hr)
1	1.75	874	49.1	784	143	53	70
2	2.30	671	49.7	784	143	55	80
3	1.82	726	49	628	115	53	70
4	1.93	887	49.4	941	172	53	80
5	2.51	511	49.7	784	143	80	40
6	2.29	805	49.4	784	143	60	40
7	2.27	581	60.1	784	143	70	60
8	2.07	872	48.2	784	143	53	55
9	3.20	676	50.1	784	143	60	60
10	1.97	900	50.1	628	115	53	70
11	2.1	794	48.6	784	143	53	70
12	1.85	905	49.2	628	115	53	60
13	1.97	901	50.1	784	143	53	70

What we will do

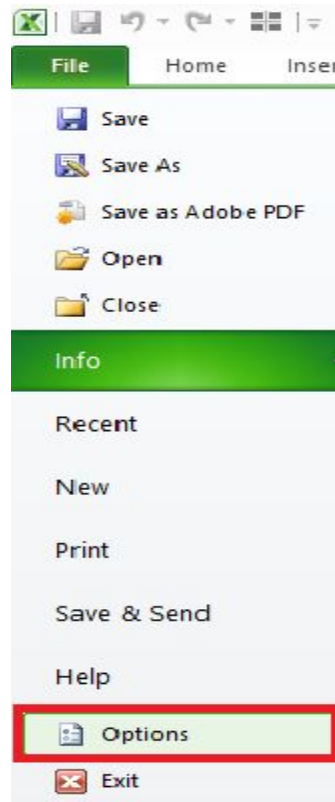
- Try to find the correlation between dependent variable and independent variables
 - Y with one X
 - Y with two Xs
 - Y with three Xs
 - Y with four Xs
 - Y with all 6 Xs

Multivariable Regression

- **Multivariable regression enables you to relate one dependent variable to multiple independent variables you've derived from measurements. This type of data analysis helps you search for the effects of your observed data on a related condition or predict a condition based on other related observations.**

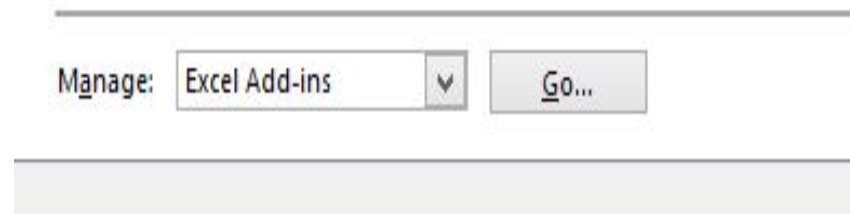
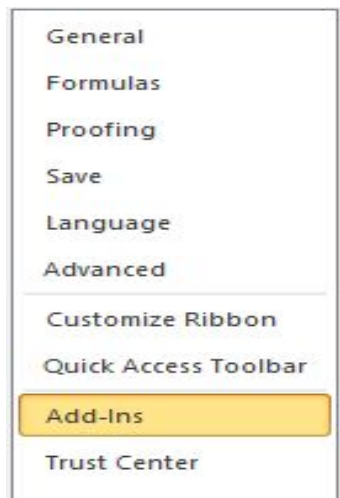
Step 1

- Launch Microsoft Excel and click on the "File" tab in the ribbon. Select "Options" to open the Excel Options dialog box.



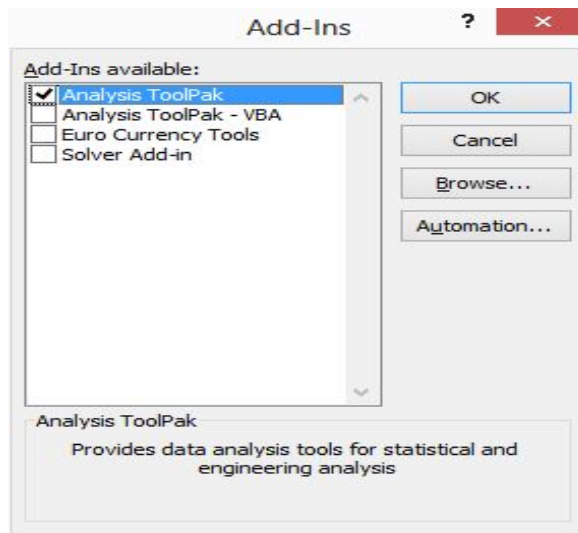
Step 2

- Click the "Add-Ins" item in the list on the left side of the dialog box. You will see "Analysis ToolPak" in the list of Inactive Application Add-Ins. Set the Manage drop-down menu to "Excel Add-Ins," and click on the "Go" button at the bottom of the dialog box to open the Add-Ins dialog box.



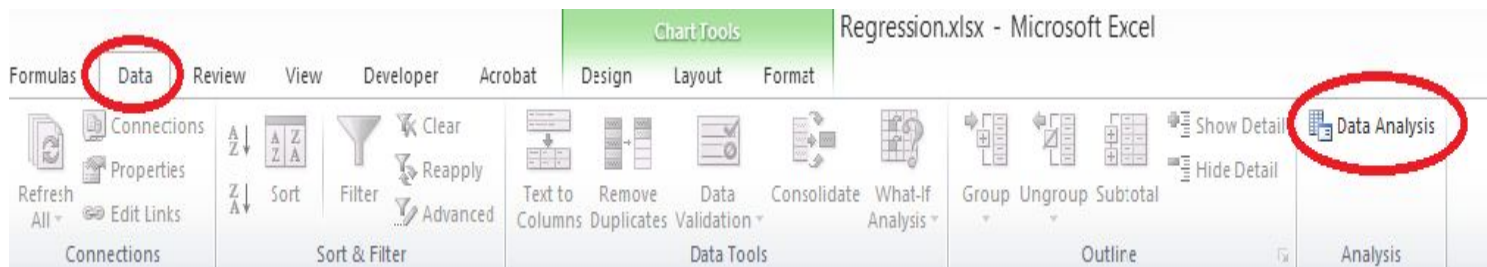
Step 3

- Tick the check box in front of "Analysis ToolPak" in the list of available add-ins. Click the "OK" button on the right side of the Add-Ins dialog box to turn on the Analysis ToolPak once you have selected it in the list of options.



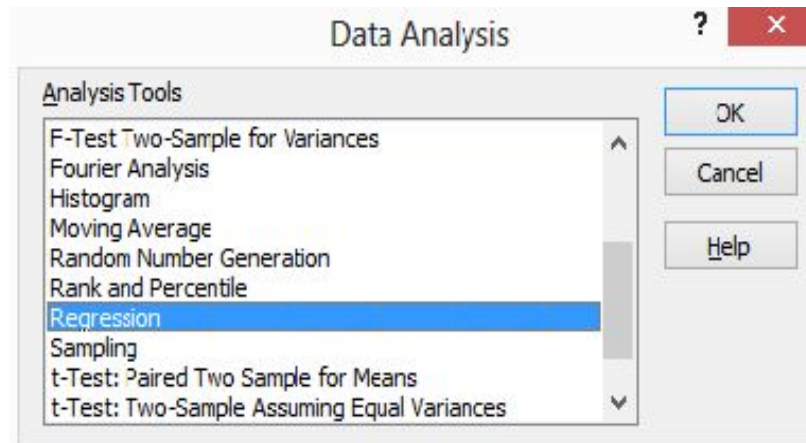
Step 4 & 5

- Enter your column headings in row 1 of your worksheet, and input your data below the respective headings. You can enter your dependent variable in the first or last column of your data. Use consecutive columns for the data defining your independent variable's components.
- Switch to the "Data" tab in the Microsoft Excel ribbon and locate the "Analysis" group. Click on the "Data Analysis" item to bring up the dialog box of the same name



Step 6

- Scroll through the list of Analysis Tools until you locate "Regression." Click on it to select it, and then click on the "OK" button at the right to open its dialog box.



Step 7

- Type the location of the cell range that contains your dependent variable into the "Input Y Range" field in the Input section of the Regression dialog box. You can click on the unlabeled "Collapse Dialog" button at the right edge of the field to reduce the dialog box height temporarily so you can fill in the field by clicking on the heading of the relevant data column. After you identify your data range, click on the "Restore Dialog" button at the right edge of the input field to regain access to the full dialog box.

Exp. No.	Drying CVs moisture content (%)	Drying CVs Time (sec)	Drying CVs Bed Temperature (degC)	Loading of Material wet Weight (g)	Loading of Material Initial water	Drying MV Inlet temperature (degC)	Drying MV Inlet flowrate (m3/hr)
1	1.75	874	49.1	784	143	53	70
2	2.30	671	49.7	784	143	55	80
3	1.82	726	49	628	115	53	70
4	1.93	887	49.4	941	172	53	80
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Regression

?

×

Input

Input Y Range:

Input X Range:

☒ Labels
 ☐ Constant is Zero

☐ Confidence Level: %

Output options

☐ Output Range:

☒ New Worksheet Ply:

☐ New Workbook

Residuals

☒ Residuals
 ☒ Residual Plots

☐ Standardized Residuals
 ☐ Line Fit Plots

Normal Probability

☒ Normal Probability Plots

OK

Cancel

Help

Step 8

Enter the location of the cell range that contains your independent variable – also called a predictor or explanatory variable – into the "Input X Range" field.

	Drying CVs	Drying CVs	Drying CVs	Loading of Material	Loading of Material	Drying MV	Drying MVs
Exp. No.	moisture content (%)	Time (sec)	Bed Tempera ture (degC)	wet Weight (g)	Initial water	Inlet temperat ure (degC)	Inlet flowrate (m3/hr)
1	1.75	874	49.1	784	143	53	70
2	2.30	671	49.7	784	143	55	80
3	1.82	726	49	628	115	53	70
4	1.93	887	49.4	941	172	53	80
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Regression

Input

Input Y Range:

Input X Range:

☒ Labels ☐ Constant is Zero

☐ Confidence Level: %

Output options

☐ Output Range:

☒ New Worksheet Ply:

☐ New Workbook

Residuals

☒ Residuals ☒ Residual Plots

☐ Standardized Residuals ☐ Line Fit Plots

Normal Probability

☒ Normal Probability Plots

OK Cancel Help

Step 9 & 10

- Click on the "Labels" check box to tell Excel that the first row of your data contains data labels. If you didn't enter a header row, leave this box unchecked.
- Click on the "Output Range" radio button in the Output Options section of the dialog box and enter a data range in the entry field to identify a location in your current worksheet for the output of your analysis. Use the "Collapse Dialog" and "Restore Dialog" buttons to click through your worksheet and identify where to put your results. Select the "New Worksheet Ply" radio button to place your results in a new sheet within your workbook, or choose "New Workbook" to put the results in a new file.

Step 11

- Choose options from the Residuals section of the Regression dialog box. Residuals summarize the statistical output of the analysis on a case-by-case basis, comparing the prediction derived from the regression equation to the difference between it and the actual score. Standardized Residuals adjust the standard deviation of Residuals to a value of 1. Tick the check box in front of the Plot options to graph your results. The Residual Plot graphs your residuals, and the Line Fit Plot compares the regression's prediction to its actual output.

The screenshot shows the 'Regression' dialog box with the following settings:

- Input:**
 - Input Y Range:
 - Input X Range:
 - ☒ Labels
 - ☐ Constant is Zero
 - ☐ Confidence Level: %
- Output options:**
 - ☐ Output Range:
 - ☒ New Worksheet Ply:
 - ☐ New Workbook
- Residuals:**
 - ☒ Residuals
 - ☐ Standardized Residuals
 - ☒ Residual Plots
 - ☒ Line Fit Plots
- Normal Probability:**
 - ☒ Normal Probability Plots

Buttons on the right: OK, Cancel, Help.

Step 12

Click on the "OK" button at the right of the Regression dialog box to process your regression. View your results in the location you specified, either on your current worksheet, elsewhere in your document or in another file.

The first part of the output is the regression statistics

SUMMARY OUTPUT	
<i>Regression Statistics</i>	
Multiple R	0.7090
R Square	0.5027
Adjusted R Square	0.0046
Standard Error	0.3545
Observations	13

The ANOVA table comes next. This gives a test of significance of the R².

ANOVA					
	<i>df</i>	<i>SS</i>	<i>MS</i>	<i>F</i>	<i>Significance F</i>
Regression	6	0.89	0.15	1.42	0.34
Residual	7	0.88	0.13		
Total	13	1.77			

Coefficients

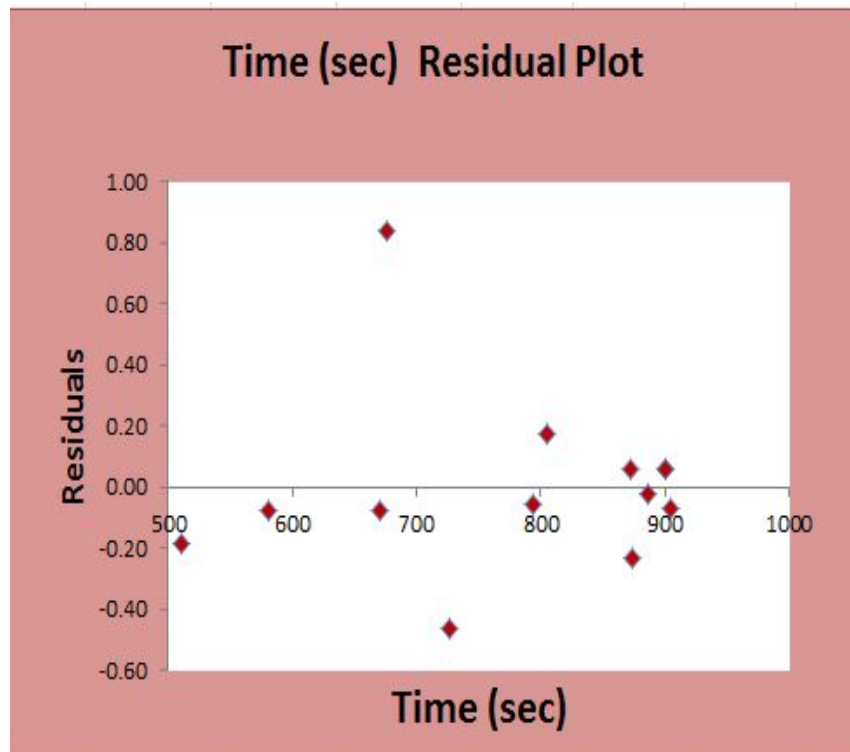
The next stage is the coefficients. It gives the coefficient for each parameter, including the intercept (the constant).

The standard errors, and the t-values follow (the t-value is the coefficient divided by the standard error). Next comes the p-value associated with the variable, and the confidence intervals of the parameter estimates

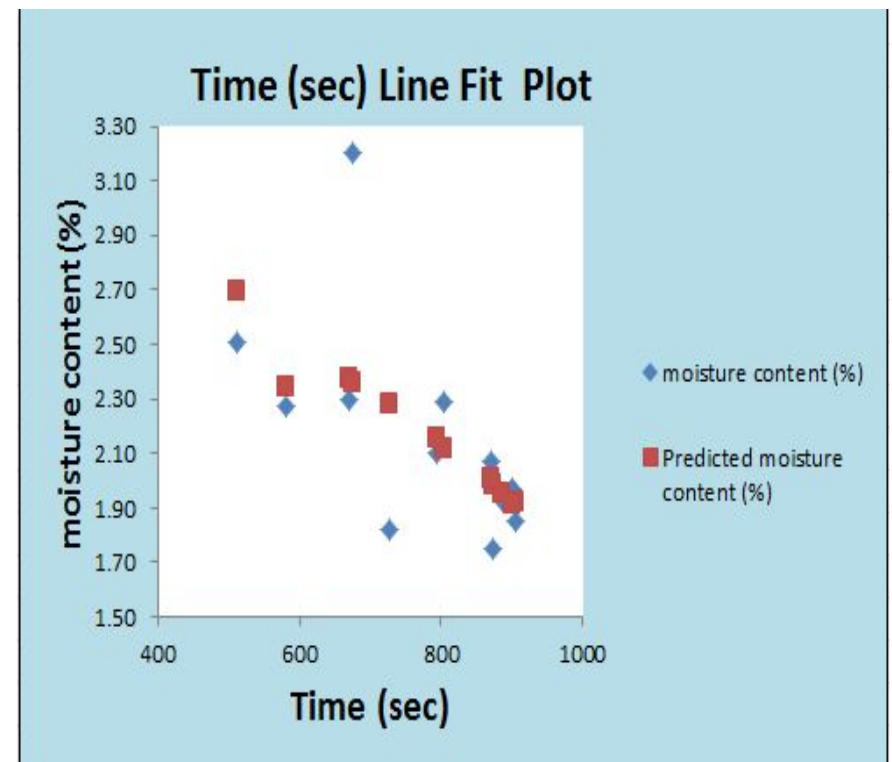
	<i>Coefficients</i>	<i>Standard Error</i>	<i>t Stat</i>	<i>P-value</i>	<i>Lower 95%</i>	<i>Upper 95%</i>	<i>Lower 95.0%</i>	<i>Upper 95.0%</i>
Intercept	6.1244	3.6291	1.6876	0.1354	-2.4571	14.7060	-2.4571	14.7060
Time (sec)	-0.0028	0.0017	-1.6654	0.1398	-0.0067	0.0012	-0.0067	0.0012
Bed Temperature (degC)	-0.0044	0.0421	-0.1039	0.9201	-0.1040	0.0952	-0.1040	0.0952
wet Weight (g)	0.0013	0.0013	0.9807	0.3594	-0.0018	0.0043	-0.0018	0.0043
Initial water	0	0	65535.0000		0	0	0	0
Inlet temperature (degC)	-0.0287	0.0365	-0.7861		-0.1151	0.0577	-0.1151	0.0577
Inlet flowrate (m3/hr)	-0.0142	0.0137	-1.0354	0.3349	-0.0466	0.0182	-0.0466	0.0182

Different Plots

The Residual Plot graphs your residuals



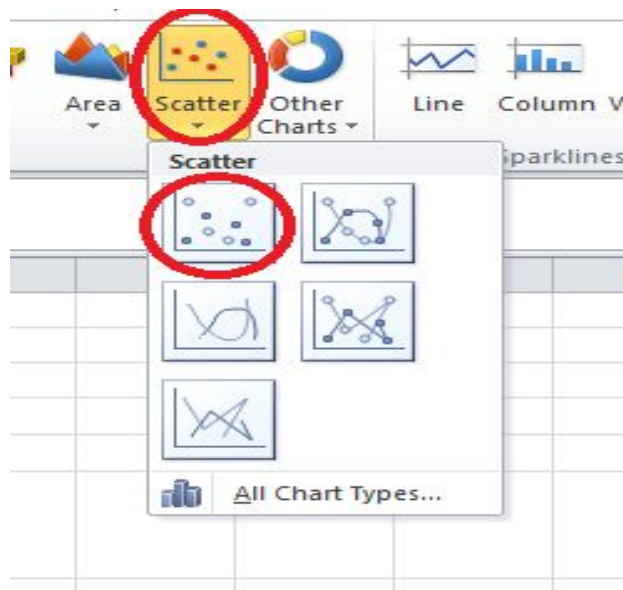
The Line Fit Plot compares the regression's prediction to its actual output.



Inserting a Scatter Diagram into Excel

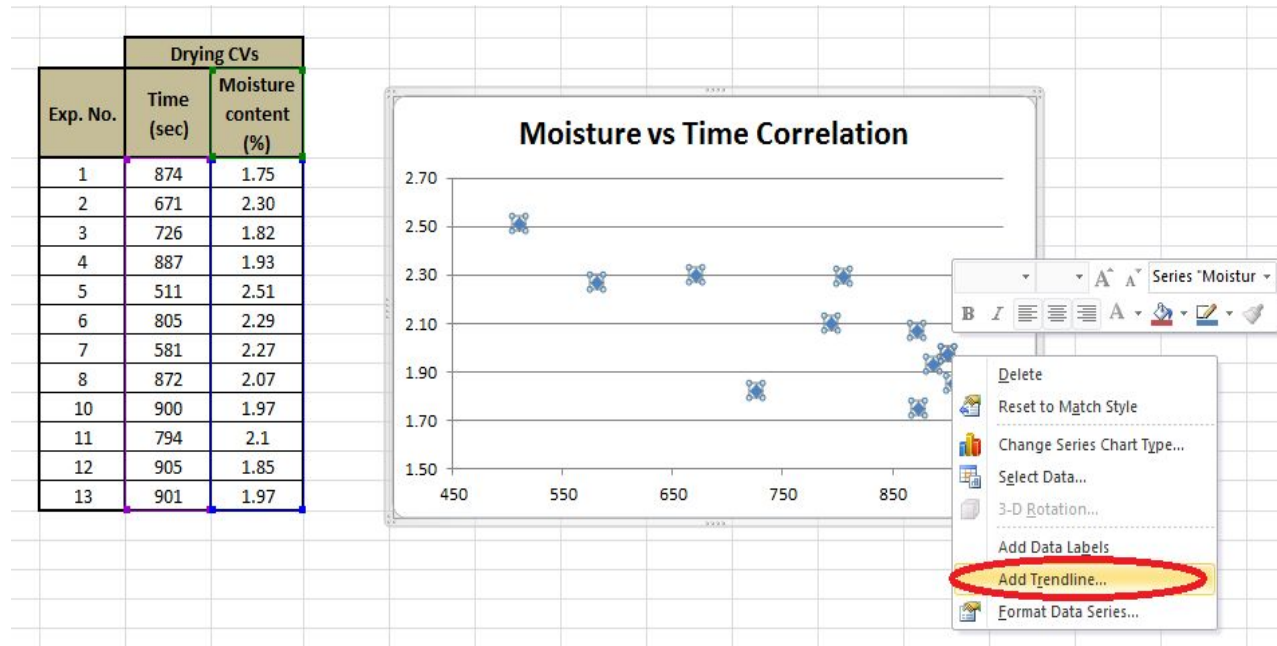
Suppose you have two columns of data in Excel and you want to insert a scatter plot to examine the relationship between the two variables.

- Begin by selecting the data in the two columns. Then, click on the Insert tab on the Ribbon and locate the Charts section. Click on the button labeled Scatter and then select the button from the menu titled Scatter with Only Markers.



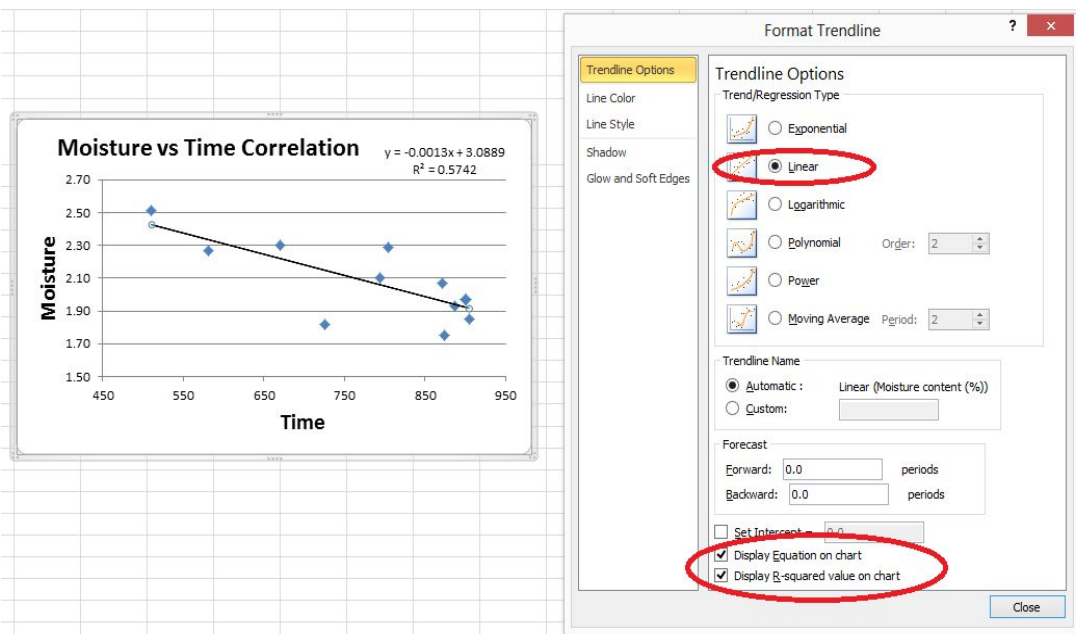
Add a Trendline to Excel

- You can now add your trendline. Begin by clicking once on any data point in your scatter plot. This can be tricky because there are many elements of the chart you can click on and edit. You will know that you have selected the data point when all of the data points are selected. Once you have selected the data points, right click on any one data point and choose add a Trendline from the menu.



Formatting an Excel Trendline

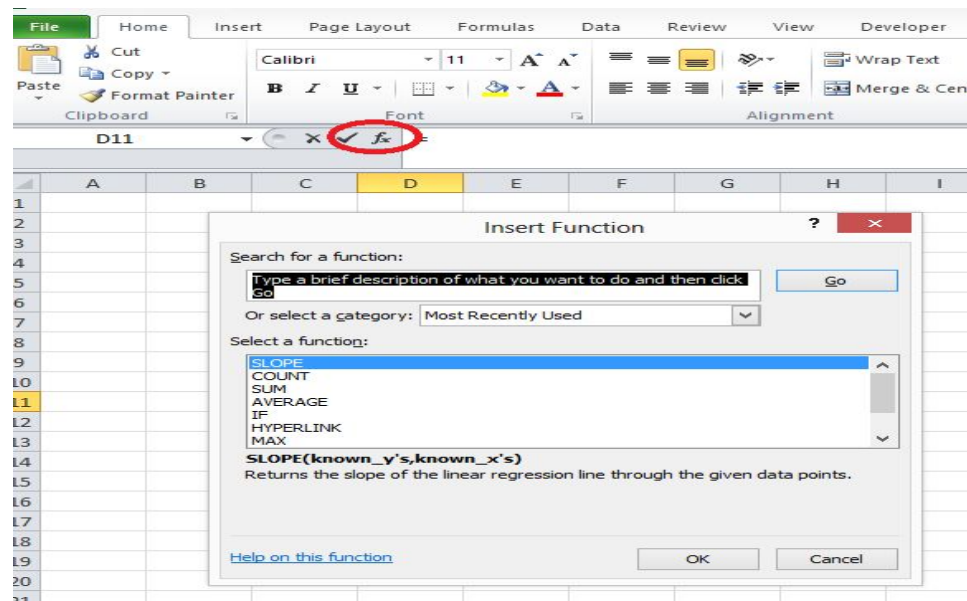
- To format your newly-created trendline, begin by right clicking on the line and selecting Format Trendline from the menu. Excel will once again open up the Format Trendline window
- One of the more popular options people use when adding a trendline to Excel is to display both the equation of the line and the R-squared value right on the chart. You can find and select these options at the bottom of the window. For now, select both of these options



Simple Linear Regression

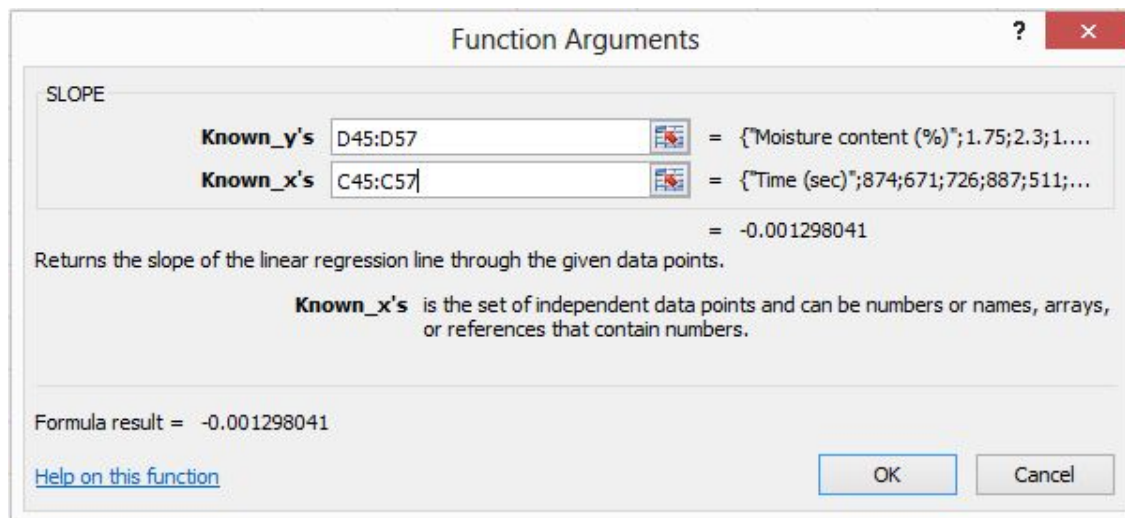
Using an Excel function

- Open the Microsoft Excel page with the data that you need to correlate. Name one column "x" and the other "y". Select an empty cell below the columns that will contain the correlation coefficient R, once calculated. Create a label above it to distinguish it from other data cells.
- Select the cell you created earlier and put an equal sign. Go to the Formula tab, select Function Library Group, and then More Function and Statistical. Select Slope, a dialog box will pop up asking you to infill the range.



Simple Linear Regression

- In array one, fill in the number of variable (named x) Repeat the procedure for array Y. Close the dialog box by clicking OK. The result will be displayed in the cell



Linear Regression Formula

Repeat the same process to get result for Intercept - Correlation and R- Squared

The syntax to calculate each of the terms in the regression is as follows:

- The SLOPE function returns the slope of the linear regression line that is used to predict Y values from X values.

Slope,m: =SLOPE(Known_Y's,Known_x's)

Linear Regression Formula

- The intercept point is based on a best-fit regression line plotted through the known x-values and known y-values. Calculates the point at which a line will intersect the y-axis by using existing x-values and y-values.

Y-intercept, b: =INTERCEPT(Known_Y's, Known_x's)

- The correlation coefficient (a value between -1 and +1) tells you how strongly two variables are related to each other. We can use the CORREL function or the Analysis Toolpak add-in in Excel to find the correlation coefficient between two variables

Correlation Coefficient, r: =CORREL(Known_Y's, Known_x's)

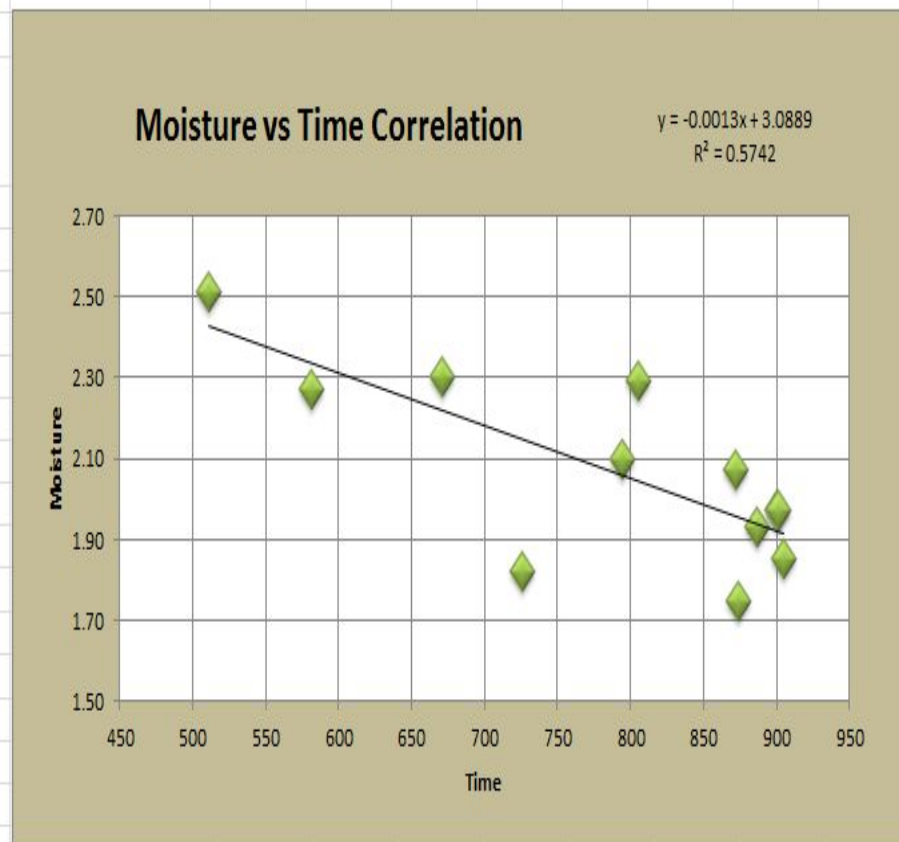
- **R-squared, r² =RSQ(Known_Y's, Known_x's)**

Chart

outlier removal

Drying CVs

Exp. No.	Time (sec)	Moisture content (%)
1	874	1.75
2	671	2.30
3	726	1.82
4	887	1.93
5	511	2.51
6	805	2.29
7	581	2.27
8	872	2.07
10	900	1.97
11	794	2.1
12	905	1.85
13	901	1.97



Regression Moisture vs Time

Slope (m)	-0.0013
Y-intercept, b	3.0889
Correlation Coefficient, r	-0.7578
R-squared, r ²	0.5742