DOYLE-FULLER-NEWMAN MODEL

NUMERICAL IMPLEMENTATION

I. Electrolyte Concentration: $c_e(x,t)$

Continuous-time/space equations

$$\begin{aligned}
\frac{\partial c_e}{\partial t}(x,t) &= \frac{\partial}{\partial x}\left[D_e \frac{\partial c_e}{\partial x}(x,t) + \frac{1-t_c^0}{\epsilon_e F} i_e(x,t)\right] && (1)\\
\left.\frac{\partial c_e}{\partial x}\right|_{x=0^-} &= 0 && (2)\\
\epsilon_e^- D_e \left.\frac{\partial c_e}{\partial x}\right|_{x=L^-} &= \epsilon_e^{sep} D_e \left.\frac{\partial c_e}{\partial x}\right|_{x=0^{sep}} && (3)\\
\epsilon_e^{sep} D_e \left.\frac{\partial c_e}{\partial x}\right|_{x=L^{sep}} &= \epsilon_e^+ D_e \left.\frac{\partial c_e}{\partial x}\right|_{x=L^+} && (4)\\
\left.\frac{\partial c_e}{\partial x}\right|_{x=0^+} &= 0 && (5)
\end{aligned}$$

CN discretization. Let $\alpha = \frac{D_e \Delta t}{2\Delta x^2}$ and $\beta = \frac{1-t_c^0}{\epsilon_e F} \cdot \frac{\Delta t}{4\Delta x}$

$$\begin{aligned}
& -\alpha c_{i+1}^{k+1} + (1+2\alpha) c_i^{k+1} - \alpha c_{i-1}^{k+1} - i_{e,i+1}^{k+1} + \beta i_{e,i-1}^{k+1} \\
= \; & \alpha c_{i+1}^{k} + (1-2\alpha) c_i^{k} - \alpha c_{i-1}^{k} - i_{e,i+1}^{k} + \beta i_{e,i-1}^{k} && (6)
\end{aligned}$$

$$\begin{aligned}
\frac{c_{n,1}}{\Delta x_n} - \frac{c_{n,0}}{\Delta x_n} &= 0 && (7)\\
-\frac{\epsilon_{e,n} D_{e,n}}{\Delta x_n} c_{n,N-1} - \frac{\epsilon_{e,s} D_{e,s}}{\Delta x_s} c_{s,1} + \left(\frac{\epsilon_{e,n} D_{e,n}}{\Delta x_n} + \frac{\epsilon_{e,s} D_{e,s}}{\Delta x_s}\right) c_{ns} &= 0 && (8)\\
-\frac{\epsilon_{e,s} D_{e,s}}{\Delta x_s} c_{s,N-1} - \frac{\epsilon_{e,p} D_{e,p}}{\Delta x_p} c_{p,1} + \left(\frac{\epsilon_{e,s} D_{e,s}}{\Delta x_s} + \frac{\epsilon_{e,p} D_{e,p}}{\Delta x_p}\right) c_{sp} &= 0 && (9)\\
-\frac{c_{p,N-1}}{\Delta x_p} + \frac{c_{p,N}}{\Delta x_p} &= 0 && (10)
\end{aligned}$$

$$\begin{aligned}
(M_1 - M_2 N_2^{-1} N_1) c^{k+1} + M_3 i_e^{k+1} &= (M_4 - M_5 N_2^{-1} N_1) c^k + M_6 i_e^k && (11)\\
F_1 c^{k+1} + F_2 i_e^{k+1} &= F_3 c^k + F_4 i_e^k && (12)
\end{aligned}$$

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