EXCEL & You in the Physical Chemistry Lab – Part I

<u>Introduction</u>

This lab is designed to familiarize you with some of the types of data analysis we will be doing in pchem lab. You will notice that it says "Part I" as part of the title. This is due to the fact that the problems delineated here are just a small sample of the types of calculations you may have to perform in the course of the physical chemistry lab. I suggest you start working on this lab now and make sure that you do not run into any difficulties.

<u>Data Analysis</u>

Project I: Graphing Data

You would be surprised how something which seems so trivial (ie. Graphing) can in fact be quite challenging when the amount of data is immense. You will be graphing three data sets of vapor pressure and temperature measurements. For consistency, please use temperature as your independent variable in all cases.

Choose one of the liquids given below and plot

a.) P in torr & T in °C
b.) P in atm & T in K
c.) Ln P in atm and 1/T in K^{-1}

Table of Vapor Pressures

			Carbon Disulfide			
P (torr)	1.00	10.00	40.00	100.0	400.0	760.0
T (°C)	-73.8	-44.7	-22.5	-5.1	28.0	46.5
			Mercury			
P (torr)	300	320	340	350	352	356
T (°C)	246.80	376.33	577.90	672.69	697.83	723.73
			Ethanol			
P (torr)	55.9	93.8	154.1	241.9	304.15	377.9
T (°C)	25.00	35.00	45.00	55.00	60.00	65.00
			Ammonia			
P (torr)	51.15	60.00	91.70	134.80	176.45	192.90
T (°C)	-76.0	-72.0	-68.0	-62.0	-58.0	-56.0
			Carbonyl Chloride			
P (torr)	1.00	10.00	40.00	100.0	400.0	760.0
T (°C)	-92.9	-69.3	-50.3	-35.6	-7.6	8.3

Project II: Fitting Curves & Differentiation

Chemists who spend their days and nights in the lab collect data points not mathematical functions. Occasionally, these sets of data may be fit with a function thereby simplifying the relationship they represent. For this project, you will take the plots you have already generated and fit them with functions.

a.) Fit the data from your first graph to a quadratic equation (2^{nd} order polynomial).
b.) Compute the derivative of your graph at the first, central and last data points.
c.) Fit the third graph with a linear equation (1^{st} order polynomial).
d.) Compute the derivative of your third graph at the first, central and last data points.

Your previous experience with derivatives has most likely been with functions. Here you differentiated a function which was derived from data points.

Project III: Curve Fitting & Integration

Now you will compute the integral of a function which is describing a data set. You are to begin by plotting the heat capacity as a function of T using the data below.

T (K)	**$C_{P,m}$ (J K^{-1} mol^{-1})**
273	28.99
321	29.01
355	29.03
388	29.05
439	29.09
544	29.20
602	29.30
771	29.62
822	29.75
901	29.94
1055	30.41
1122	30.64
1203	30.97
1339	31.50
1488	32.30

Next, you fit the data to a quadratic equation of the form $C_{P,m} = a + bT + cT^2$ where *a*, *b*, and *c* are constants. The physical significance of this problem we have already talked a bit about in class. The data above is the energy that is needed to heat 1 mol of $H_{2(g)}$ from T_1 to T_2. Once you determine the constants you will integrate the functional form of $C_{P,m}$ over the temperature range I assign to you shown below.

T_1	T_2
301	671
404	881
511	899
619	903
299	543
366	662
449	765

Project IV: Graphing Functions

Up to this point we have been dealing with data that was collected from experiments. Sometimes we must used a function which is based on theory in order to determine the success of your data. Later in the semester we will introduce the compression factor, Z_m, which is a measure of deviation from ideality of a gas. As you will learn Z = 1 for a perfect/ideal gas. There are a number of equations which address real gases, one of which you probably saw in general chemistry - van der Waals. Below is the compression factor equation for a van der Waals gas.

$$Z_m = 1 + \left(b - \frac{a}{RT}\right)\frac{1}{RT}P + \left(2b - \frac{a}{RT}\right)\frac{a}{(RT)^3}P^2$$

I will assign you a gas from the list below and I will expect you to find a reference for the van der Waals constants *a* and *b*.

Gases: N_2, O_2, Ne, Ar, Kr, Xe, CO_2, SO_2

a.) Plot the compression factor over the pressure range 0 to 400 atm using 10 atm intervals. Assume T = 200 K.

b.) Repeat the plot in a.) assuming a temperature of 300 K.

c.) Repeat the plot in a.) assuming a temperature of 400 K.

All three plots should be placed in the same graph so you can clearly see the trends.

Project V. Extrema of Functions

Hopefully you learned from calculus that the minima and maxima of a function is determined by taking the first derivative of the equation and setting it equaled to zero. There will be times that taking the derivative will be prove difficult and so it is necessary to determine the extrema graphically.

The Maxwell Boltzmann distribution of molecular speeds is

$$F(v) = 4\pi v^2 \left(\frac{m}{2\pi kT}\right)^{3/2} e^{-\frac{mv^2}{2kT}}$$

This is an example of a statistical distribution, in particular, a probability distribution. We can substitute any speed, v, into this function and determine the probability that a molecule in our system possesses this speed. To make this clear, if $F(\mathrm{v}_1) > F(\mathrm{v}_2)$ then we would say that it is more likely the molecule is traveling at a speed of v_1 than a speed of v_2. The “k” symbol in the equation is the Boltzmann constant. The “m” is the mass of the molecule. I would strongly encourage you to make sure you understand all units before you perform the plots below. HINT: make sure m is in kg.

a.) Plot the MBD at 300 K for the gas you were assigned int the previous project. Use speeds of 0 to 2000 m/s at an interval of 20 m/s. What is the most probable speed at this temperature?

b.) Repeat a.) for a temperature of 700 K. What is the most probable speed this time?

References

[1]R. Hudson, Eckerd College – This lab was adapted from him.