04-02-2020 Meeting Minutes – Nanoparticles Case Study

General Notes

- Nondimensionalisation
    - We have found that by using the change of variables $\hat{r} = kr$ and $\hat{t} = Dk^2 t$ our equations simplify:
        - We get that our partial differential equation simplifies so that the diffusion constant D is removed.
        - We get that the $\frac{1}{k}$ factor in the robin boundary conditions at $r = R(t)$ is removed.
    - When using the suggested scaling: $\hat{c}_3(\hat{r},\hat{t}) = \frac{c_3(\hat{r},\hat{t})}{c_\infty(0)}$ we found:
        - Our PDE does not change.
        - The right hand side of the boundary condition at $r = R(t)$ is divided by a factor of $c_\infty(0)$.
        - The right hand side of the boundary condition at infinity becomes: $\frac{c_\infty(\hat{t})}{c_\infty(0)}$.
        - The right hand side of our initial condition reduces to 1.
    - When using the suggested scaling: $\hat{c}_3(\hat{r},\hat{t}) = \frac{c_3(\hat{r},\hat{t}) - c_\infty(0)}{\Delta c}$ we found:
        - Our PDE does not change.
        - The right hand side of the boundary condition at $r = R(t)$ becomes: $\frac{c_1(t) - c_\infty(0)}{\Delta c}$.
        - The right hand side of the boundary condition at infinity becomes: $\frac{c_\infty(t) - c_\infty(0)}{\Delta c}$.
        - The right hand side of the initial condition reduces to 0.
    - We are unsure how to pick Δc since there is no natural choice.
        - Ask supervisor on Thursday how we are supposed to pick this scaling factor.
- Timescales
    - The Damköhler number in out model corresponds to the ratio: $\frac{k}{D}$.
        - When this quantity is very large it corresponds to the chemical reaction dominating the system (i.e. $D \ll k$).
        - When this quantity is very small it corresponds to the diffusion process dominating the system (i.e. $k \ll D$).
        - Would be useful to see if we can perform a substitution that introduces a factor of either $\frac{k}{D}$ or its reciprocal into our governing equations, so that we may use asymptotics to analyse the behaviour of this system in the two extremes.

Plan of Action

- William will update the Overleaf document so that the equations are consistent with those provided by our supervisor.
- Lewis will update the Overleaf document to explain how our change of variables from (r, t) to $(\hat{r}, \hat{t})$ simplifies our system. He will also add the equations we get when using the substitutions for $\widehat{c_3}$ suggested by our supervisor, so that we can show him why it is not clear how to pick Δc.

- Shyam and Piefeng will attempt to see if there is a time scaling (change of variable for t) which can be made to introduce either a factor of $\frac{k}{D}$ or $\frac{D}{k}$ into our governing equation and look at any asymptotic analysis (i.e. setting either $0 \ll \frac{k}{D} < 1$ or $0 \ll \frac{D}{k} < 1$).