Soft Matter and Biological Physics Coursework

Given data

Nx = 200

Ny = 155

A = 0.0075

B = 1.5 (Kelvins)

T = 320 (Kelvins)

1)a) Calculating Critical Composition

-Critical Composition ($Ø_c$) can be found using the following equation along with the above given data:

$$\phi_c = \frac{\sqrt{N_y}}{\sqrt{N_x} + \sqrt{N_y}}$$

$$\phi_c = \frac{\sqrt{155}}{\sqrt{200} + \sqrt{155}}$$

$$\phi_c = 0.468$$

-Critical Interaction Parameter (X_c) can be found using the following equation:

$$X_c = \frac{1}{2}\left[\frac{1}{\sqrt{N_x}} + \frac{1}{\sqrt{N_y}}\right]^2$$

$$X_c = \frac{1}{2}\left[\frac{1}{\sqrt{200}} + \frac{1}{\sqrt{155}}\right]^2$$

$$X_c = 0.01141$$

-Critical Temperature (T_c) can be found using the following equation:

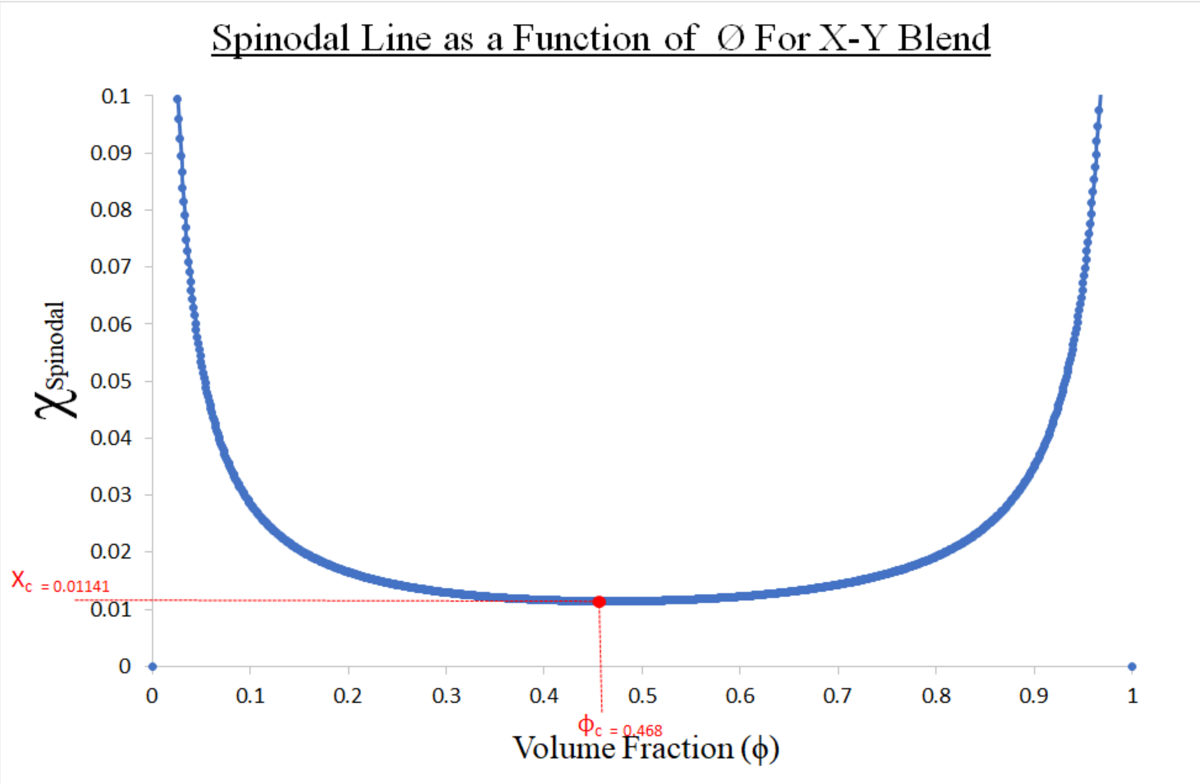
$$T_c = \frac{B}{X_c - A}$$

$$T_c = \frac{1.5}{0.01141 - 0.0075}$$

$$T_c = 384.1\ Kelvins\ (K)$$

<u>1)b) Constructing a graph of X on the spinodal as a function of ϕ</u>

-Below is the graph showing X on the Spinodal (X_s) as a function of (ϕ).



-The following equation was used to graph it:

$$X_s = \frac{1}{2}\left(\frac{1}{N_x \phi} + \frac{1}{N_y(1-\phi)}\right)$$

-With (X_s) limit from 0-1 in increments of 0.001 to obtain a smooth graph. With (ϕ) limits 0-1 representing concentration from 0% to 100% (expressed in decimal form).

-The critical points can be found in three ways:

- Using the graph
- Taking the 1st derivative, setting it equal to zero and solving for variable ϕ
- The calculations in 1.a.

-All these methods were done and the same values were found for the critical points.

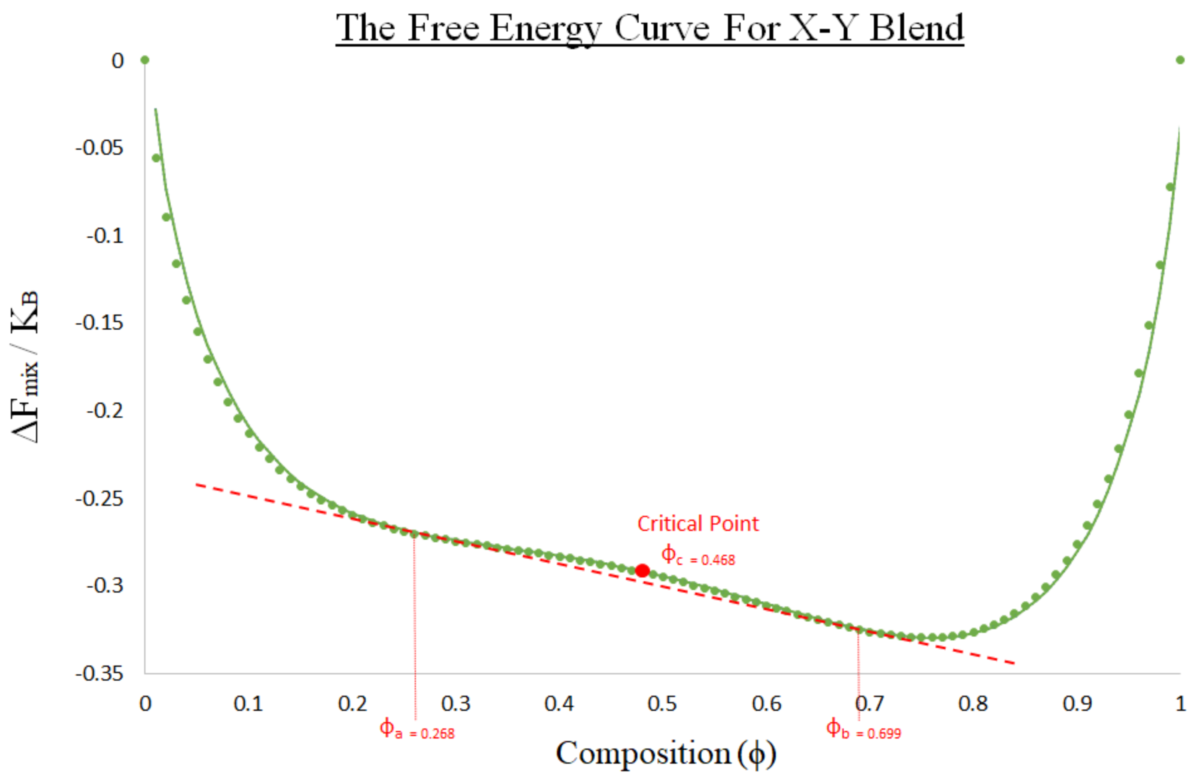
1)c) Finding the two equilibrium compositions

-The two equilibrium compositions for the assigned X-Y blend can be found by using the gradient of the common tangent on the following graph:

Composition (ϕ) vs Free energy of mixing (ΔF_{mix})

-First, ΔF_{mix} needs to be calculated using the equation below then it can be plotted:

$$\Delta F_{mix} = K_B T \left[\frac{\phi}{N_x} \ln \phi + \frac{1-\phi}{N_y} \ln(1-\phi) + X\phi(1-\phi)\right]$$



-Once graphed, the common tangent was added (red dotted line), then using two points the gradient was found to be:

Common Tangent Gradient = 0.298

-From this graphed tangent the equilibrium points can approximately found to be :

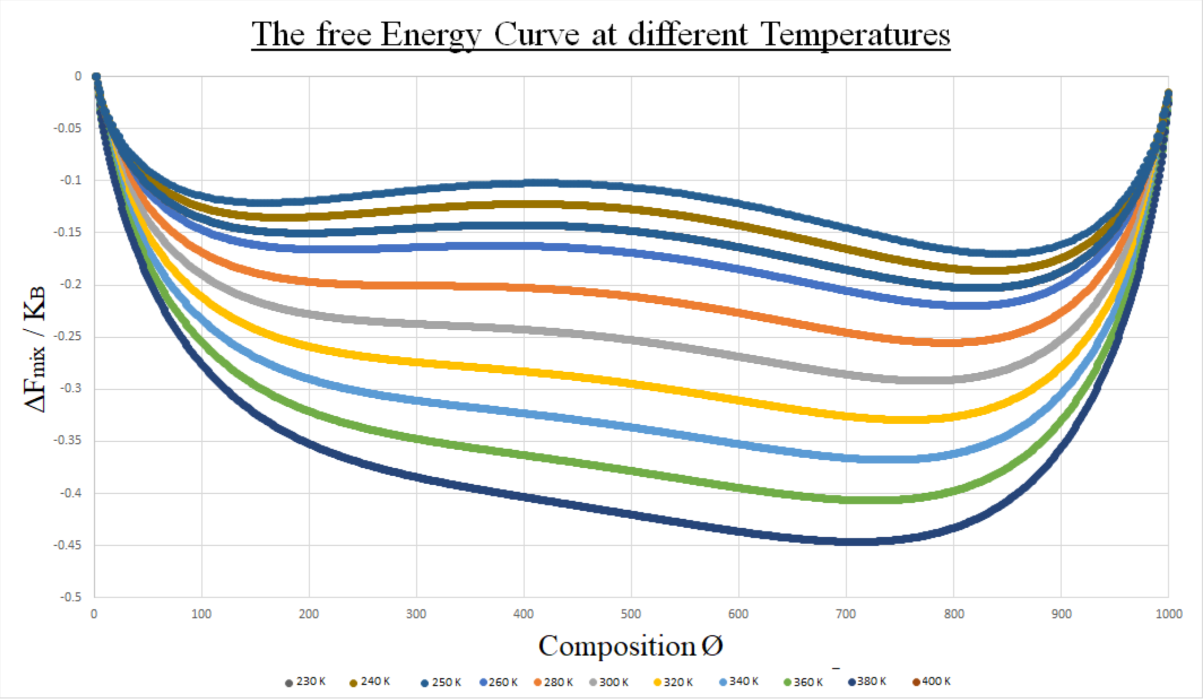
$\phi_1 = 0.268$ $\phi_2 = 0.699$

-To find the exact value for the equilibrium compositions the above equation is set equal to the gradient above, and solved for ϕ, of course finding two values:

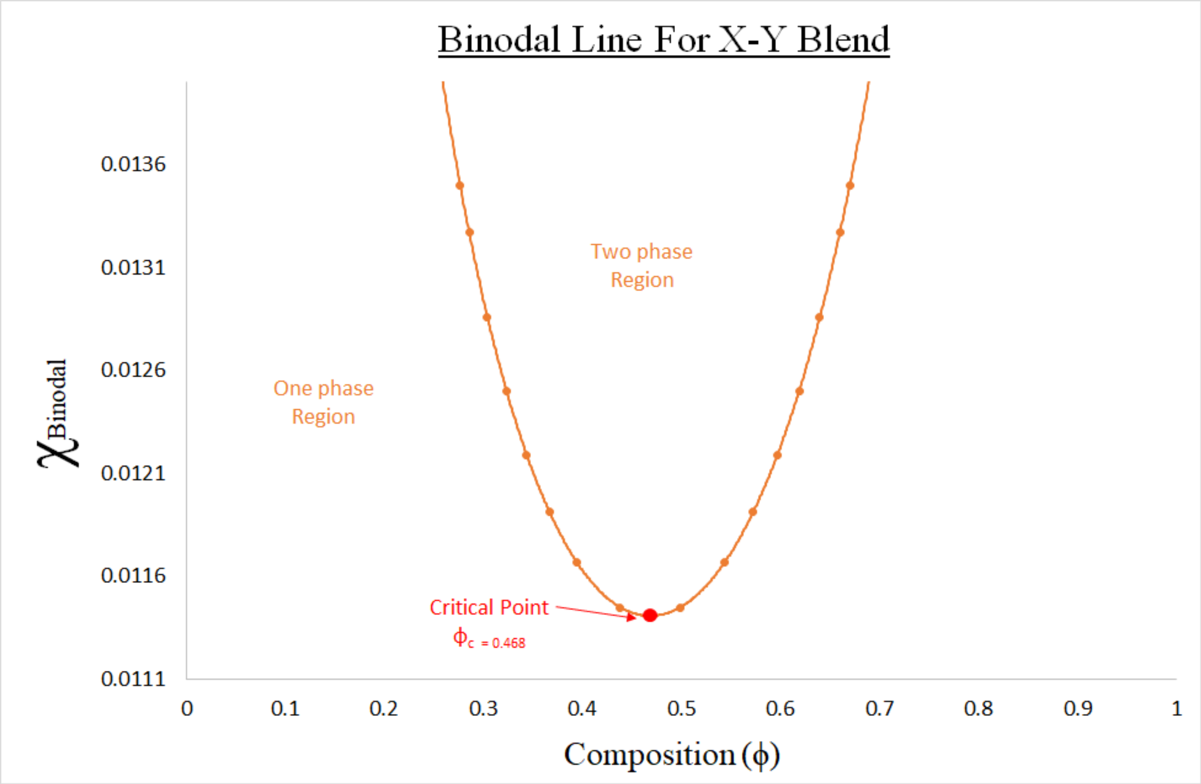
$\phi_1 = 0.268$ $\phi_2 = 0.699$

1)d) Contructing a binodal line for the x-y blend

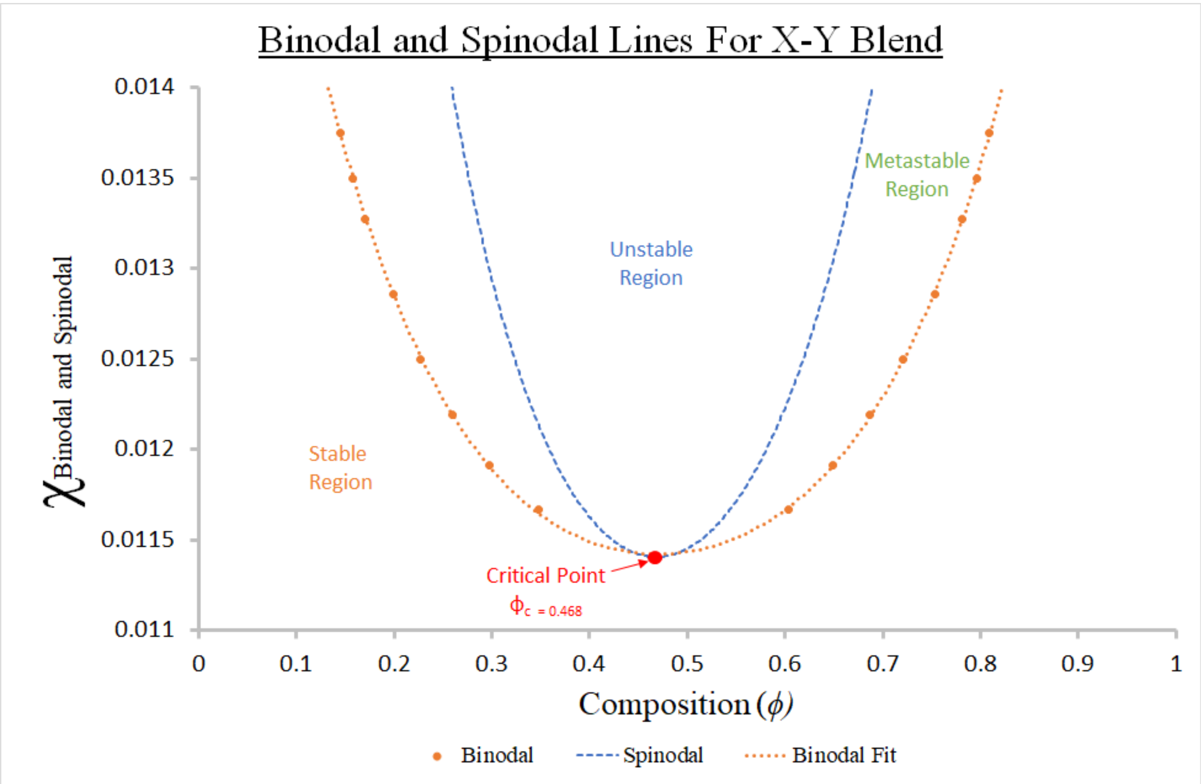
-To get the points we first plotted $(\Delta Fmix)/K_b$ vs Ø as in Q.1. but this time at varying temperatures and hence gaining two equilibrium points for each temperature.



-These equilibrium points were then used to plot the following graph which shows the binodal line for the X-Y blend.



-Now the spinodal line from Q.1.b. can be plotted with this binodal line which will enable us to see the metastable region of the X-Y blend:

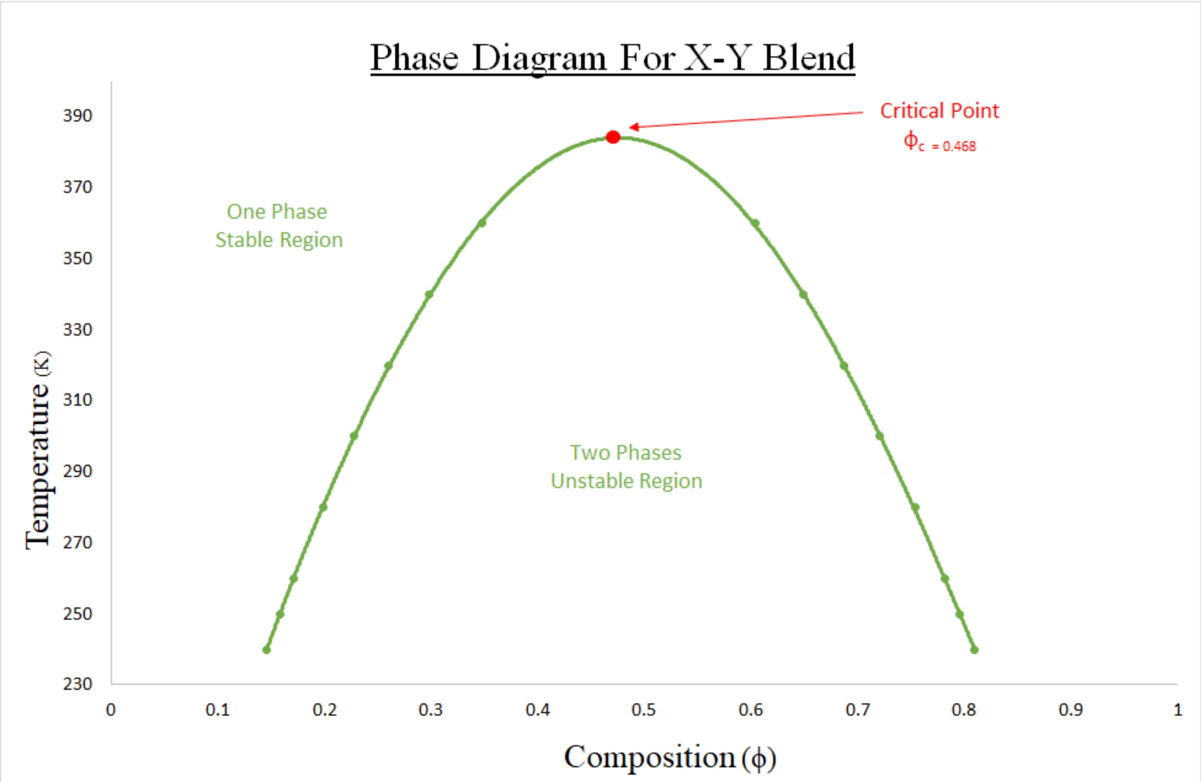


-Now using the binodal (X_b) values from above, values for temperature can be found using the following rearranged equation:

$$T = \frac{B}{X_b - A}$$

$$T = \frac{1.5}{X_b - 0.0075}$$

-Using this information, the following final phase diagram was able to be created showing the critical point and phase regions.



1)e)

-Heterogeneous nucleation will most likely occur due to the impurities in the blend X-Y hence will nucleate at a higher temperature.

Normal temperature at: Ø= 0.3 is T=360 K

-So with nucleation it will phase separate at a different temperature, in this case most likely around 380 K.

2) a)i) Estimating the value for the lewis number

-The equation for the Lewis number is as follows:

$$L_e = \frac{Thermal\ diffusivity\ (\alpha)}{Mass\ diffusivity\ (D)}$$

$$= \frac{Thermal\ Conductivity(\Lambda)}{Density(\rho)\ x\ Diffusion\ Coefficient(D_{im})\ x\ Specific\ Heat\ Capacity(C_p)}$$

-Gaining the following value from the below sources and plugging it into the above equation, the value for the relevant Lewis number can be calculated.[1] [2]

-Thermal diffusivity (α), of water (H_2O) is = $1x10^{-7}$ m^2/s

-Mass diffusivity (D), of ATP = $1x10^{-10}$ m^2/s

$$L_e = \frac{1x10 - 7\ m2/s}{1x10 - 10\ m2/s} = 1{,}000$$

-The reason H_2O was used was because the human body and the cell is essentially water, so one can assume most qualities for water such as mass density and in this case thermal diffusivity is that of the same of a human cell.

2)a)ii) Naming a species of molecule in a cell with a lewis number smaller than ATP's

-We know from above that the mass diffusivity (D), of ATP is $1x10^{-10}$ m^2/s, we also know from the same sources as above that the mass diffusivity for Oxygen is $1x10^{-9}$ m^2/s. Showing its value for D is larger, hence in the equation:

$$L_e = \frac{Thermal\ diffusivity\ (\alpha)}{Mass\ diffusivity\ (D)}$$

[1] Ballas SK. Erythrocyte concentration and volume are inversely related. Clin Chim Acta. 1987 Apr 30 164(2):243-4. p.243 https://bionumbers.hms.harvard.edu/bionumber.aspx?id=107602&ver=2&trm=red+blood+cell+surface+area&org=

[2] "Physical Biology of the Cell", Rob Phillips, Jane Kondev and Julie Theriot (2009). Page 26 https://bionumbers.hms.harvard.edu/bionumber.aspx?id=101792&ver=6&trm=e+coli+surface+area&org=

-This will make the Lewis number smaller, hence we can conclude that oxygen has a smaller Lewis number than ATP.

2)b) Obtaining a Fermi estimate for the fraction of the food energy you eat, that is used by the bacterial cells in your gastrointestinal tract.

-The food we eat contains glucose which can be broken down into ATP. It is then used in the body to give cells and bacteria energy. Each ATP when used by a cell contains approximately 1 eV of energy - assuming that all the food we eat is transferred to glucose and then ATP without any loss.

-We can then assume that ATP on a random walk must "bump" into a cell or bacteria to receive this energy. We also assume that all the ATP must eventually encounter either a cell or a bacteria and only a cell or a bacteria.

-The frequency at which ATP encounters a cell or a bacterium will depend on their respective surface areas. The surface area of a typical human cell, i.e. a red blood cell is 140 μm^2 and a typical bacteria such as E.coli has a surface area of 6 μm^2.[3] [4]

-If we assume that there are the same numbers of cells and bacteria in the body (10^{13}) then we would expect approximately 4 % of the ATP molecules to encounter a bacteria before a cell.

-Probability of ATP meeting a bacteria = $6\ \mu m^2/140\ \mu m^2 \approx 4\%$

-Hence this is the fraction of the food energy you eat that is used by the bacteria cells.

3) Diffusion of Oxygen in the body

-The diffusion coefficient of oxygen (D_{o2}) in cells, in cartilage is around $1\text{x}10^{-9}$ m^2/s with a range of:

$$1\text{x}10^{-10}\ m^2/s < D_{o2} < 1\text{x}10^{-8}\ m^2/s$$

-There are two data sets given of twelve measurements of the average distance that oxygen has diffused across a sample of cartilage at twelve different times.

-One of these sets is consistent with the diffusion coefficient of oxygen in cartilage, while the other set looks unlikely to be the same.

-The task here is to determine which set of data is consistent with the diffusion above and which is not.

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[3]Ballas SK. Erythrocyte concentration and volume are inversely related. Clin Chim Acta. 1987 Apr 30 164(2):243-4. p.243
https://bionumbers.hms.harvard.edu/bionumber.aspx?id=107602&ver=2&trm=red+blood+cell+surface+area&org=

[4] "Physical Biology of the Cell", Rob Phillips, Jane Kondev and Julie Theriot (2009). Page 26
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3)a) Finding the Diffusion constant

-Here is the equation to say how the diffusion distance (d) varies with diffusion time (t):

$$d = \sqrt{\Lambda t}$$

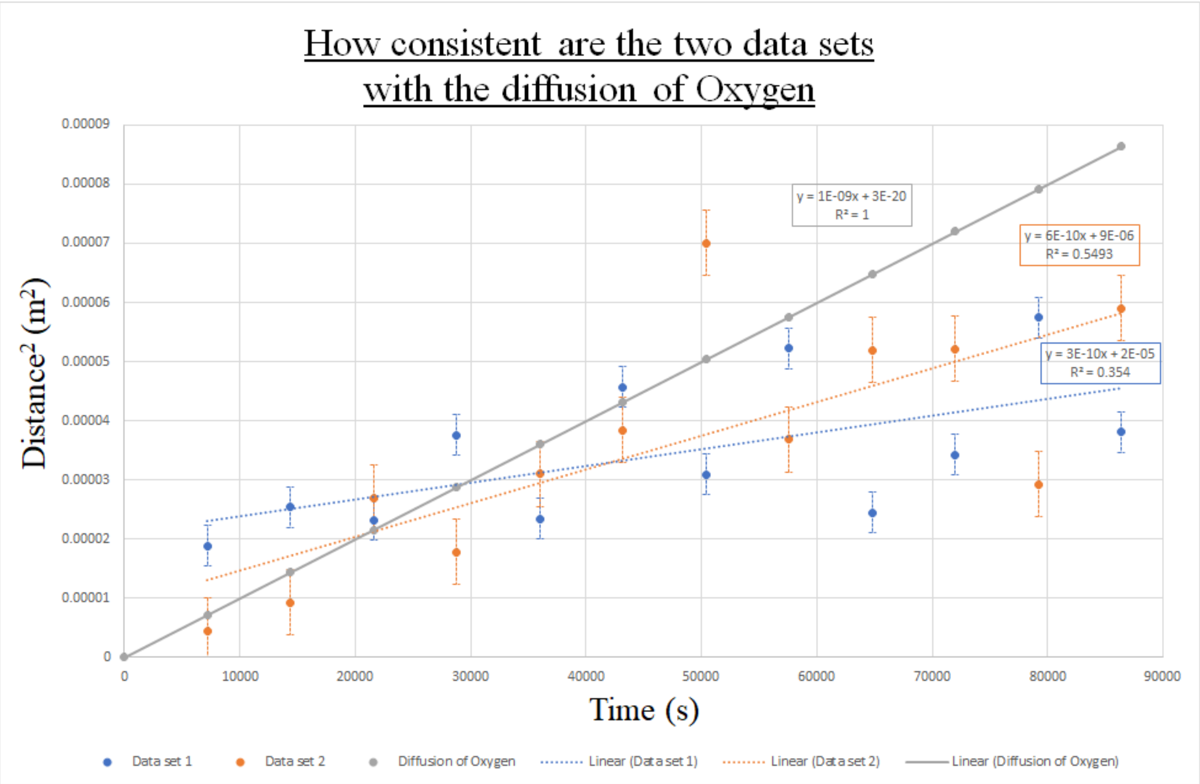
-Rearranging so that the equation can be graphed to find a value for the diffusion constant (Λ):

$$d^2 = \Lambda t$$

3)b) i) ii) iii) Which data set is consistent with diffusion

-Both sets of data have noise in them so neither one will follow the functional form perfectly. Hence we must look for the best fitted data set, this will be done using various methods, as per below.

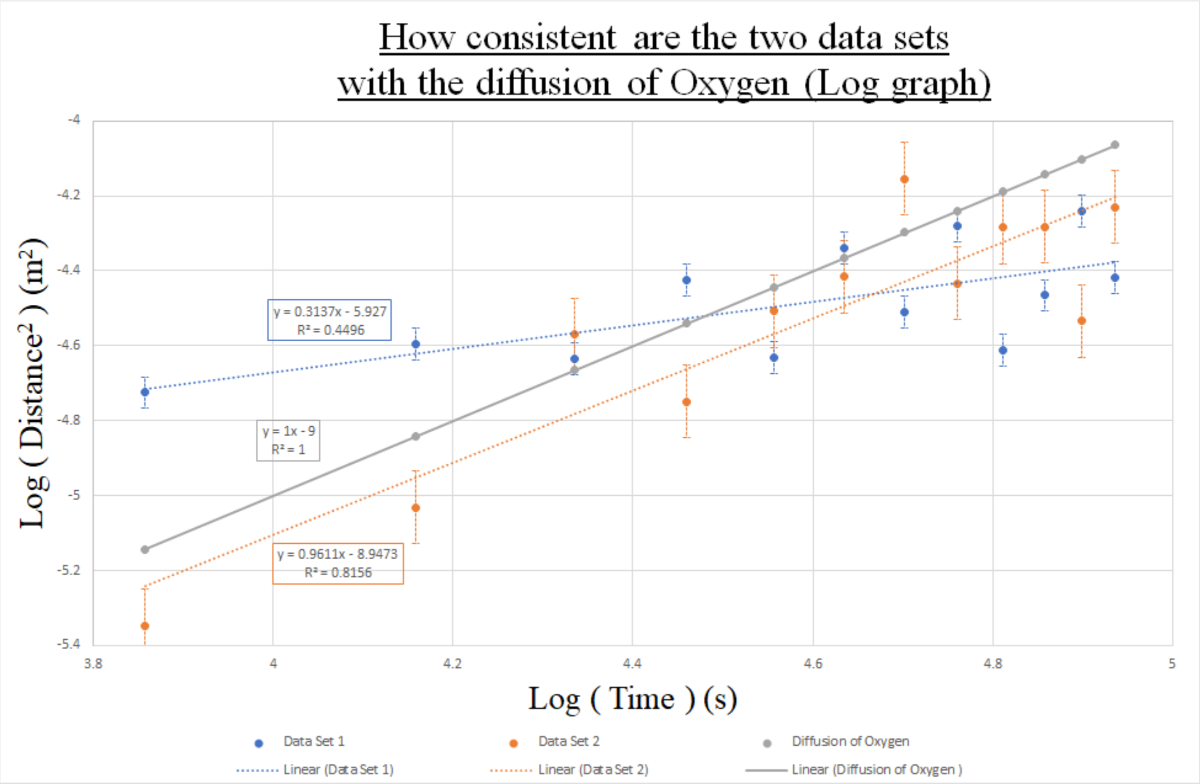
-The following graph has both data sets plotted along side the diffusion data set taken from the theoretical values given and the above equation in 3)a)



-The error bars were created from standard error of the given data sets. From this graph it can already be seen that data set 2 (in orange) is a much closer fit then that of data set 1. Not only having more data points falling within the error margin but also with the line of best fit showing to fit better with the diffusion line of best fit.

-It can also be seen that data set 2 is approaching zero much more than data set 2. Of course, this could still be just noise so more analysis is needed.

-A log graph was then plotted to further see the relationship between the two data sets and the diffusion.



-As seen in this graph the theory that data set 2 is the one consistent with diffusion is definitely backed up here. Aligning it self with the data from the diffusion constant $1x10^{-9}$.

-Looking at the gradient values and R^2 values from the above graphs it can also be seen the gradient from data set 1 is further from the standard, and hence not the one that is consistent with diffusion

Linear graph

	Data set 1	Data set 2	standard
gradient	3x10^-10	6x10^-10	1x10^-9
R^2	0.354	0.5493	1

log graph

	Data set 1	Data set 2	standard
gradient	0.3137	0.9611	1
R^2	0.4496	0.8156	1

To conclude data set 2 is clearly the consistent set with diffusion. Even with its observed noise, its main points show it to clearly be consistent. Data set 1 even with noise disregarded still does not have enough to represent it as a data set consistent with diffusion.