1 The Transport Model

$$\nabla[\varepsilon\nabla v] = -\sum_i z_i c_i \tag{1}$$

We do everything in SI units:

- c_i is in $c_i[1/\mathrm{m}^3] = N_\mathrm{A} 10^3 c_i[\mathrm{mol/L}]$
- D_i is in $D_i[\mathrm{m}^2/\mathrm{s}] = 1/100^2 D_i[\mathrm{cm}^2/\mathrm{s}]$
- $\varepsilon = \varepsilon_r \varepsilon_0$ with $\varepsilon_0 = 8.854187817 \cdot 10^{-12}\,\mathrm{F/m}$
- $z_i = q_i e$ with $e = 1.60217662 \cdot 10^{-19}\,\mathrm{C}$
- $\beta = (k_\mathrm{B} T)$ with $k_\mathrm{B} = 1.38064852 \cdot 10^{-23}\,\mathrm{J/K}$
- v is in $v[J/C]$
- u is in $u[m/s]$

The coupled transport-PNP equations read:

$$\dot{c}_i = -u c_i' + D_i c_i'' + D_i z_i \beta \left[c_i' v' + c_i v''\right] + R_i \tag{2}$$

with v and c_i connected via the PBE:

$$v'' = \begin{cases} \varepsilon_\mathrm{s}^{-1} \sum_i z_i c_i, & \text{for } x > 0 \\ 0, & \text{for } 0 \geq x > -d_\mathrm{OHP} \end{cases} \tag{3}$$

The concentrations at $x > 0$ are given by:

$$c_i = c_{i,\mathrm{s}} \exp\left(-z_i \beta v\right), \quad \text{for } x > 0 \tag{4}$$

So we can also calculate v from an arbitrary c_i:

$$v = -\left(z_i \beta\right)^{-1} \ln\left(\frac{c_i}{c_{i,\mathrm{s}}}\right), \quad \text{for } x > 0 \tag{5}$$

This gives us v' from c_i' as

$$v' = \frac{\partial v}{\partial c_i} c_i' = -\left(z_i \beta\right)^{-1} c_i^{-1} c_i', \quad \text{for } x > 0 \tag{6}$$

For the second case that we are at the inside of the OHP, v' which depicts the electric field, is constant and we can therefore set it to the value of v' at $x = 0$. In total we then get:

$$\dot{c}_i = \begin{cases} -u c_i' + D_i \left[c_i'' - c_i^{-1} {c_i'}^2 + z_i \beta c_i \varepsilon_\mathrm{s}^{-1} \sum_i z_i c_i\right] + R_i, & \text{for } x > 0 \\ -u c_i' + D_i \left[c_i'' - \left.\frac{c_i'}{c_i}\right|_{x=0} c_i'\right] + R_i, & \text{for } 0 \geq x > -d_\mathrm{OHP} \end{cases} \tag{7}$$

Check the units!

What is remaining now are the initial and boundary conditions.

2 Discretization