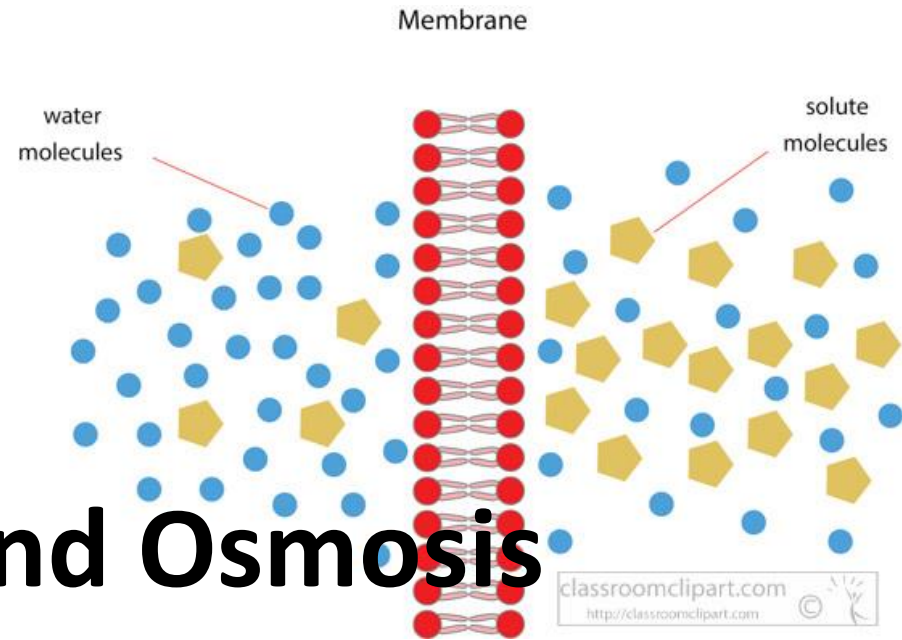


Diffusion and Osmosis



EGA219 – CONTINUOUS ASSESSMENT 2022

Lab session 1 and 2

MATLAB modelling of diffusion and osmosis

You will write a short scientific report based on your model and outputs

30% of module mark

Lab sessions will run on **Thursday the 1st December and 8th December from 12.00 to 14.00 in Y Twyni PC lab 101.**

During the remaining time you can focus on formulating your results and writing your report

Lab session 1

- Recap on the main principles of diffusion
- Lab session – MATLAB modelling of diffusion
- Population level analysis of molecular diffusion in time and space

Diffusion & Osmosis

1. Create a MATLAB model
2. Write a technical report on the model and its outputs

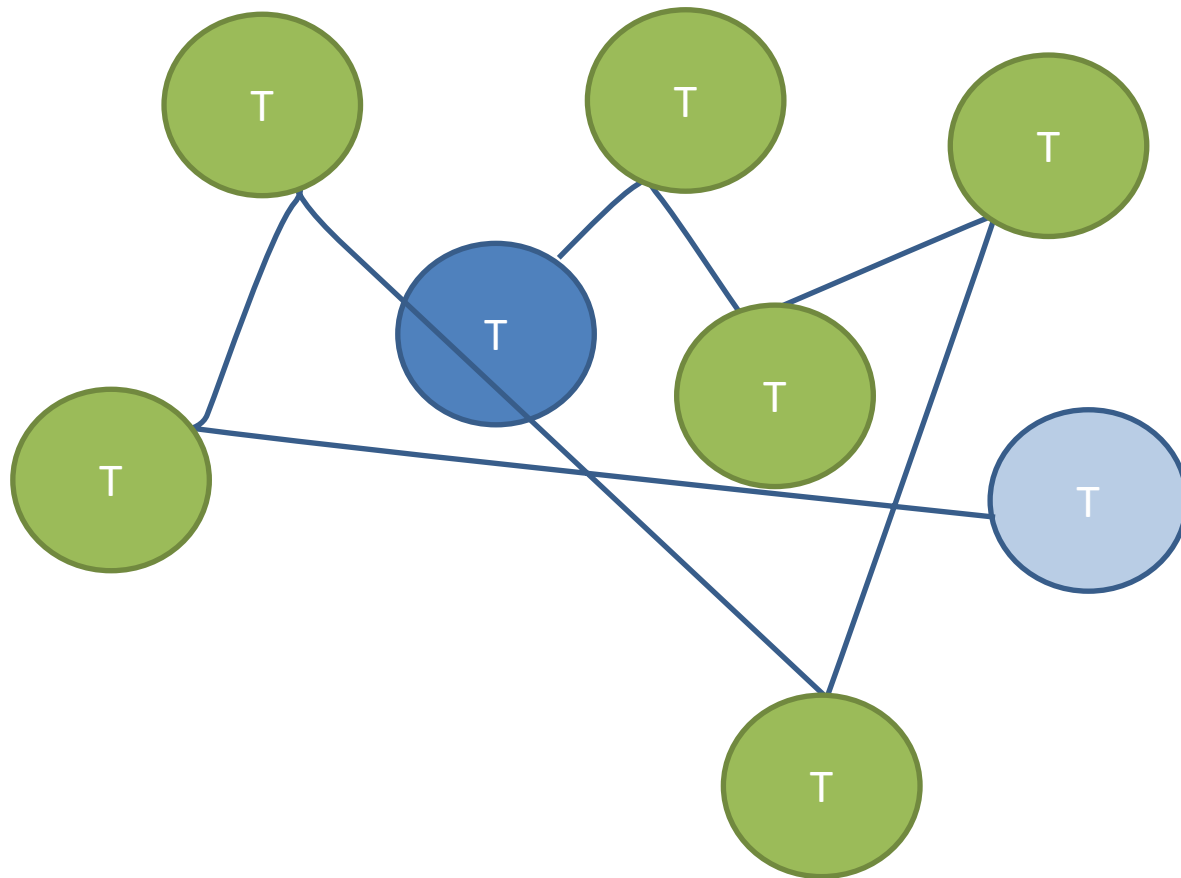
The 30% marks will be based on the written report and the **inclusion of a fully working code as part of the appendix**

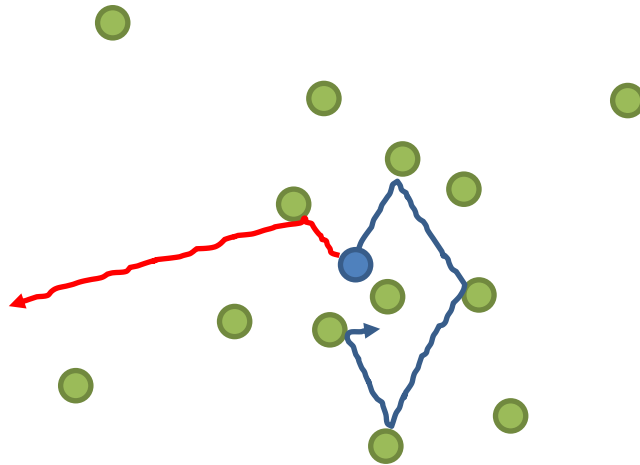
Recap – Diffusion

<https://www.youtube.com/watch?v=2psBnet1VXg>

Background

The biology of the cell is determined by molecular interactions. So fundamentally, we need to understand the motion of molecules due to their thermal energy.





Molecules move in random directions

BUT

Due to density differences there is an overall **diffusion** of molecules

Diffusion

The term *diffusion* relates to any particulate system, in this course we specifically use it to refer to molecular diffusion –

‘the motion of molecules due to their thermal energy’

In particular the thermal motion of molecules leads to a net flux of molecules from regions of high concentration to regions of lower concentration, i.e. there is an overall flow of molecules *down a concentration gradient*.

Mathematically this net flux is described by Fick’s laws of diffusion (Adolf Fick, 1855):

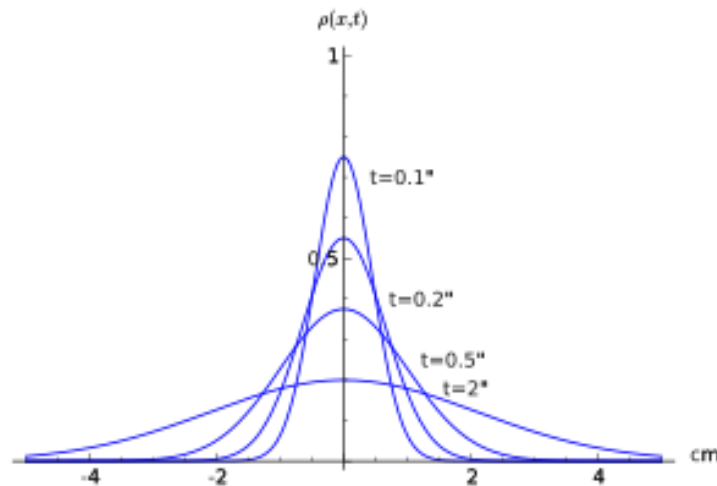
1st law – diffusive transport is driven by concentration differences: $J = -D \frac{\delta\Phi}{\delta x}$

J – flux, D – diffusion constant, Φ – concentration

2nd law – the rate of change in concentration over time is dependent upon the change in slope of the concentration gradient:

$$\frac{\delta \Phi}{\delta t} = -D \frac{\delta^2 \Phi}{\delta x^2}$$

Change in Φ over time



What is the diffusion coefficient, D ?

1906, Albert Einstein provided a theoretical explanation of Brownian motion based on atomic and molecular collisions. In this he defined, D :

$$D = \frac{k_B T}{6\pi\eta r}$$

k_B - Boltzmann's constant, η - viscosity, r - particle radius

Stokes-Einstein equation

$k_B T$ - the thermal energy available (drives molecular collisions)

r - the size of the molecule

$$D = \Delta x^2 / 2\Delta t$$

for small molecules, $D = 6 \times 10^{-8} \text{ cm}^2 \text{ s}^{-1}$

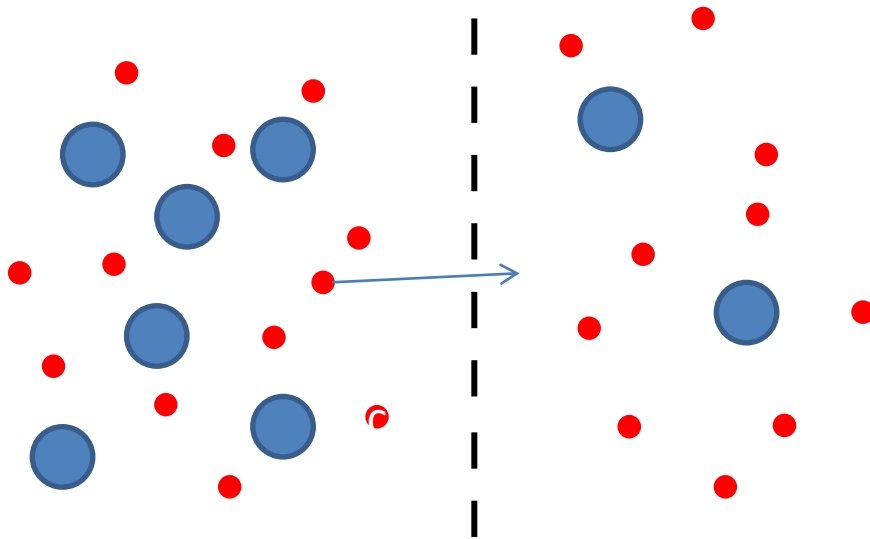
So for

$$\Delta x = 1 \mu\text{m}$$

$$\Delta t = 83 \text{ ms}$$

Consider the diffusion of molecules of 2 types, the molecule of interest (e.g. sugar) AND the solvent molecules which surround it (e.g. H_2O)

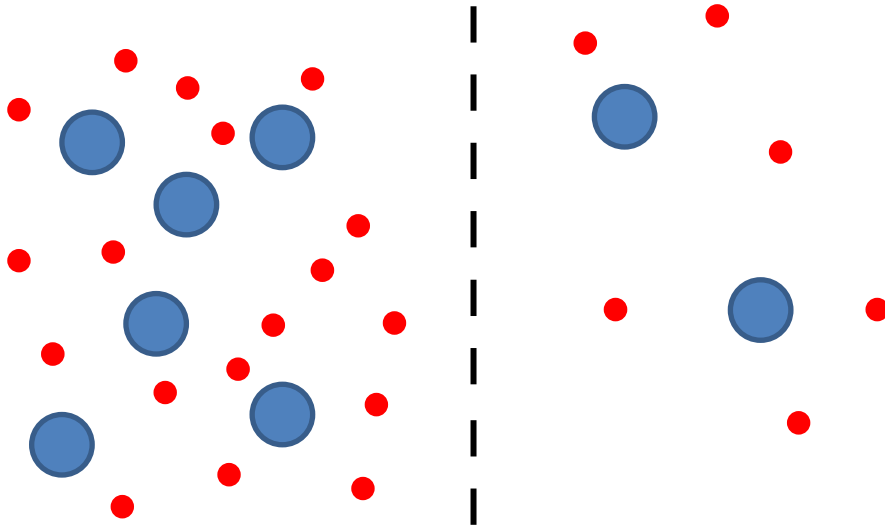
Also, imagine a semi-permeable membrane through which solvent molecules can pass but solute molecules cannot



Over time both molecular species will diffuse due to concentration gradients

BUT

Only the solvent molecules can pass through the membrane



The solvent molecules will move across the membrane to produce an equilibrium state (no further change) in which there is an equal concentration of solute on both sides

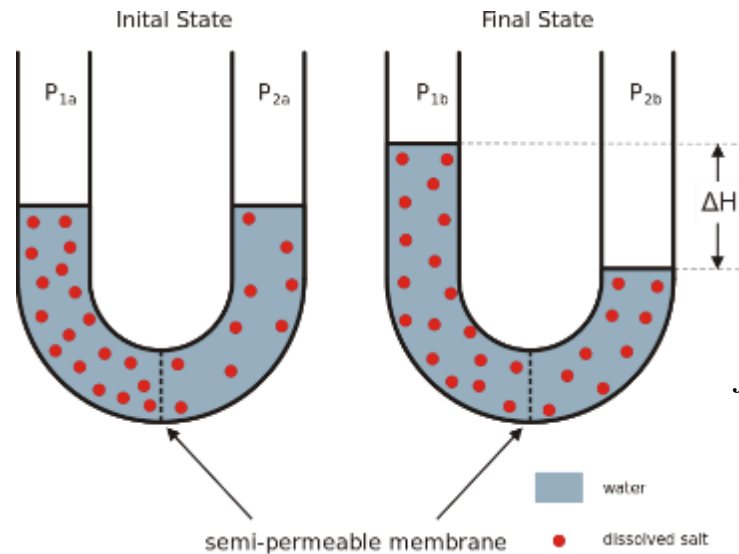
This is the process of OSMOSIS

Osmosis

Osmosis occurs in solutions in which there is a semi-permeable membrane allowing passage of solvent (e.g. water) but not solute (e.g. Na^+ ions).

The process operates to equalise the solution concentration, e.g. water transport into a cell due to high concentration of sugars, ions, proteins etc. in the cell.

The transport of the solvent across the membrane creates a pressure difference – *osmotic pressure*.



from Wikipedia

Cells are bound by a semi-permeable membrane through which water molecules may pass

Thus water flows in or out of the cell depending upon whether the ion/sugar/salt concentration is greater inside the cell than the surrounding environment

Typically cells build up local concentrations of molecules and have a positive osmotic pressure as a result

Recommended watching:

<http://www.khanacademy.org/video/diffusion-and-osmosis?playlist=Biology>

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Diffusion and Osmosis

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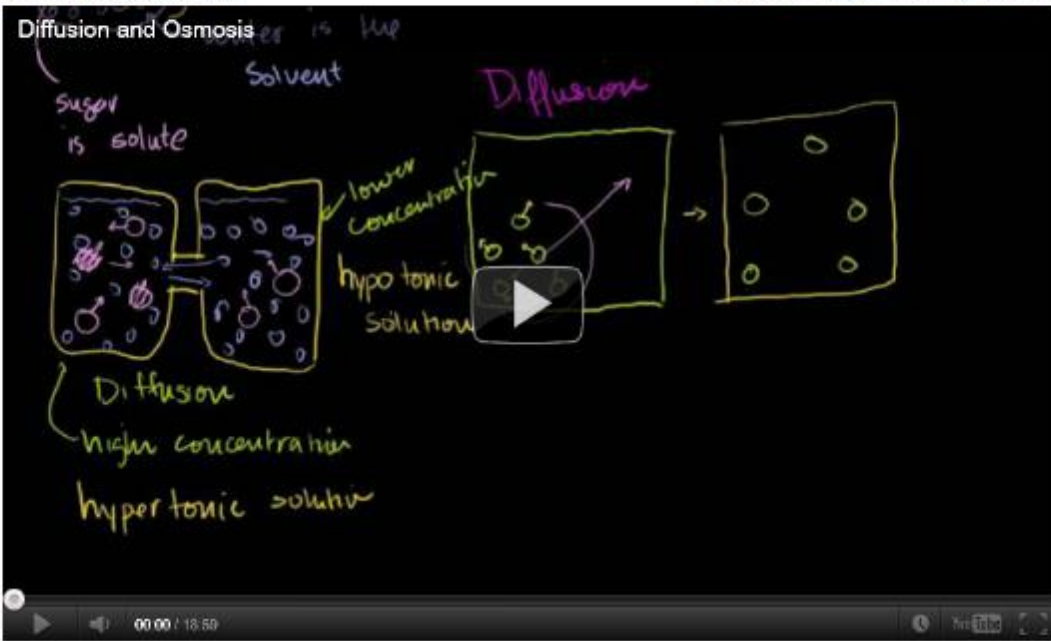
Diffusion and Osmosis

Solvent is the
sugar is solute

Diffusion

lower concentration
hypo tonic solution

higher concentration
hyper tonic solution



- You should aim to complete this assignment by next week
- Final deadline for this assignment, along with assignment 1 will be **Monday December 19th at 16.30.** A link will be provided on blackboard
- You should provide working code for the questions to gain all of the available marks

Analysis of molecular diffusion in time and space

In this assignment you will develop a computer model that mimics the random steps of molecules undergoing Brownian motion.

Create a MATLAB programme which:

- Tracks the motion of 300 molecules within a 2-D space, over a series of time steps
- On each time step every molecule will move by a random amount in the x and y directions
- Your model needs to calculate the steps in space for all 300 molecules, store them in an array and repeat this for 100 time steps
- Start the model with all molecules at the $[0,0]$ point
- At each time point plot the position of the molecules in a scatter plot and run this for all time points so that a 'movie' of the molecular motion is created

Population level analysis of molecular diffusion in time and space

In this assignment you will consider the motion of molecules as a collection rather than as individuals. This will allow you to compare behaviour to Fick's laws.

Amend your MATLAB model of a single set of diffusing molecules (no membrane) :

- Create a histogram of the x-position values at each time point
- Plot out the histogram for each time point, again as a movie so that you can visualise the sequence
- Create a 2-D histogram so that you can visualise the spread in molecular concentration in x and y directions
- You should also plot out the mean and standard deviation of the x and y position of your particles through time

Additional step

- You should assign units to each time step and step size being enforced by your code, clearly state these units and adjust these to increase the Diffusion coefficient being applied by a factor of two.

Analysis of molecular diffusion in time and space – with a semi-permeable membrane - Osmosis

In this assignment you will adapt your computer model to mimic Osmosis – the diffusion of two molecular species in the presence of a semi-permeable membrane.

Alter your MATLAB code to:

- Track the motion of two sets of 300 molecules within a 2-D space, over a series of time steps
- Model the effect of a membrane placed at $x=-2$, one of the molecule types can diffuse through the membrane, the second is reflected by it
- You will need to think about what happens to Δx and Δy upon reflection
- At each time point plot the position of the molecules in a scatter plot and run this for all time points so that a 'movie' of the molecular motion is created. Represent the two molecule types with different markers so that you visualise the different movement of solvent and solute molecules.
- Remember to place each type of molecule either side of the membrane
- At the end of 40 time steps consider the **net** flux of the solute molecules across the membrane. (Number of particles moving past a given region per unit area per unit time))

Technical Report

You need to write a short report

- deadline for submission **FRIDAY 10th DECEMBER**

This should include:

1. A description of the processes of diffusion and osmosis
2. An explanation of how you created a model that mimics these processes and the underlying theory
3. A description of the simulations that you ran with the model
4. Presentation of the results from the simulations
5. A brief discussion on what the results show

The purpose of the exercise is to learn about:

- building a computer model
- Using the model to simulate a specific situation
- Explaining the outputs from the model in technical language
- **You should discuss some limitations associated with your simplified model**

Marks will be awarded for

1. Clear and precise explanation of the processes and the coding used to model them
2. High quality presentation of data, figures, equations and references
3. Discussion on why the particular algorithms were chosen and how they mimic the processes of diffusion and osmosis