Addendum 1

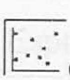
Spreadsheet Data Analysis

This analysis is the same as the manual analysis, except that all the graphs are drawn using Excel 97 (other spreadsheets will also work, but the commands required to plot the data will be different).

1. Open an Excel spreadsheet. Enter your data in two vertical columns. Label column A time (including units), and record the measured times. Label column B mass (including units). Enter the experimentally measured masses at each time interval into these two columns.

2. Plot an XY scatter plot of your experimental data. Put the mass on the vertical (y) axis, and time on the horizontal (x) axis.

a. Select the entire set of data using your mouse. Then click on the Chart Wizard

b. Chart Wizard Step 1: Choose **XY (Scatter)** and the **no line**  chart sub type, then press [Next].

c. Chart Wizard Step 2: Press [Next] (assuming that you have correctly selected the data in step a).

d. Chart Wizard Step 3:

i) Select the **titles** tab, and enter appropriate titles, including units for each axis

ii) Click the **gridlines** tab, and turn on major gridlines on both the x and y axis.

iii) Click the **legend** tab, and turn off the legend (there will only be one set of data on the graph)

e.Chart Wizard Step 4: Select **Place chart as new sheet**, and press [Finish]

f. Turn on the chart toolbar. Select menu item View|Toolbars|Chart and click it on. This is really useful to locate the data series later on.

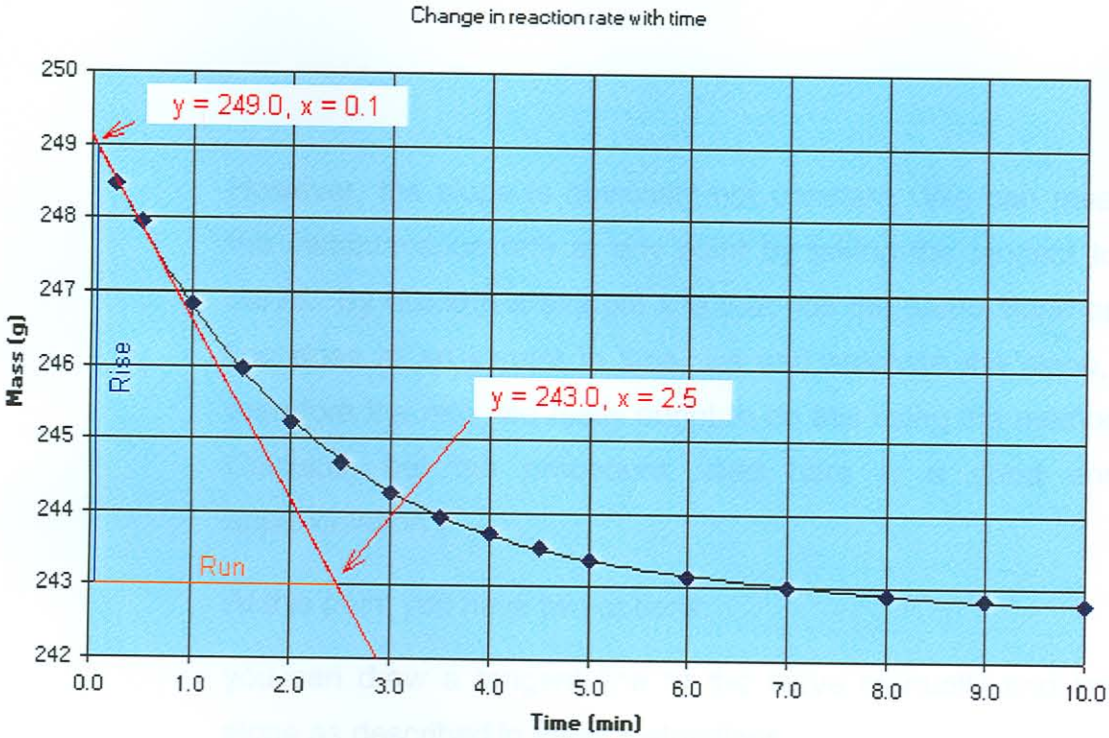
3. Add a trendline to your data. You will use Excel's ability to generate a "least squares" fit to the data.

Hints: We want a smooth curve through the data. It is impossible to find the tangent to the curve unless the data has been smoothed. **DO NOT join the data point to point**. This is almost never done in scientific graphing.

a. Select Series 1 from the Chart Toolbar. Select menu item Chart|Add Trendline and use polynomial type fitting. Experiment with the results when you change the order. (An order of 4 usually gives good results for this type of graph. Going to a higher order will not give much better fit, and will make your work in the next step harder.)

b. Select Series 1 Trendline 1 from the Chart Toolbar. Select Format Trendline (either right click on the trendline on the graph, or the Toolbar), and set its options to:

i) Forecast backwards (extrapolate) to time = 0 (in other words, if your first data point is recorded at 0.25 min, then enter a forecast backwards value of 0.25 units). You need to



extrapolate the graph back to time = 0, so that you will be able to calculate the initial rate of the reaction. Note: if you select too far a projection, you will change the scale of the graph. If this happens, reduce the forecast.

ii) Turn on the option Display equation on chart and click [Ok]

iii) Click on the equation, and drag it to a blank area on the screen. Write the equation on a piece of paper for reference, as you will need it in a later step.

Reaction rate for this reaction can be defined as $\frac{\Delta \text{mass}}{\Delta t}$ which, since mass is on the vertical (y axis) and time on the horizontal (x axis), is actually the slope of the line.

The rise on the graph is measured in mass units. The run on the graph is measured in time units. Therefore the slope – the rise over the run – is mass over time.

However, the slope is obviously not constant. We can measure the instantaneous rate at any point by taking the tangent to the curve. By drawing a straight line that has the same slope as the line does at an instant in time, we can estimate the slope, and therefore the rate (we really ought to do this using the methods of Calculus, but the procedure used here is a good enough approximation.)

At this point you have two options:

you can draw a tangent line to the curve manually and find its slope as described in these instructions

you can use the plotted least squares fit equation to calculate the slope as described in the following steps

2. Use Excel to draw a tangent to the curve at the very beginning of the reaction (t = 0). To do this:

a) Click the Sheet 1 tab. Go to column D and label it X. Go to column E and label it Y

b) Enter a time = 0 in cell D2. Enter a small increment of time in cell D3 (it should be small enough that the graph appears straight over this period of time at the start of the reaction, perhaps about 0.1 minutes).

c) Enter the equation for your trendline in cell E2. You must do this as follows:

Suppose that the equation is: $y = 0.0016x^4 - 0.0478x^3 + 0.5409x^2 - 2.8772x + 249.2$

Since the value of x is in cell D2, we will enter this formula in cell E2 for Y as:

=0.0016*(D2^4)-0.0478*(D2^3)+0.5409*(D2^2)-2.8772*D2+249.2

d) Copy this formula into cell E3.

e) Click the Chart 1 tab to display the graph. Right click on the plotting area (not on the data or line), and select Source Data from the menu.

f) Click the [Add] button to put on a new series (series 2). Click on the X-values range button. Click on the Sheet 1 tab, and select the cells D2, and D3. Click on the Y-values range button. Click on the Sheet 1 tab, and select the cells E2, and E3.

g) Using the Chart toolbar, select series 2. Press the Toolbar Format data button. Select Marker None on the patterns tab.

h. Select menu item Chart|Add Trendline, chose Series 2, select the Linear type, and set the options to project forward 2 or 3 units, and to display the equation. Note: if you select too far a projection, you will change the scale of the graph. If this happens, reduce the forecast.

The equation for this trend line is of the form y = mx + b, where m is the slope. This slope is the initial rate (the slope, in units of g/min).

2. Repeat the above procedures to calculate the slope of the graph halfway through the measured time, at 5 minutes.

a) Enter a time = 4.95 in cell D4. Enter a small increment of time in cell D5, centered on 5 minutes (it should be small enough that the graph appears straight over this period of time at the start of the reaction, perhaps about 5.05 minutes).

b) Copy the formula for cell E3 into cells E4 and E5.
c) Draw the trendline for these points, extending it both forward and backwards a few units.

Notice that there has been a significant decrease in the slope (the rate at t = 5.0 minutes).

4. Repeat these steps to calculate the slope of a line at the end of the time interval. Project this line backwards for a few units.

Complete your graph by checking its formatting. You may wish to adjust the colors, or the scale on the axis. You can do this by selecting the part of the graph you wish to change with a right click, or from the chart toolbar. Save and print your graph.

5. Summarize you results and explain why the rate changes with time.

Notice that in the sample set of data shown, the rate has decreased by a factor of about 10 in every five minutes. Don't however read too much into this. While the rate has gone down a lot, it is just a coincidence that it went down by this amount. Other reactions, and other concentrations in this reaction would give very different results. In general though, the rate will decrease with time.

http://www.carlton.paschools.pa.sk.ca/chemical/chem30/ReactionRate/spreadsheet.htm Monday, 09 February 2004