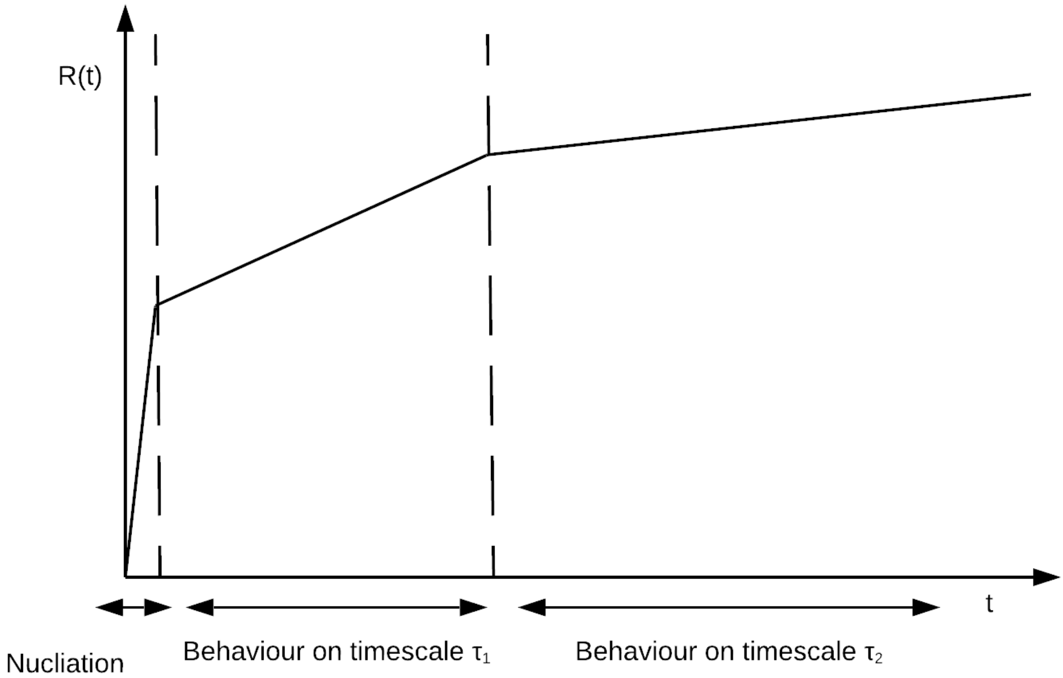
06-02-2020 Meeting Minutes – Nanoparticles Case Study

General Notes

- Our attempted non-dimensionalisation was incorrect as our length scaling was not right.
- The value of k is generally unknown, so it is not a good idea to use any scaling that involves D/k or any terms involving k.
    - We don't know the size of the Damköhler number ($D_a = \frac{D}{R(0)k}$), so we can't use it in our parameter scaling.
    - By looking at the cases when $D_a \gg 1$ and $0 < D_a \ll 1$ (which correspond to either reaction or diffusion dominating), our boundary condition at $r = R(t)$ becomes either Dirichlet or Neumann.
- It makes more sense to scale r in terms of $R(0)$, since that is the natural length scale of the problem.
- Using this length scaling will result in two different time scales τ_1 and τ_2, which may be obtained by balancing the order of each of the terms in our governing equations.
    - By looking at our system on each of the two different timescales, we should be able to find an analytic solution to our equations.



- Although nanoparticle growth is continuous, the nucleation stage is so rapid, that we can collapse it to $t = 0$.
- $\Delta c = c_\infty(0)$ is not a good scaling because an order 1 change in the non-dimensional c_3 corresponds to an order $c_\infty(0)$ change in the dimensional quantity $\hat{c_3}$.
- We should choose Δc in order to balance the order of terms in equation.
    - The choice of Δc should come from balancing the magnitude of terms in the boundary condition at $r = R(t)$.

- The solubility c^* is not known, but we might be able to determine this quantity from experimental data.
- There is data in the peng paper which we may be able to compare our numerical results to
- Ultimate case study goal:
    - Predict how $R(t)$ behaves for different $c_\infty(t)$ functions, so that we can find an optimal choice of $c_\infty(t)$ that best facilitates nanoparticle growth.
- Scaling space with the moving boundary $R(t)$ is essential for producing numerical solutions however, it is not helpful when trying to find analytical solutions.

<u>Non-dimensionalisation Remarks</u>

- The idea of non-dimensionalisation is to make our problem more convenient in terms of expressing the underlying physics which is driving the system.
- Don't necessarily want to remove all the constants in non-dimensionalisation.
- In our particular problem, the non-dimensionalisation will allow us to identify the dominant behaviour of the system.
    - Our system will contain two timescales
        - One is associated with diffusion (comes from the PDE).
        - One is associated with the growth of the nanoparticle (comes from the ODE).
- What should you have in mind when non-dimensionalising?
    - Want to make our system simpler.
    - Want to capture the main physical processes driving the system.
    - Want to eliminate physical constants from the equations.
    - In non-dimensionalised form we want all the terms to be of the same order/magnitude.
    - When done correctly, non-dimensionalisation allows us to see which terms may be neglected in particular limits (e.g. because they are very small).

<u>Tasks from Supervisor</u>

- Attempt to non-dimensionalise our system correctly:
    - We may begin by considering the case where the boundary condition at infinity is time independent (i.e. $c_\infty(t) = c_\infty(0)$).
    - Use the length scale $r = \frac{\hat{r}}{R(0)}$.
    - Find two distinct timescales τ_1 and τ_2 for our system.
        - One timescale is given by the Damköhler number, which is the nondimensional number: $D_a = \frac{D}{R(0)k}$.
    - We should use the boundary condition at $r = R(t)$ to find a natural choice for Δc.
        - This should be of the form: $\frac{D\Delta c}{R(0)} = k\big(c_1(0) - c_3(0)\big)$
- We should then be able to introduce a parameter $0 < \varepsilon \ll 1$, which is the ratio between our two timescales τ_1 and τ_2. This parameter should appear in the left hand side of our PDE, so that it is of the form:
    - $\varepsilon \frac{\partial c_3}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial c_3}{\partial x}\right)$
    - We then use this to set the left hand side equal to zero, which gives us an ODE for c_3, which corresponds to its quasi-steady state.
    - We will then get an ODE for R.

- We should then look at using MATLAB to find solutions to the ODE for R.
- We should then think about how to incorporate multiple nanoparticles into our system and note that in this case c_∞ will depend on time.