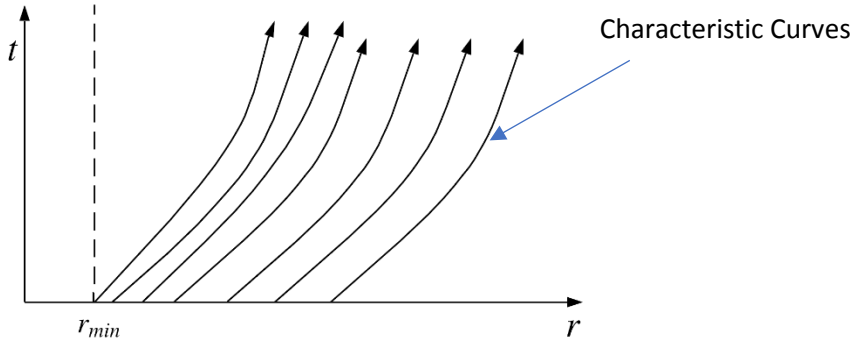
27-02-2020 Meeting Minutes – Nanoparticles Case Study

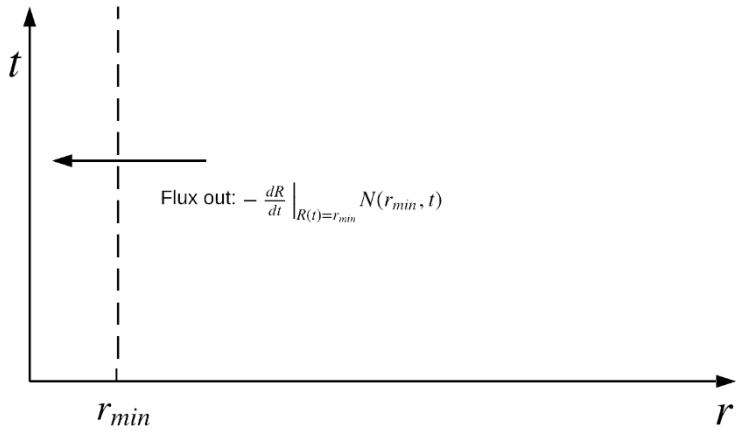
Remarks from Supervisor

- We have derived a PDE model which describes the evolution of the distribution of nanoparticles in our system:
  - $\frac{\partial N}{\partial t}(r,t) + \frac{\partial}{\partial r}\left(\frac{dR}{dt}|_{R(t)=r}\, N(r,t)\right) = 0$
  - Not an obvious way to nondimensionalise/identify the natural timescales in our PDE.
    - Perhaps we can pick out the Ostwald ripening timescale heuristically.
  - This is a first order quasilinear equation, so we can use the method of characteristics to seek a solution.
    - If we write $f(r) \coloneqq \frac{dR}{dt}|_{R(t)=r}$ (which we can do since $\frac{dR}{dt}$ has no direct dependence on t), then the characteristic equations for our PDE are given by:
      - $\frac{dt}{d\tau} = 1,$ with initial condition $t(0) = 0.$
      - $\frac{dr}{d\tau} = f(r),$ with initial condition $r(0) = s,\ r_{min} \leq s \leq r_{max}.$
      - $\frac{dN}{d\tau} = -\frac{\partial f}{\partial r}N,$ with initial condition $N(0) = N_0(s).$
    - A change in sign of $\frac{\partial f}{\partial r}$ could be responsible for the change of behaviour that occurs when Ostwald ripening starts to kick in.



  - We may produce simulations of our PDE model by solving the characteristic ODEs numerically.
    - By solving these characteristic equations for several initial conditions: $t(0) = 0$, $x(0) = s$ and $N(0) = N_0(s)$, we can construct the solution surface for the entire PDE.
    - It is recommended that we use the central difference approximation: $\frac{dy}{dx}(x_i) \approx \frac{y(x_{i+1}) - y(x_{i-1})}{x_{i+1} - x_{i-1}}$ for computing numerical solutions to the characteristic ODEs.
    - Choose a sufficiently large grid so that r_{max} not attained at any time.
  - It is important to note that numerical simulations of our PDE could possibly lead to a loss in the total number of particles in the system (i.e. the constraint $\int_{r_{min}}^{r_{max}} N(s,t)ds = const$ may be violated).
    - We may wish to investigate numerical schemes that conserve this quantity.

- Asymptotics of PDE model:
  - Just after the nucleation stage, when the nanoparticles initially grow, we have that $\frac{\partial}{\partial r}(\frac{dR}{dt}|_{R(t)=r}) \approx 0$ and hence our PDE reduces to: $\frac{\partial N}{\partial t} + \frac{dR}{dt}|_{R(t)=r}\frac{\partial N}{\partial r} = 0.$
    - Therefore, the characteristics of this system are given by: $\frac{dt}{d\tau} = 1$, $\frac{dr}{d\tau} = \frac{dR}{dt}|_{R(t)=r}$ and $\frac{dN}{d\tau} = 0.$
    - This should yield travelling wave solutions.
  - For large times, when the Ostwald ripening occurs, we get that $\frac{dR}{dt}|_{R(t)=r}\frac{\partial N}{\partial r} \approx 0$ and hence our PDE reduces to: $\frac{\partial N}{\partial t} = -\frac{\partial}{\partial r}(\frac{dR}{dt}|_{R(t)=r})N.$
    - By integrating with respect to t on both sides, we have that N has the analytic solution: $N(r,t) = N_0(r)\exp(-\frac{\partial}{\partial r}(\frac{dR}{dt}|_{R(t)=r})t).$
- Remarks about the derivation of the PDE for N.
  - It is not entirely clear what non-dimensionalisation procedure you have used in the governing equations for the derivation of the PDE.
  - It is a good idea to use the same length non-dimensionalisation for the radius of each of the nanoparticles in the system.
  - Equation (67) in the derivation of the PDE, needs modification.
    - Currently we have $c_\infty(t) = c_\infty(0) - \frac{4\pi N_0(\hat{R}_k(0))^3}{3V_m}\sum_{i=1}^{n}(R_i(t))^3$, however, this needs to be expressed in terms of our new quantity N, in order to produce simulations of our PDE.
    - Intuitively we should have that the sum generalises to an integral when we switch to the continuous case to get $c_\infty(t) = c_\infty(0) - \frac{4\pi N_0(\hat{R}_k(0))^3}{3V_m}\int_{r_{min}}^{r_{max}} s^3 N(s,t)\,ds$ however, this needs proper mathematical justification.
- We need to resolve the issue caused by the presence of particles of a very small size occurring in simulations of our model.
  - Instead of removing individual particles from the simulation that are below a certain threshold size, we should mathematically describe the process of small particles dissolving back into the solution.
    - The Taylor series approach used in the provided paper should not be used. This is because the sum diverges as we take the limit as $R \to 0$, so the idea of truncating the Taylor series is nonsensical.
  - We should fix the lower bound $r_{min} > 0$ in our PDE for N, so that particles cannot be arbitrarily small.
    - We need to adjust the expression for $c_\infty(t)$ to account for the flux of particles that are being lost through the boundary $r = r_{min}$.
    - Use a hyperbolic conservation law, where the flux out of r_{min} is $-\frac{dR}{dt}|_{R(t)=r_{min}}N(r_{min},t)$.



- Would be good to model both the discrete model for $R_1, R_2, \dots, R_n$ nanoparticles and the continuous model $N(r,t)$ and then compare the results.
- Priority now is dealing with the small particle issue.
- Optimal control Theory
    - Extension of Calculus of Variations.
    - This provides a framework of how to optimally vary $c_\infty(0)$ so that we achieve the desired terminal nanoparticle distribution (we want a tall thin distribution so that the nanoparticles are virtually all the same size).
    - Perhaps this is too ambitious to put into the presentation.
- Once we have simulations of the N and R models, we have enough to make a reasonable conclusion and start putting a presentation together.
- In the Peng paper, they plot the mean of R, which should agree with the average of our quantity N.
- The next and final meeting with our supervisor will take place at 11am on the 5th of March in room C2.

Additional Notes

- Next group meeting is scheduled for 3pm on Monday the 2nd of March in the MMSC room.
- Everyone should go through the derivation of the PDE for N before our next meeting.
    - How might we generalise our conservation of mass expression for $c_\infty(t)$ in terms of $R(t)$, to an expression in terms of $N(t)$?
    - How might we account for the particles lost through the boundary $r = r_{min}$ in our boundary?
    - Can we explicitly derive a travelling wave solution for $N(r,t)$, when we consider the behaviour of the particle shortly after the nucleation stage?
    - Can we find a natural timescale on which the Ostwald ripening takes place?
    - How might we mathematically describe the process of a small nanoparticles dissolving back into the solution?
- If incomplete, Shyam and Lewis may wish to continue working on adjusting the numerical simulations of the R model so that sufficiently small nanoparticles are removed.
- Someone may wish to start working on the preliminary work for the presentation.
    - The important equations in the derivation and non-dimensionalisation of the governing equations in Sections 1 and 2 of the LaTeX document need to be converted to a suitable presentation format (e.g. Microsoft PowerPoint or a LaTeX presentation format).

- It would be useful to create a brief description/list of all the relevant information that we want to include so far in the presentation, so that we have a structure that we are working to.