18-02-2020 Meeting Minutes – Nanoparticles Case Study

General Notes

- Mistake in the previous minutes:
    - The ODE for R on our long timescale is given by: $\frac{dR}{dt}(t) = \frac{\hat{c}_\infty(0) - c_s^* \, e^{\frac{l_m}{\hat{R}(0)R(t)}}}{\Delta c \, (D_a + R(t))}$.
- Asymptotics
    - When $D_a \gg 1$ the right-hand side of our governing ODE becomes zero and hence the nanoparticle remains the same size.
    - When $D_a \ll 1$ and we assume that there is a constant boundary condition at infinity (i.e. $c_\infty(t) = c_\infty(0)$) we can use that for large values of t and $R(t)$ we may approximate our exponential term by a constant.
        - This gives us that for large time and small Damköhler number, the growth of our nanoparticle has a square root dependence on time (i.e. $R(t) \sim \sqrt{t}$).
    - We can find an expression for the boundary condition at infinity by using a conservation of mass argument, which yields:
        - $c_\infty(t) = c_\infty(0) - \frac{4\pi N_0}{3V_m}\left(\hat{R}(0)R(t)\right)^3$ for the case of one nanoparticle.
    - By substituting out time dependent boundary condition at infinity into our ODE for R we get more complicated asymptotic behaviour.
- Numerics
    - Initially found that when using the constant boundary condition at infinity, our nanoparticle never saturates, it simply continues to grow forever.
    - It is more appropriate to use a time dependent boundary condition at infinity (even when we are considering only a single nanoparticle), which is given by Equation (26) in: https://arxiv.org/pdf/1901.08990.pdf?fbclid=IwAR0pAeutJR0zm74UTRQ6YDZfAY5i42AYoy_JS-QHBgld4u4qXSrswl96D3g and can be derived by using conservation of mass.
    - Are now able to better replicate the simulation data provided by our supervisor.

Plan of Action

- William
    - Write up the derivation of the asymptotic behaviour when $D_a \gg 1$ for large time, when the boundary condition c_∞ depends on time.
    - Bring a copy of this derivation to our meeting on Thursday.
- Peifeng
    - Write up the derivation of the asymptotic behaviour when $D_a \gg 1$ for large time, when the boundary condition c_∞ does not depend on time.
    - Bring a copy of this derivation to our meeting on Thursday.
- Shyam and Lewis
    - Produce a numerical simulation of our ODE model for the growth of a single nanoparticle, by using the parameters provided in the Peng paper and compare with the data provided by our supervisor.
    - Bring a copy of the code on a laptop to our meeting on Thursday so that it can be demonstrated.

- If time permits, then try and work on developing a numerical simulation for the case when there are multiple nanoparticles in the solution.