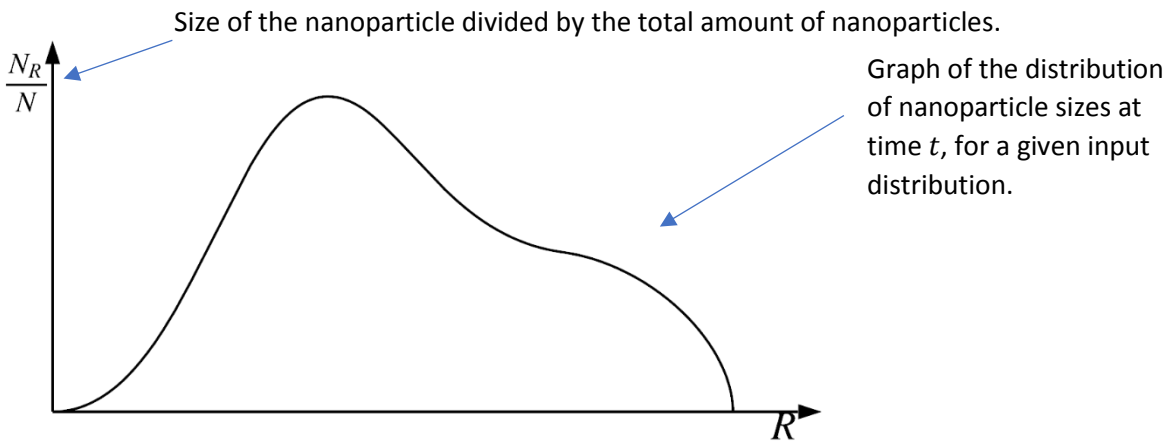
13-02-2020 Meeting Minutes – Nanoparticles Case Study

General Notes

- The derivation that we sent to our supervisor was correct, however in our substitution for c_1 we didn't include the scaling and translation terms that arise from the non-dimensionalisation process.
    - Therefore, in terms of non-dimensionalised variables, our ODE for R can be written as: $\frac{dR}{dt} = \frac{\hat{c}_\infty(0) - c_s^* e^{\frac{l_m}{R}}}{\Delta c\,(D_a + R)}$.
    - l_m is the capillary length.
    - D_a is the Damköhler number.
    - $\hat{c}_\infty(0)$ is the concentration of the solute in the solution at our boundary at infinity.
    - Δc is the scaling factor $\Delta c = \hat{c}_\infty(0) - \hat{c}_1(R(0))$.
        - This scaling factor corresponds to the initial concentration gradient in our system, which is the driving force in our system.
    - It is important to note that $\hat{c}_1$ in non-dimensional form ($c_1(R(t)) = \frac{\hat{c}_1(R(t) - \hat{c}_\infty(0)}{\Delta c}$) is negative.
- Since we are considering the case where $\hat{c}_\infty(t)$ is constant, our existing model may be used to describe the growth of n independent nanoparticles in our solution (e.g. by introducing $R_1, R_2, \dots, R_n$ which all satisfy our ODE for R as above).
    - It is important to note that the individual particles only interact through (are coupled by) the boundary term $\hat{c}_\infty(t)$.
- It would be useful to understand the dynamics of the one nanoparticle case/system with constant boundary condition $\lim_{\hat{r}\to\infty} \hat{c}(\hat{r}, \hat{t}) = \hat{c}_\infty(0)$, before proceeding to model multiple nanoparticles.
- For our complete system, the free boundary dynamics problem is very similar to Stephan problems, which will be covered in our Further Partial Differential Equations class this week.
    - Therefore, it would be useful for everyone to either go to the Further Partial Differential Equation lectures next week (or look at Section 2 in the corresponding lecture).
- Is it worth generalising our model to the case when we do not have radial symmetry?
    - The governing equations become very complicated when we introduce dependence on the angles θ and ϕ, so it may not be useful to pursue this direction.
- Now that we have devised the main system of governing equations, there are lots of different directions in which we can take the project.
    - It may be useful to divide our team in order to pursue different directions concurrently.
- It is important to not lose sight of the original goal of the project.
    - The ultimate aim is to use mathematical models to determine a size distribution of nanoparticles for an arbitrary function $\hat{c}_\infty(t)$.
        - $\hat{c}_\infty(t)$ corresponds to the concentration of solute at the boundary $r \to \infty$.
        - We want to find the optimal way to vary the boundary concentration $\hat{c}_\infty(t)$ (which is controlled by adding solute to the solution), in order to produce a uniform distribution of nanoparticles.



- It is important to note that for the case when we have multiple particles, we start with a distribution of initial sizes $\hat{R}_1(0), \hat{R}_2(0), \dots, \hat{R}_n(0)$ (which is not the same for all n).
  - When our initial size distribution is uniform, the nanoparticle sizes remain uniform (for all time) and we have that Ostwald ripening does not occur.

<u>Possible Project Directions to Consider</u>

- Necessary conditions for Ostwald ripening
  - Is there a necessary size difference threshold in order for Ostwald ripening to take place in the two particle version of our model?
  - Can use liner stability analysis to classify any fixed points for the radius of our nanoparticle.
- Asymptotics
  - Could try to find analytic solutions in the cases when either when $D_a \gg 1$ or $0 < D_a \ll 1$.
- We can consider the case when $\hat{c}_\infty$ has time dependence and see how this changes our model.
  - $\hat{c}_\infty$ time dependence does not have a significant affect on the case when we are only considering a single nanoparticle in our system.
  - In the case when we have multiple nanoparticles, $\hat{c}_\infty$ is very important as nanoparticles are only coupled via the $\hat{c}_\infty$ term in our ODE.
  - Could attempt to model two nanoparticles in our solution to observe Oswald ripening.
- Numerical Solutions
  - This would be useful because we can only find an expression for the solution to our ODE in terms of the exponential integral (which is not something that can be easily computed).
  - Parameter Recovery (using the Peng data set)
    - It is important to note that in order to compare our data with the experimental data provided, we must either non-dimensionalise the Peng data or dimenisonalise the output from our numerical simulations of the non-dimensional model.
    - We can infer values for parameter c_s^* from the Peng paper (the data has been emailed to use by our supervisor).

        - We can therefore eliminate the free parameter c_s^* from our model, so that the only free parameter it contains is the Damköhler number D_a.
            - In practice we may have more parameters to play with, since our non-dimensionalisation scaling depends on physical parameters.
        - We can do parameter fitting manually, by looking at the solution curves for our ODE and adjusting the parameters by hand.
        - We could alternatively formulate the parameter minimisation process as an optimisation problem and attempt to solve.
        - Useful to see if we get something that is the same shape as the provided data.
    - Can solve for both the full system and the simplifies ODE for R numerically.
        - We can then compare the two results to see when our simplified system is valid.
        - For solving the full system, we need to solve for both R and c_3 at each time step.
        - We also need to scale the mesh grid so that the free boundary is no longer moving. (e.g. could use the change of variables $\rho = \frac{r}{R(t)}$ and substitute into our ODE and PDE).
        - We can also use special numerical methods to deal with shifting boundaries.
            - However, these are computationally expensive, because we need to constantly re-mesh and re-interpolate at every time step of the process.

<u>Possible Plan of Action</u>

- Group has been divided into two sub-groups:
    - Lewis and Shyam
        - Focusing on Numerical simulations of existing work.
    - Peifeng and William
        - Focusing on asymptotic analysis of the equations.
- Everyone should choose a particular item from the list of possible project directions provided by our supervisor (or any other direction that they think is appropriate) and pursue it.
- It would be useful for us to meet again early next week to discuss the progress we have made in our chosen area, prior to the meeting with our supervisor on Thursday.