

Mathematical Fundamentals for Electrochemical Energy Storage Systems

Exercise 5

Task 1: Forward Euler

- a) Implement the forward euler method to solve the following initial value problems
- $y' + \left(\frac{y}{1+x}\right) + 6x = 0, y(0) = 3$
 - $y' \sin(x) = y \cos(x), y\left(\frac{\pi}{6}\right) = 1$
 - $y' x \ln(x) = y, y(e^2) = 2$
- b) A solid electrolyte interface is a layer that grows on top of an electrode of a lithium-ion battery that consists of decomposition products from the electrolyte. This side reaction happens throughout the life of a battery and causes loss of lithium ions when cycling.

Assume that the SEI reaction is limited by the speed of diffusion of solvent molecules to the reaction site. Therefore, the flux of solvent molecules N_{sol} is defined by the fick's law as shown in the equation below,

$$N_{sol} = -\frac{D_{sol}(T)dc_{sol}}{dl}$$

Here, l represents a point in the SEI layer, $D_{sol}(T)$ represents the diffusion coefficient of the solvent, c_{sol} is the concentration of the solvent. Assume that the solvent concentration in the SEI varies linearly with the following two conditions

$$c_{sol} = 0 \text{ at } l = 0$$

$$c_{sol} = c_{sol,0} \text{ at } l = L_{SEI}$$

Assume that the growth of SEI thickness can be described the following equation,

$$\frac{dL_{SEI}}{dt} = -\frac{1}{2}N_{sol}\bar{V}_{SEI} = c_{sol,0} \cdot D_{sol}(T) \cdot \frac{\bar{V}_{SEI}}{2L_{SEI}}$$

In this equation, \bar{V}_{SEI} is the molar volume of the SEI. Solve the equations using forward euler and odeint. Consider the following parameters for the model.

$$\bar{V}_{SEI} = 9.585 \times \frac{10^{-5}m^3}{mol}$$

$$c_{sol,0} = 2636 \frac{mol}{m^3}$$
$$D_{sol} = 1.25 \times 10^{-20} \frac{m^2}{s}$$