New PE degradation model

Applied current I^*_{app} Applied current density $I^* = \frac{I^*_{app}}{A^*_{cc}}$

Typical current $I^*_{app,typ}$ Typical current density $I^*_{typ} = \frac{I^*_{app,typ}}{A^*_{cc}}$

Dimensionless current = dimensionless current density $I = \frac{I^*_{app}}{I^*_{app,typ}} = \frac{I^*}{I^*_{typ}}$

Discharge timescale $\tau^*_d = F^* C^*_{n,max} L^*_x / I^*_{typ}$

L^*_x cell thickness

Scaling timescale t^*_{sca} $(= \tau^*_d)$

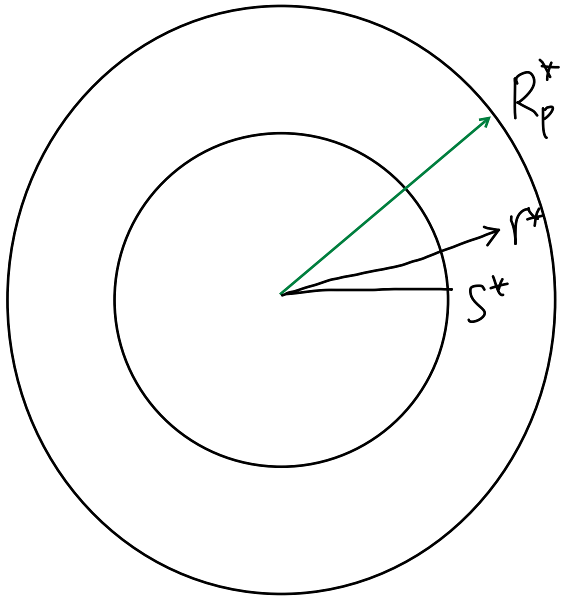
Diffusion timescales $t^*_c = \frac{R^{*2}_{p,typ}}{D^*_{c,typ}}$ $t^*_o = \frac{R^{*2}_{p,typ}}{D^*_{o,typ}}$

$D^*_c = D_c D^*_{c,typ}$, $D^*_o = D_o D^*_{o,typ}$, $C^*_c = C_c C^*_{p,max}$, $C^*_o = C_o C^*_{o,typ}$

Timescale ratios $C_c = t^*_c / t^*_{sca}$ $C_o = t^*_o / t^*_{sca}$ $C_d = \tau^*_d / t^*_{sca}$

Typical interface current density $j^*_{p,typ} = \frac{I^*_{typ} \cdot A^*_{cc}}{a^*_p L^*_x A^*_{cc}} = \frac{I^*_{typ}}{a^*_p L^*_x}$

$j^*_p = j_p j^*_{p,typ}$



$R_p^* = R\, R_{p,typ}^*$, $R_{p,typ}^* = R_p^* (x=1)$

$r^* = r R_p^*$ $s^* = s R_p^*$

$\eta = \dfrac{r^*}{s^*}$, $\chi = \dfrac{r^* - s^*}{R_p^* - s^*}$

Variable change to fix moving phase boundary — old (t^*, r^*)

for core (t, η)

$$t = \frac{t^*}{t^*_{scale}} \qquad \eta = \frac{r^*}{S^*(t^*)}$$

$$t^* = t\, t^*_{sca} \qquad r^* = \eta\, S^*(t^*)$$

$$\frac{\partial}{\partial t^*} = \frac{\partial}{\partial t}\frac{\partial t}{\partial t^*} + \frac{\partial}{\partial \eta}\frac{\partial \eta}{\partial t^*}$$

$$= \frac{1}{t^*_{scale}}\frac{\partial}{\partial t} - \frac{r^*}{(S^*)^2}\frac{dS^*}{dt^*}\frac{\partial}{\partial \eta}$$

$$= \frac{1}{t^*_{scale}}\frac{\partial}{\partial t} - \frac{\eta}{S^*}\frac{dS^*}{dt^*}\frac{\partial}{\partial \eta}$$

$$= \frac{1}{t^*_{scale}}\left(\frac{\partial}{\partial t} - \frac{\eta}{S}\frac{dS}{dt}\frac{\partial}{\partial \eta}\right)$$

$$\frac{\partial}{\partial r^*} = \frac{\partial}{\partial t}\frac{\partial t}{\partial r^*} + \frac{\partial}{\partial \eta}\frac{\partial \eta}{\partial r^*}$$

$$= \frac{1}{S^*}\frac{\partial}{\partial \eta} = \frac{1}{R_p^*}\frac{1}{S}\frac{\partial}{\partial \eta}$$

for shell (t, χ)

$$t = \frac{t^*}{t^*_{sca}} \qquad \chi = \frac{r^* - S^*}{R_p^* - S^*}$$

$$t^* = t\, t^*_{sca} \qquad r^* = [(1-S)\chi + S]R_p^*$$

$$\frac{\partial}{\partial t^*} = \frac{\partial}{\partial t}\frac{\partial t}{\partial t^*} + \frac{\partial}{\partial \chi}\frac{\partial \chi}{\partial t^*}$$

$$= \frac{1}{t^*_{sca}}\frac{\partial}{\partial t} + \frac{-\dot{S}^*(R_p^* - S^*) + (r^* - S^*)\dot{S}^*}{(R_p^* - S^*)^2}\frac{\partial}{\partial \chi}$$

$$= \frac{1}{t^*_{sca}}\frac{\partial}{\partial t} + \frac{\chi - 1}{R_p^* - S^*}\frac{dS^*}{dt^*}\frac{\partial}{\partial \chi}$$

$$= \frac{1}{t^*_{sca}}\left(\frac{\partial}{\partial t} - \frac{1-\chi}{1-S}\frac{dS}{dt}\frac{\partial}{\partial \chi}\right)$$

$$\frac{\partial}{\partial r^*} = \frac{\partial}{\partial t}\frac{\partial t}{\partial t^*} + \frac{\partial}{\partial \chi}\frac{\partial \chi}{\partial r^*}$$

$$= \frac{1}{R_p^* - S^*}\frac{\partial}{\partial \chi} = \frac{1}{R_p^*}\frac{1}{1-S}\frac{\partial}{\partial \chi}$$

Gradient/divergence operators in Spherical coordinate

$$\nabla^*(\circ) = \frac{\partial}{\partial r^*}(\circ) = \frac{1}{R_p^*}\frac{1}{S}\frac{\partial}{\partial \eta}$$

$$\nabla^*\cdot(\circ) = \frac{1}{r^{*2}}\frac{\partial}{\partial r^*}(r^{*2}\circ)$$

$$= \frac{1}{R_p^*}\frac{1}{S}\frac{1}{\eta^2}\frac{\partial}{\partial \eta}(\eta^2\circ)$$

$$\nabla^*\cdot(\nabla^*\circ) = \frac{1}{R_p^{*2}}\frac{1}{S^2\eta^2}\frac{\partial}{\partial \eta}\left(\eta^2\frac{\partial}{\partial \eta}\circ\right)$$

$$\nabla^*(\circ) = \frac{\partial}{\partial r^*}(\circ) = \frac{1}{R_p^*}\frac{1}{1-S}\frac{\partial}{\partial \chi}$$

$$\nabla^*\cdot(\circ) = \frac{1}{r^{*2}}\frac{\partial}{\partial r^*}(r^{*2}\circ)$$

$$= \frac{1}{R_p^*}\frac{1}{1-S}\frac{1}{[(1-S)\chi + S]^2}\frac{\partial}{\partial \chi}\left([(1-S)\chi + S]^2\circ\right)$$

$$\nabla^*\cdot(\nabla^*\circ) =$$

$$\frac{1}{R_p^{*2}}\frac{1}{(1-S)^2}\frac{1}{[(1-S)\chi + S]^2}\frac{\partial}{\partial \chi}\left([(1-S)\chi + S]^2\frac{\partial}{\partial \chi}\circ\right)$$

Lithium diffusion in core

$$\frac{\partial C_c^*}{\partial t^*} + \nabla^* \cdot \left(-D_c^* \nabla^* C_c^* \right) = 0$$

$$\frac{\cancel{C^*_{p,max}}}{t^*_{sca}} \left(\frac{\partial C_c}{\partial t} - \frac{\eta}{s} \frac{ds}{dt} \frac{\partial C_c}{\partial \eta} \right)$$

$$+ \frac{\cancel{C^*_{p,max}}\, D^*_{c,typ}}{R_p^{*2}} \frac{1}{s^2 \eta^2} \frac{\partial}{\partial \eta} \left(-\eta^2 D_c \frac{\partial C_c}{\partial \eta} \right) = 0$$

$$\frac{\partial C_c}{\partial t} - \frac{\eta}{s} \frac{ds}{dt} \frac{\partial C_c}{\partial \eta} +$$

$$\frac{t^*_{sca}}{R^{*2}_{p,typ} / D^*_{c,typ}} \frac{1}{R_p^{*2} / R^{*2}_{p,typ}} \frac{1}{s^2 \eta^2} \frac{\partial}{\partial \eta} \left(-\eta^2 D_c \frac{\partial C_c}{\partial \eta} \right) = 0$$

$$\frac{\partial C_c}{\partial t} - \frac{\eta}{s} \frac{ds}{dt} \frac{\partial C_c}{\partial \eta} + \frac{1}{C_c} \frac{1}{R^2} \frac{1}{s^2 \eta^2} \frac{\partial}{\partial \eta} \left(-\eta^2 D_c \frac{\partial C_c}{\partial \eta} \right) = 0$$

Oxygen diffusion in shell

$$\frac{\partial C_o^*}{\partial t^*} + \nabla^* \cdot \left(-D_o^* \nabla^* C_o^* \right) = 0$$

$$\frac{\cancel{C^*_{o,typ}}}{t^*_{sca}} \left(\frac{\partial C_o}{\partial t} - \frac{1-\chi}{1-s} \frac{ds}{dt} \frac{\partial C_o}{\partial \chi} \right) +$$

$$\frac{\cancel{C^*_{o,typ}}\, D^*_{o,typ}}{R_p^{*2}} \frac{1}{(1-s)^2} \frac{1}{[(1-s)\chi + s]^2} \frac{\partial}{\partial \chi} \left(-[(1-s)\chi + s]^2 D_o \frac{\partial C_o}{\partial \chi} \right)$$

$$= 0$$

$$\frac{\partial C_o}{\partial t} - \frac{1-\chi}{1-s} \frac{ds}{dt} \frac{\partial C_o}{\partial \chi} +$$

$$\frac{t^*_{sca}}{R^{*2}_{p,typ} / D^*_{o,typ}} \frac{1}{R_p^{*2} / R^{*2}_{p,typ}} \frac{1}{(1-s)^2} \frac{1}{[(1-s)\chi + s]^2} \frac{\partial}{\partial \chi} \left(-[(1-s)\chi + s]^2 D_o \frac{\partial C_o}{\partial \chi} \right)$$

$$= 0$$

$$\frac{\partial C_o}{\partial t} - \frac{1-\chi}{1-s} \frac{ds}{dt} \frac{\partial C_o}{\partial \chi} +$$

$$\frac{1}{C_o} \frac{1}{R^2} \frac{1}{(1-s)^2} \frac{1}{[(1-s)\chi + s]^2} \frac{\partial}{\partial \chi} \left(-[(1-s)\chi + s]^2 D_o \frac{\partial C_o}{\partial \chi} \right) = 0$$

Boundary conditions

at core-shell interface

$$\vec{h}_c^* - \vec{h}_s^* - \dot{s}^*(C_c^* - C_s^*) = 0$$

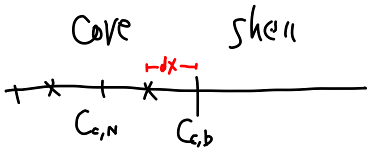
$$-D_c^* \frac{\partial C_c^*}{\partial y^*} - \frac{1}{F^*}\frac{1}{s^2} j_p^* - \dot{s}^*(C_c^* - C_s^*) = 0$$

$$-D_{c,typ}^* \frac{C_{p,max}^*}{R_p^*} \frac{1}{s} D_c \frac{\partial C_c}{\partial \eta} - \frac{1}{F^*}\frac{1}{s^2}\frac{I_{typ}^*}{a_p^* L_x^*} j_p - \frac{R_p^*}{t_{sca}^*} C_{p,max}^* \frac{ds}{dt}(C_c - C_s) = 0$$

$$-D_c \frac{\partial C_c}{\partial \eta} - \frac{I_{typ}^*}{F^* C_{n,max}^* L_x^*}\frac{C_{n,max}^*}{C_{p,max}^*}\frac{s}{a_p^* R_{p,typ}^*}\frac{R_{p,typ}^* R_p^*}{D_{c,typ}^*}\frac{j_p}{s^2} - \frac{R_{p,typ}^{*2} R^2}{D_{c,typ}^*}\frac{s}{t_{sca}^*}\frac{ds}{dt}(C_c - C_s) = 0$$

$$-D_c \frac{\partial C_c}{\partial \eta} - \frac{1}{T_d^*}\frac{1}{\gamma_p}\frac{s}{a_p} t_c^* R \frac{j_p}{s^2} - \frac{t_c^*}{t_{sca}^*} R^2 s\dot{s}(C_c - C_s) = 0$$

$$-D_c \frac{\partial C_c}{\partial \eta} - \frac{C_c}{C_d}\frac{RS}{\gamma_p a_p}\frac{j_p}{s^2} - C_c R^2 s\dot{s}(C_c - C_s) = 0$$



$$-D_c \frac{C_{c,b} - C_{c,N}}{dx} - \frac{C_c}{C_d}\frac{RS}{\gamma_p a_p}\frac{j_p}{s^2} - C_c R^2 s\dot{s}(C_{c,b} - C_s) = 0$$

$$C_{c,b} - C_{c,N} + \frac{dx}{D_c}\frac{C_c}{C_d}\frac{RS}{\gamma_p a_p}\frac{j_p}{s^2} + \frac{dx}{D_c} C_c R^2 s\dot{s}(C_{c,b} - C_s) = 0$$

$$\left(1 + \frac{dx}{D_c} C_c R^2 s\dot{s}\right) C_{c,b} = C_{c,N} - \frac{dx}{D_c}\left(\frac{C_c}{C_d}\frac{RS}{\gamma_p a_p}\frac{j_p}{s^2} - C_c R^2 s\dot{s} C_s\right)$$

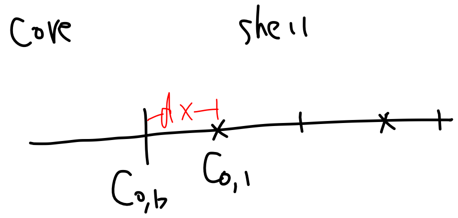
Oxygen generation at the interface

$$-D_o^* \frac{\partial C_o^*}{\partial r^*} + \dot{S}^*(C_{oc}^* - C_o^*) = 0$$

$$-D_{o,typ}^* C_{o,typ}^* \frac{1}{R_p^*(1-S)} D_o \frac{\partial C_o}{\partial x} + \frac{R_p^*}{t_{sca}^*} \dot{S} C_{o,typ}^* (C_{oc} - C_o) = 0$$

$$-D_o \frac{\partial C_o}{\partial x} + \frac{R_p^{*2}}{D_{o,typ}^*} \frac{1}{t_{sca}^*} (1-S)\dot{S}(C_{oc} - C_o) = 0$$

$$-D_o \frac{\partial C_o}{\partial x} + C_o R^2 (1-S)\dot{S}(C_{oc} - C_o) = 0$$



$$-D_o \frac{C_{o,1} - C_{o,b}}{dx} + C_o R^2 (1-S)\dot{S}(C_{oc} - C_{o,b}) = 0$$

$$C_{o,1} - C_{o,b} - \frac{dx}{D_o} C_o R^2 (1-S)\dot{S}(C_{oc} - C_{o,b}) = 0$$

$$\left(1 - \frac{dx}{D_o} C_o R^2 (1-S)\dot{S}\right) C_{o,b} = C_{o,1} - \frac{dx}{D_o} C_o R^2 (1-S)\dot{S}\, C_{oc}$$

Phase boundary location evolution

$$\frac{ds^*}{dt^*} = \begin{cases} -(k_1^* - k_2^* \, C_0^*) , & C_c^* < C_{thrd}^* \\ 0 , & \text{otherwise} \end{cases}$$

$$C_0^* = C_0 \, C_{0,typ}^* \qquad s^* = s \, R_p^* \qquad t^* = t \, t_{sca}^*$$

$$k_1^* = k_1 \, k_{1,typ}^* \qquad k_2^* = k_2 \, k_{2,typ}^* \qquad R_p^* = R \, R_{p,typ}^*$$

$$\frac{R_p^*}{t_{sca}^*} \frac{ds}{dt} = -(k_1 \, k_{1,typ}^* - k_2 \, k_{2,typ}^* \, C_0 \, C_{0,typ}^*)$$

$$\frac{ds}{dt} = -\left(\frac{k_{1,typ}^* \, t_{sca}^*}{R_{p,typ}^* \, R} k_1 - \frac{k_{2,typ}^* \, t_{sca}^*}{R_{p,typ}^* \, R} C_{0,typ}^* \, k_2 \, C_0 \right)$$

$$= -(K_1 \, k_1/R - K_2 \, k_2/R \, C_0)$$

$$K_1 = \frac{k_{1,typ}^* \, t_{sca}^*}{R_{p,typ}^*} \qquad K_2 = \frac{k_{2,typ}^* \, t_{sca}^*}{R_{p,typ}^*} C_{0,typ}^*$$