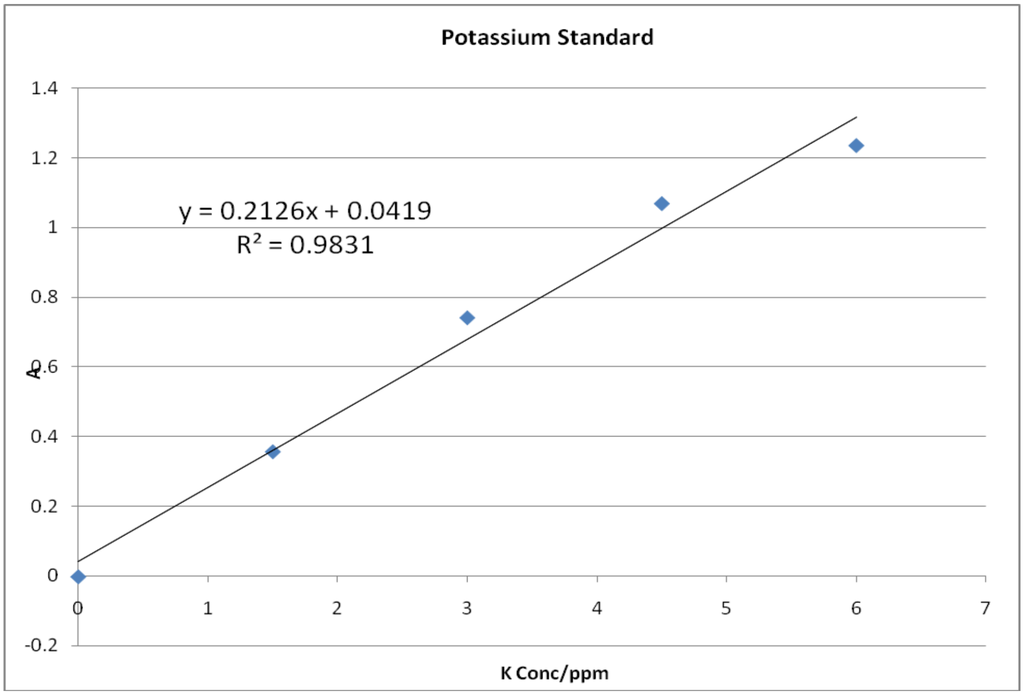
Designing An Exeriment: Potassium

For the standard solution, choose a potassium concentration that will give absorbance values in a good range.

Absorbance values much over 1 are not always reliable due to sensitivity (or lack thereof) of the detector.

Absorbance values should be in the range where the unknown potassium concentration will be. It is also possible to adjust the potassium concentration in the unknown so there are two possible variables here; the concentration of the standard and the concentration of the unknown.

Here is a standard curve for potassium ion with a concentration of 6 mg/L (or 6 ppm).



Notice that the last two points have absobance values greater than one.
Also notice that the line is not straight, and the R^2 value is not too close to 1 which also tells us it is not linear.

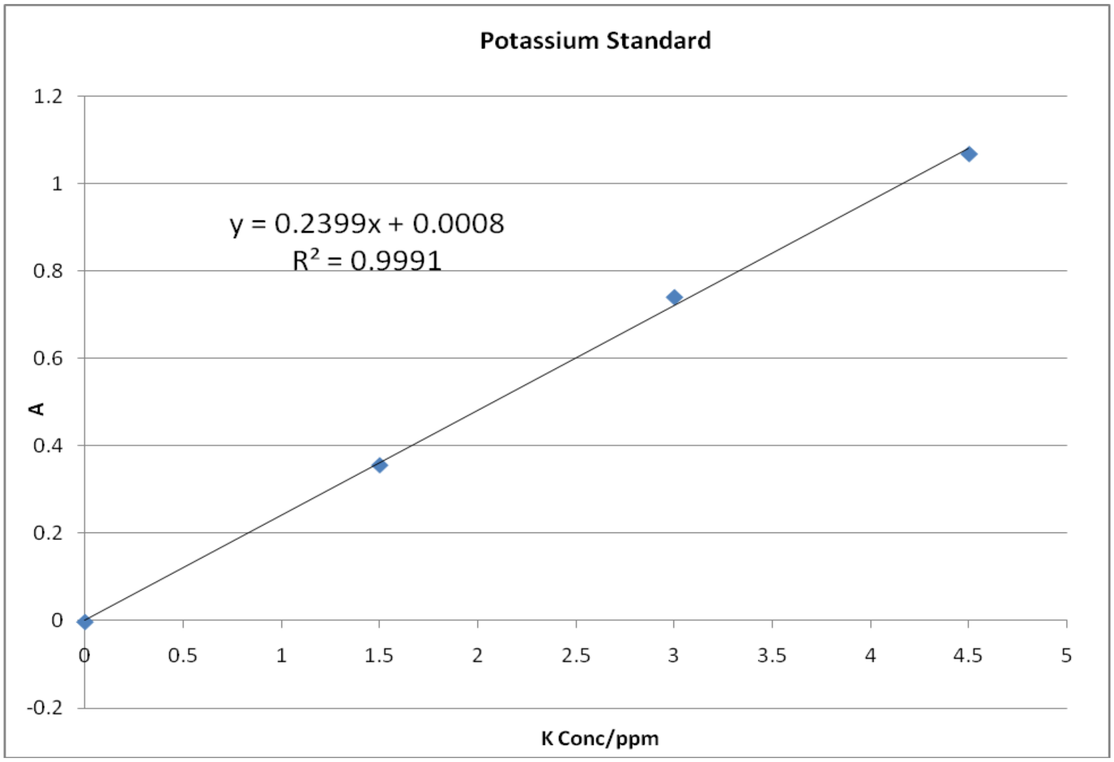
Most atomic absorption spectrometers can handle nonlinear lines but they must be set to do that; default is often linear.

So what can we do?

We can use a standard solution with a lower concentration of potassium.

Or we can treat the data by hand rather than letting the instrument do the calculation.

1. What if we leave off the last point?



This is an Excel plot with a linear Trendline.

Now we have a nice straight line with an excellent R^2 value. We can then use the equation of the line to convert absorbance values to concentrations.

$A = 0.2399\, C + 0.0008$

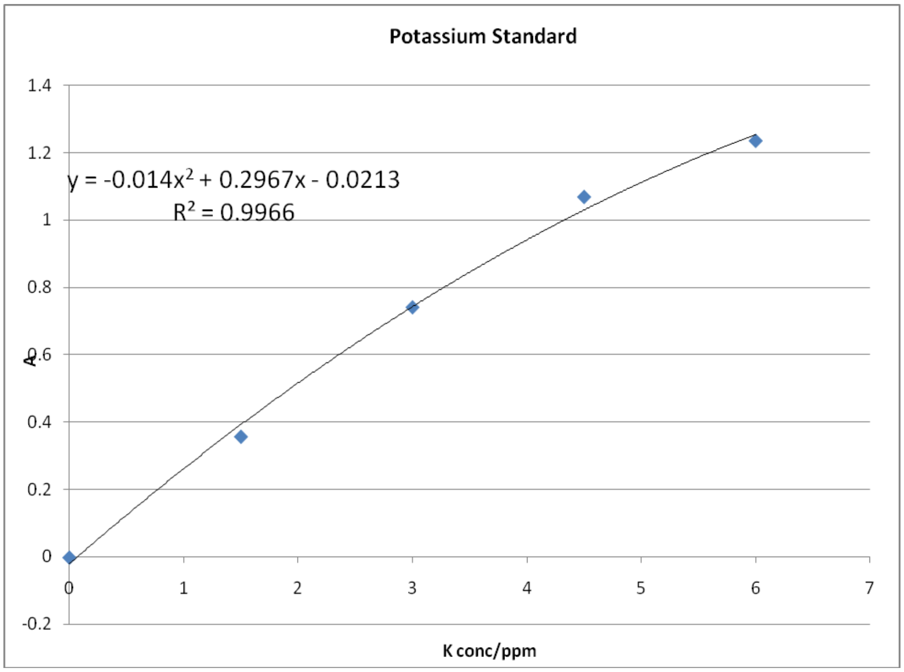
or $C = 5.168\, A - 0.0033$

This is good and easy.

2. Do a nonlinear fit to all the data.

But remember that we decided that the last point may not be too reliable.

This option is given because leaving off a point or two doesn't always result in a linear fit.



Excel will do nonlinear fits. Here the equation which fits well is a quadratic. The R^2 value is very close to 1.

$$A = -0.014\,C^2 + 0.2967\,C - 0.0213$$

This presents a greater challenge to solve for concentration.

Method 1. Use the quadratic formula. Set *A* to the value you want to use. For this example, set *A* = 0.800

Arrange the equation so that all the terms are on the left, with *A* = 0.800.

$$-0.014\,C^2 + 0.2967\,C - 0.8213 = 0$$

The Quadratic Formula

$$X = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

Using this Formula, the roots of the equation are 3.339 and 17.568. Looking at the graph, the correct root must be the 3.339.

There are web sites that will solve quadratics. Three examples are as follows. All were accessed on 9/8/2009.

www.1728.com/quadratc.htm
www.coolmath.com/calculators/quadratiac.htm
www.freewebs.com/brianjs/ultimateequationsolver.htm

This last one also solves quartic and cubic equations.

Method 2. Use Excel to make succession approximations.

Assume that the *A* value is 0.800. Look at the graph and approximate the value of *C*: about 3.1.

If we move A to the right side of the equation and combine terms, then the equation becomes:

$$-0.014\ C^2 + 0.2927\ C – 0.8213 = 0$$

In an Excel spreadsheet, enter 3.1 into cell A3 and = -0.014*A3^2 + 0.2927*A3 – 0.8213 into cell A5.

Cell A5 will now read -0.04847. Since this value is less than zero, 3.1 is too small.

Change the value in A3 to 3.3. The value in cell A5 will now read -0.00785. The value is closer to zero. Try 3.4; it is too large since the result is now positive. So we know the answer is between 3.3 and 3.4.

Keep changing the value in cell A3 until the value in cell A5 is close to zero. To three significant figures, the answer lies between 3.34 and 3.35 (closer to 3.34).

Method 3. Use a graphing calculator.

Plot $y = -0.014\ x^2 + 0.2927\ x – 0.8213$. Determine the value of the *x* intercept (this is where $y = 0$.

Analyze Some Data

Using the standard graph, the solution to be measured should have an absorbance value between 0.2 and 0.9. It may take more than one try to get a solution in this range. On the second try, the following solution was close to the the desired *A* value. 0.212 g of maple syrup was dissolved in water to give 100.0 mL of solution. The absorbance values for 5 measurements of the potassium concentration were:

0.9645	0.9500	0.9614	0.9785	0.9890

Using the linear equation given earlier, calculate the potassium ion concentrations in these 5 solutions. The concentrations will be in mg/L. Note that these are not the concentrations in maple syrup but in the maple syrup solution prepared and measured.

Also, calculate the mean concentration and the standard deviation.

Answers (all in mg/L):

3.987 3.927 3.974 4.045 4.089   Mean = 4.004   Std.Dev. = 0.0635

If we assume an uncertainty of ±one standard deviation, then the concentration is
4.00 ± 0.06 mg/L