Model equations

Electrochemical modelling

The simulation app is based on the Doyle-Fuller-Newman model and consists of a set of coupled partial differential equations describing the transport of Li^+ ions in the electrolyte, carbon binder, and the active material.

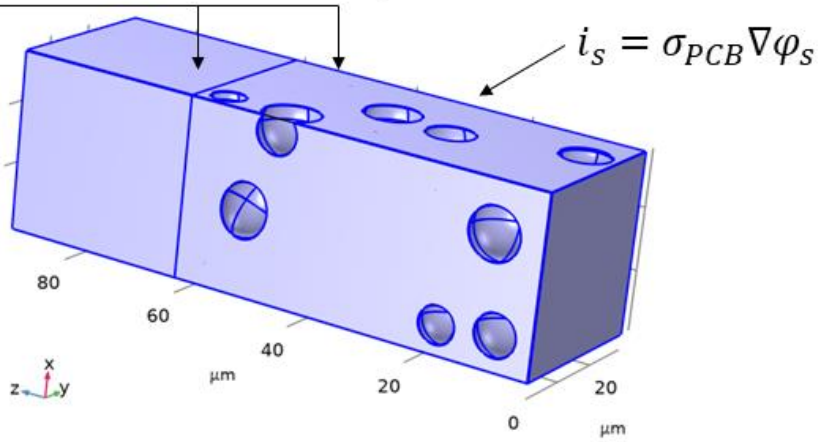
Porous conductive binder and separator

The equations describing the lithium ions transport in the electrolyte phase of the separator and the porous conductive binder (PCB) are shown below, together with an additional equation describing the electron transport in the PCB.

$$\frac{\partial c_l}{\partial t} = \nabla\left(D_l \nabla c_l - \frac{i_l t_+}{F}\right)$$

$$i_l = \sigma_l \nabla \varphi_l + \frac{2\sigma_l RT}{F}\left(1 + \frac{\partial lnf}{\partial lnc_l}\right)(1 - t_+)\nabla lnc_l$$

$$i_s = \sigma_{PCB} \nabla \varphi_s$$



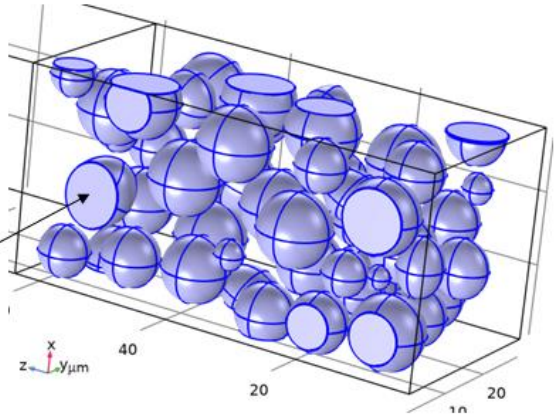
c_l is the Li^+ concentration in the electrolyte, D_l is Li^+ diffusion coefficient in the electrolyte, F – Faraday constant, t^+ – transference number, i_l is the electrolyte current density, R – universal gas constant, σ_l – ionic conductivity, φ_l – electrolyte potential, and $\partial lnf/(\partial lnc_l)$ is the electrolyte thermodynamic factor, σ_{PCB} – is the electric conductivity of the PCB, and φ_S – the electrode potential, and i_s is the electron current density in the PCB.

Particles (active material)

The diffusion of lithium in the active material particles is driven by the concentration gradient and it is described by Fick's law. The electronic transport, driven by the electrical potential gradient, is described by Ohm's law. Both equations are shown below, where D_l is Li^+ diffusion coefficient in the particles, c_s is the Li^+ concentration in the particles, σ_{NMC} – is the electric conductivity of the particles, i_s is the electron current density in the particles.

$$\frac{\partial c_s}{\partial t} = \nabla(D_s c_s)$$

$$i_s = \sigma_{NMC} \nabla \varphi_s$$



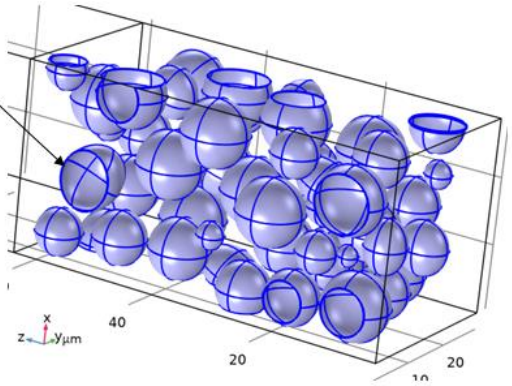
Interface coupling between the electrolyte and the active material particles

The coupling between the lithium transport in the electrolyte and the active particles at the interface of the particles is described by the Butler-Volmer equation of charge transfer reaction.

$$i_{ct} = i_{0,ref}\left(1 - \frac{c_s}{c_{s,max}}\right)^{\alpha}\left(exp\left(\frac{(1-\alpha)F\eta}{RT}\right) - exp\left(\frac{\alpha F\eta}{RT}\right)\right)$$

$$i_{0,ref} = Fkc_l^{\alpha} c_s^{1-\alpha}$$

$$\eta = \varphi_s - \varphi_l - E_{eq}$$



i_{ct} is the charge transfer current, $i_{0,ref}$ is the reference exchange current density, $c_{s,max}$ – maximum Li^+ concentration in particles, α– transfer coefficient, η – activation overpotential, and E_{eq} is the equilibrium potential.

Solid mechanics modelling

The principle of mechanical equilibrium governs the stress field in both the active (particles) and inactive materials (separator and binder).

$$\nabla \cdot \sigma = 0$$

The Hook's law is used to calculate the stress (σ) – $\sigma = \mathbf{C}: \boldsymbol{\varepsilon_{el}}$, where **C** is the stiffness matrix and ε_{el} is the elastic strain.

The total strain ε is connected to the displacement field u by: $\boldsymbol{\varepsilon} = \frac{\mathbf{1}}{\mathbf{2}}\left((\boldsymbol{\nabla u})^{\boldsymbol{T}} + \boldsymbol{\nabla u}\right)$