Mathematical Fundamentals for Electrochemical Energy Storage Systems

Exercise 7

Task 1: PDE solve

a) Consider the equation for diffusion through a sphere along the radial direction,

- $\frac{\partial c_s}{\partial t} = \frac{D_s}{r^2} \cdot \frac{\partial}{\partial r}\left(r^2 . \frac{\partial c_s}{\partial c_r}\right)$

1. How would you discretize this sphere using the finite volume method?

2. Implement your method of discretization in Python and convert this PDE into a system of ODEs

3. Assume the following boundary conditions. There is an intercalation reaction that happens at the boundary that results in a flux J of ions into the particle. The ions diffuse through the particle and come to a rest at the centre. What would be the boundary conditions for your system of ODEs based on this information?

4. Augment your state variable that you have developed in question 2 with the boundary conditions.

5. Now, solve your system of ODEs using scipy's odeint or solve_ivp function. Assume that the flux J is always constant and is 1 $mol\ m2.s$. Assume that the diffusion constant is 1 × 10−14 ($m2/\ s$) and radius is 8.5 × 10−6 (m)

Task 2: Single Particle Model

a) Implement the single particle model for a lithium-ion battery in Python