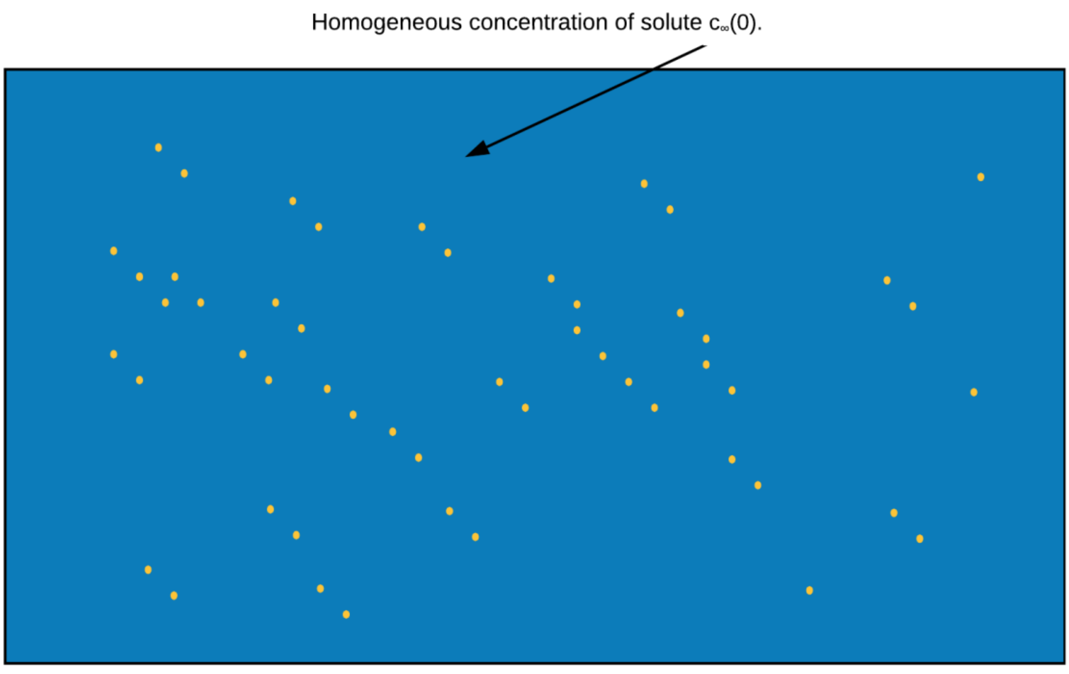
<u>30-01-2020 Meeting Minutes – Nanoparticles Case Study</u>

<u>General Remarks</u>

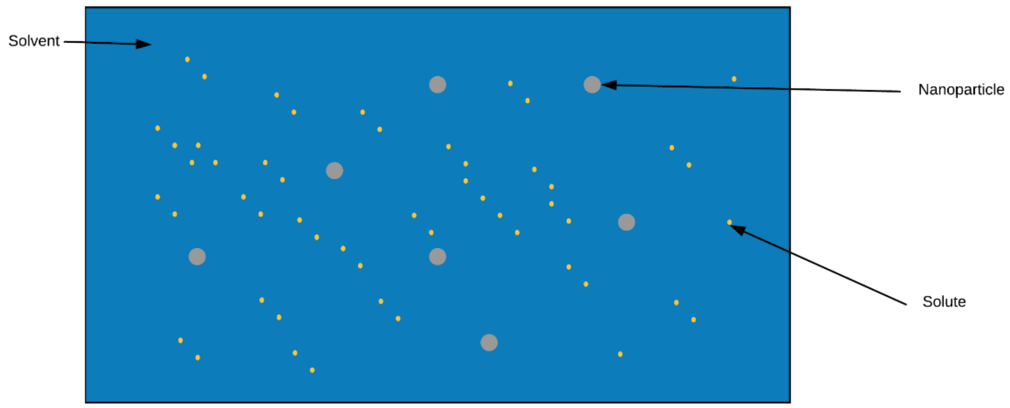
- The case studies for this course are loosely structured.
    - There is not a fixed plan of exactly what we need to produce/investigate.
    - We have the freedom to take the project in any direction we want.
- The idea of this project is to harness modelling skills and apply them to a physically motivated scenario.
    - We need to derive a system of governing equations from first principals.
    - We need to perform analysis of the resulting equations.
- In this session we begin by discussing the physical system of interest, which is essentially a precipitation reaction.

<u>Physical Scenario (the formation of Nanoparticles)</u>

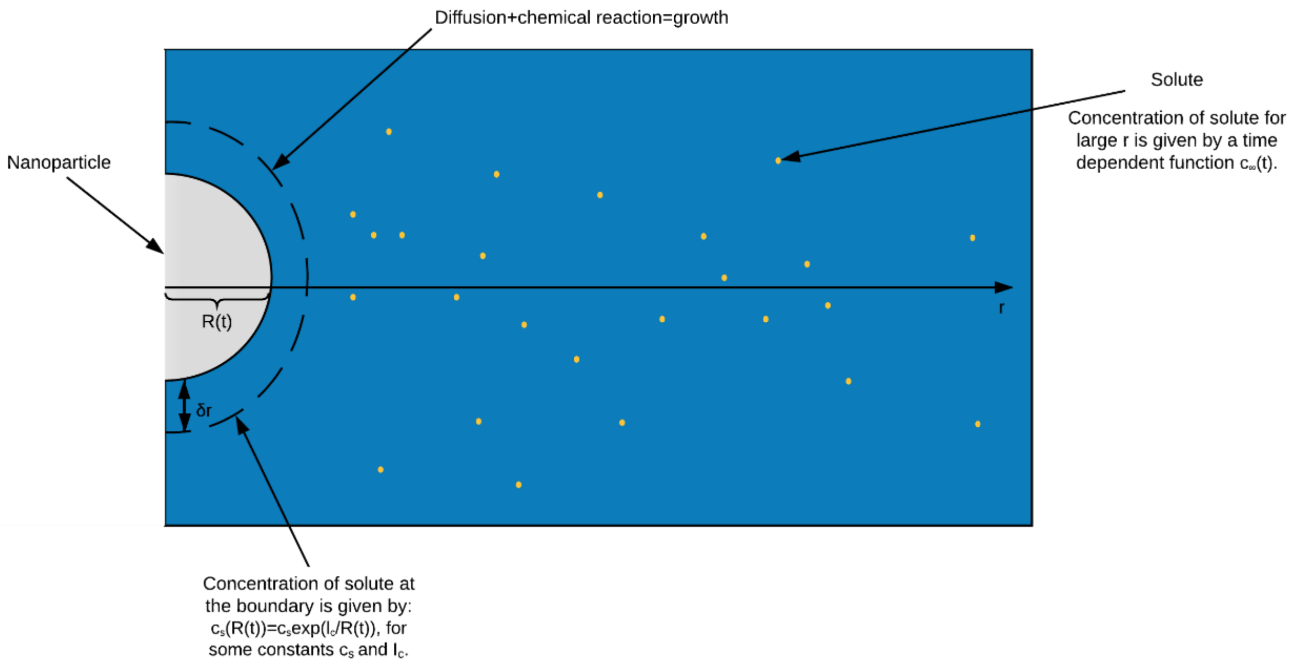
- We begin with a homogeneous solution of a solid material (the solute) which has been dissolved in a fluid (the solvent).



- Via a change in temperature or some external force, this reaction nucleates to form larger clusters/balls of solute particles (which are known as nanoparticles)

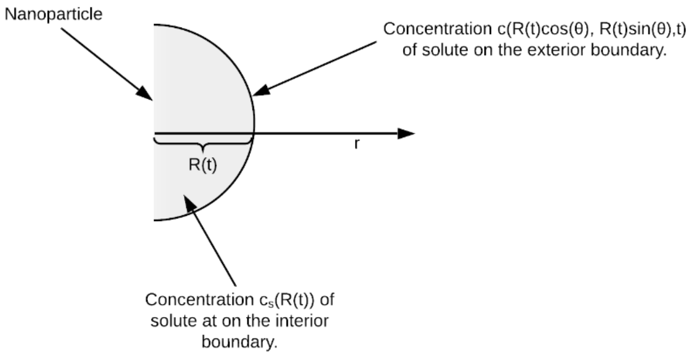


- We note that the transition from spatially homogeneous concentration, to inhomogeneous concentration occurs on a much faster time scale then the reactions governing the growth of the nanoparticles. Therefore we may neglect the origin of these nanoparticles in our model.
- These nanoparticles then begin to grow in accordance with the concentration of the solute on their external boundary.

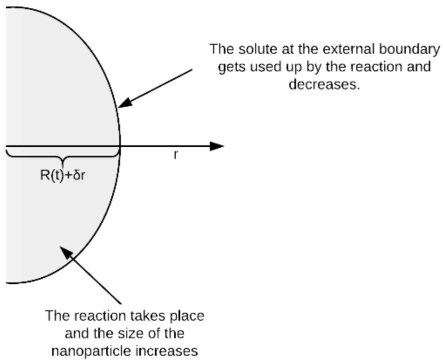


- For simplicity we look at a single nanoparticle which is growing in the fluid.
  - The nanoparticle grows until it reaches as equilibrium in which the concentration of the solute on the edge of the nanoparticle ($c_s(R(t))$) is equal to the concentration of the solute in the fluid at a large distance away from the nanoparticle ($c_\infty(t)$).
  - If the solubility of the nanoparticle is less than the concentration of the solute in the fluid on the external boundary r=R(t) then the nanoparticle grows.
  - Otherwise it dissolves back into the fluid.

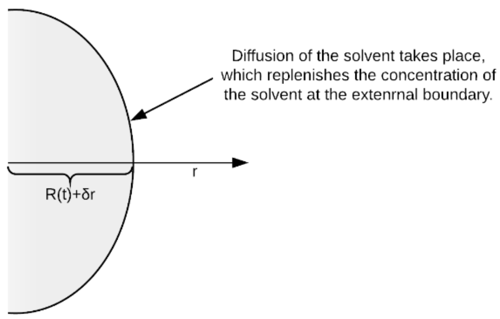
- We initially assume constant position (i.e. the nanoparticle is stationary) but could extend our model later to consider the case when the fluid is moving.
    - The growth process of the nanoparticle proceeds as follows:



- Assuming that the concentration is sufficiently high at the boundary, the nanoparticle expands and consumes the solvent particles on the boundary.



- The natural diffusion of the solvent then replenishes the consumed solute particles at the boundary.



- Equilibrium is reached when $c_s(R(t))=c_\infty(t)$.

Possible Project Progression

- Start by considering a single nanoparticle and formulate it as a PDE.
  - Initially we assume that the nanoparticle is stationary in the fluid and position the coordinate axes at this centre.
  - We can then investigate to see if there is a critical initial size $R(0)=R_0$ such that when the initial size is larger than this the nanoparticle grows and otherwise it dissolves back into the fluid.
  - We can look at how the behaviour of the system changes by adjusting the limiting factor in the reaction (i.e. what happens when diffusion is much faster than the reaction or vice versa).
  - Can then look at generalising our model to consider the case when the nanoparticle may move in the fluid, or the fluid has a specific flow (e.g. do certain types of flow help with nanoparticle growth).
- We can then consider how to expand our model so that it contains lots of particles, where each particle is governed by a PDE.
- We can then look at simplifying the model so that we have a single governing PDE, instead of a vast system of them.
- We can then look at computing numerical simulations, additional analysis and comparison with real world data.

Additional Notes

- Can think of this problem in terms of energy:
  - The system gains energy from diffusion but has a cost of surface growth.
  - Classical nucleation theory explains the balance between energy gain and surface cost.