

# Thermal Model for a Lithium Ion Cell

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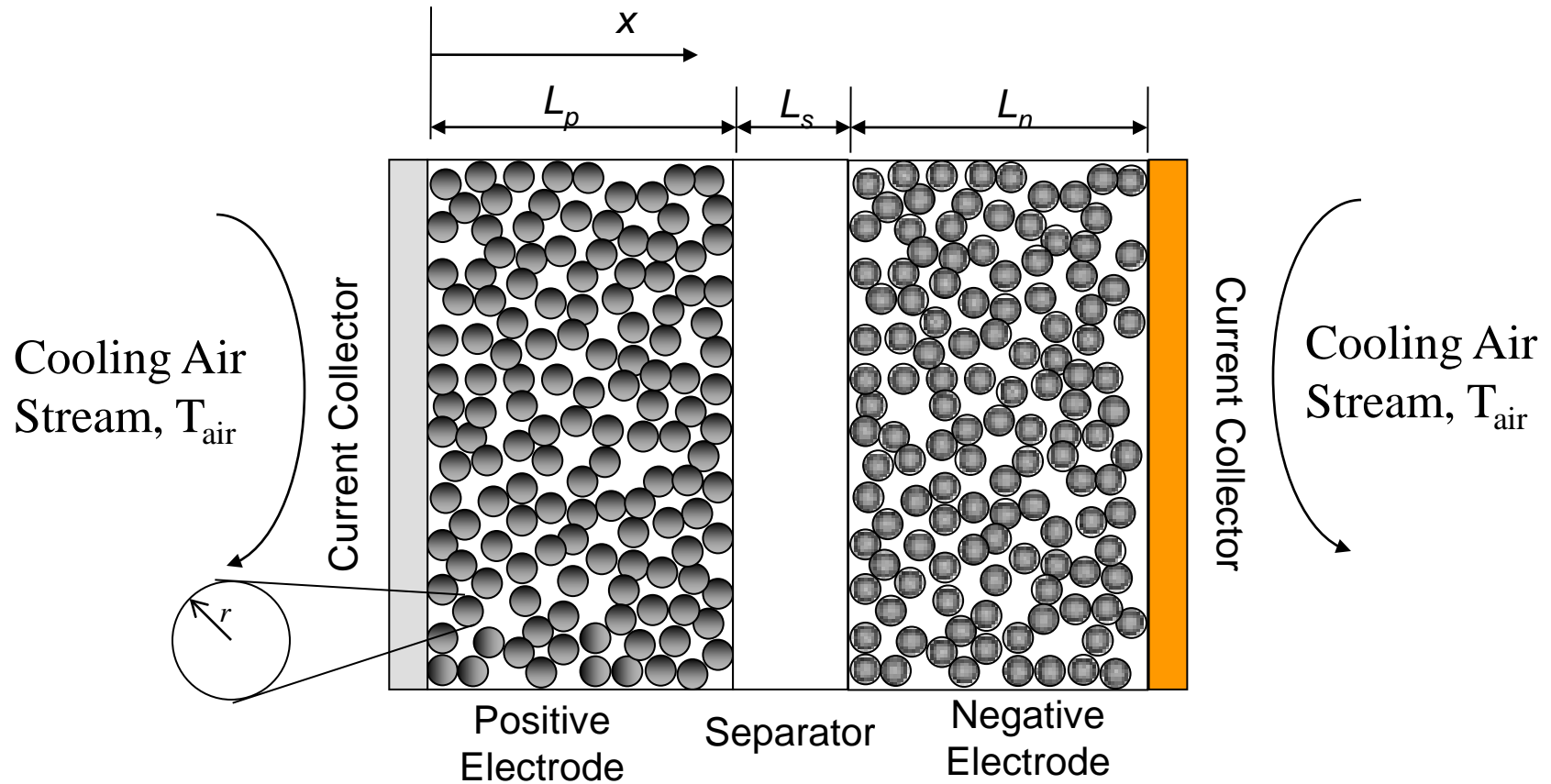
# Objective

- The existing lithium ion battery model in COMSOL's Multiphysics (MP) software is extended to include the thermal effects. The thermal behavior of a lithium ion cell is studied during the galvanostatic discharge process with and without a pulse.



# Schematic of a Lithium Ion Cell

- Problem Description





# Thermal Model of the Lithium Ion Battery

- **Governing Equation: Electrochemical Model**

- Positive Electrode

$$\frac{\partial c_{s,p}(r,t)}{\partial t} = D_{s,p} \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial c_{s,p}(r,t)}{\partial r} \right)$$

$$\varepsilon_1 \frac{\partial c}{\partial t} = D_{\text{eff,p}} \frac{\partial^2 c}{\partial x^2} + (-t_+) a_p j_p$$

$$\sigma_{\text{eff,p}} \frac{\partial^2 \Phi_1}{\partial x^2} = a_p F j_p$$

$$\kappa \frac{\partial}{\partial x} \left( \kappa_{\text{eff,p}} \frac{\partial \Phi_2}{\partial x} \right) + \beta \frac{\partial}{\partial x} \left( \kappa_{\text{eff,p}} \frac{\partial \ln c}{\partial x} \right) = a_p F j_p$$

- Negative Electrode:

$$\frac{\partial c_{s,n}(r,t)}{\partial t} = D_{s,n} \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial c_{s,n}(r,t)}{\partial r} \right)$$

$$\varepsilon_n \frac{\partial c}{\partial t} = D_{\text{eff,n}} \frac{\partial^2 c}{\partial x^2} + (-t_+) a_n j_n$$

$$\sigma_{\text{eff,n}} \frac{\partial^2 \Phi_1}{\partial x^2} = a_n F j_n$$

$$\kappa \frac{\partial}{\partial x} \left( \kappa_{\text{eff,n}} \frac{\partial \Phi_2}{\partial x} \right) + \beta \frac{\partial}{\partial x} \left( \kappa_{\text{eff,n}} \frac{\partial \ln c}{\partial x} \right) = a_n F j_n$$

- Separator:

$$\varepsilon_s \frac{\partial c}{\partial t} = D_{\text{eff,s}} \frac{\partial^2 c}{\partial x^2}$$

$$\kappa \frac{\partial}{\partial x} \left( \kappa_{\text{eff,s}} \frac{\partial \Phi_2}{\partial x} \right) + \beta \frac{\partial}{\partial x} \left( \kappa_{\text{eff,s}} \frac{\partial \ln c}{\partial x} \right) =$$

- BV:  $j_i = 2k_i \left( c_{s,\text{max},i} - c_s(R_{s,i}) \right)^{0.5} c_s(R_{s,i})^{0.5} c^{0.5} \sinh \left[ \frac{0.5F}{RT} (\Phi_1 - \Phi_2 - U_i) \right]$



# Thermal Model of the Lithium Ion Battery

- Governing Equation: Thermal Model

$$\rho C_p \frac{dT}{dt} = \lambda \frac{\partial^2 T}{\partial x^2} + Q_{\text{rxn}} + Q_{\text{rev}} + Q_{\text{ohm}}$$

$$Q_{\text{rxn}} = Faj(\phi_1 - \phi_2 - U)$$

$$-\lambda \left. \frac{\partial T}{\partial x} \right|_{x=0} = h(T_{\text{air}} - T)$$

$$Q_{\text{rev}} = FajT \frac{\partial U}{\partial T}$$

$$-\lambda \left. \frac{\partial T}{\partial x} \right|_{x=L} = h(T - T_{\text{air}})$$

$$Q_{\text{ohm}} = \sigma_{\text{eff}} \left( \frac{\partial \phi_1}{\partial x} \right)^2 + \kappa_{\text{eff}} \left( \frac{\partial \phi_2}{\partial x} \right)^2 + \frac{2\kappa_{\text{eff}} RT}{F} (1 - t_+) \frac{1}{c_e} \frac{\partial c_e}{\partial x} \frac{\partial \phi_2}{\partial x}$$

$T_{\infty}$  is the temperature of the cooling stream,  $Q_{\text{rxn}}$  is the total reaction heat generation rate,  $Q_{\text{rev}}$  is the total reversible heat generation rate,  $Q_{\text{ohm}}$  is the total ohmic heat generation rate.



# Thermal Model of the Lithium Ion Battery

- Temperature Dependent Variables

$$U_{n,\text{ref}} = 0.7222 + 0.1387\theta_n + 0.029\theta_n^{0.5} - \frac{0.0172}{\theta_n} + \frac{0.0019}{\theta_n^{1.5}} + 0.2808\exp(0.90 - 15\theta_n) - 0.7984\exp(0.4465\theta_n - 0.4108)$$

$$U_{p,\text{ref}} = \frac{-4.656 + 88.669\theta_p^2 - 401.119\theta_p^4 + 342.909\theta_p^6 - 462.471\theta_p^8 + 433.434\theta_p^{10}}{-1.0 + 18.933\theta_p^2 - 79.532\theta_p^4 + 37.311\theta_p^6 - 73.083\theta_p^8 + 95.96\theta_p^{10}}$$

$$\left[ \frac{dU}{dT} \right]_p = 1.0 \times 10^{-3} \frac{0.199521039 - 0.928373822\theta_p + 1.3645506890000003\theta_p^2 - 0.61154489399999998\theta_p^3}{1.0 - 5.6614798869999997\theta_p + 11.47636191\theta_p^2 - 9.824312135999998\theta_p^3 + 3.048755063\theta_p^4}$$

$$\left[ \frac{dU}{dT} \right]_n = 1.0 \times 10^{-3} \frac{0.5269056 \times 10^{-2} + 3.299265709\theta_n - 91.79325798\theta_n^2 + 1004.911008\theta_n^3 - 5812.278127\theta_n^4 + 19329.7549\theta_n^5 - 37147.8947\theta_n^6 + 38379.18127\theta_n^7 - 16515.05308\theta_n^8}{1 - 48.09287227\theta_n + 1017.234804\theta_n^2 - 10481.80419\theta_n^3 + 59431.3\theta_n^4 - 1.958816488 \times 10^5 \theta_n^5 + 3.745773152 \times 10^5 \theta_n^6 - 3.858211607 \times 10^5 \theta_n^7 + 1.657058597 \times 10^5 \theta_n^8}$$

$$U_n = U_{n,\text{ref}} + (T - T_{\text{ref}}) \left[ \frac{dU}{dT} \right]_n \quad U_p = U_{p,\text{ref}} + (T - T_{\text{ref}}) \left[ \frac{dU}{dT} \right]_p$$

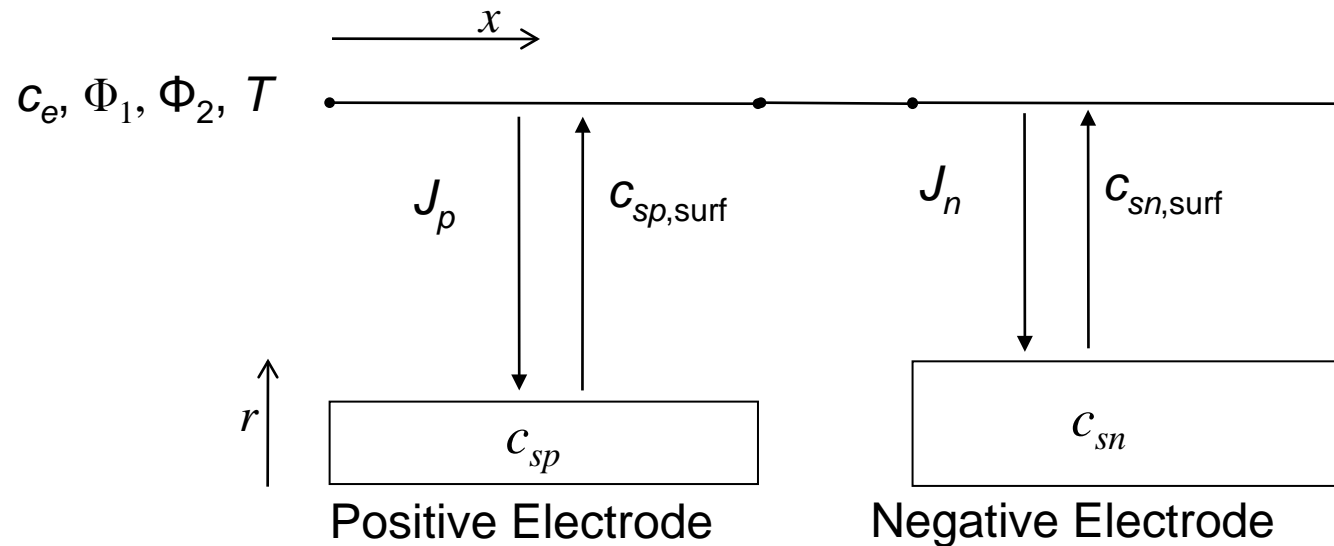
$$\varphi = \varphi_{\text{ref}} \exp \left( \frac{Ea^\varphi}{R} \left( \frac{1}{T_{\text{ref}}} - \frac{1}{T} \right) \right) \quad \varphi \text{ denotes: } D_s, \text{ and } k.$$

$$D_e = 1 \times 10^{-4} \times 10^{-4.43 - \frac{54}{T - 229 - 5.0 \times 10^{-3} c_e} - 0.22 \times 10^{-3} c_e}$$

$$\kappa = 1.0 \times 10^{-4} \times c_e \left( \begin{array}{l} -10.5 + 0.668 \times 10^{-3} c_e + 0.494 \times 10^{-6} c_e^2 + 0.074T - \\ 1.78 \times 10^{-5} c_e T - 8.86 \times 10^{-10} c_e^2 T - 6.96 \times 10^{-5} T^2 + 2.80 \times 10^{-8} c_e T^2 \end{array} \right)^2$$



# Variable Coupling in Multiphysics

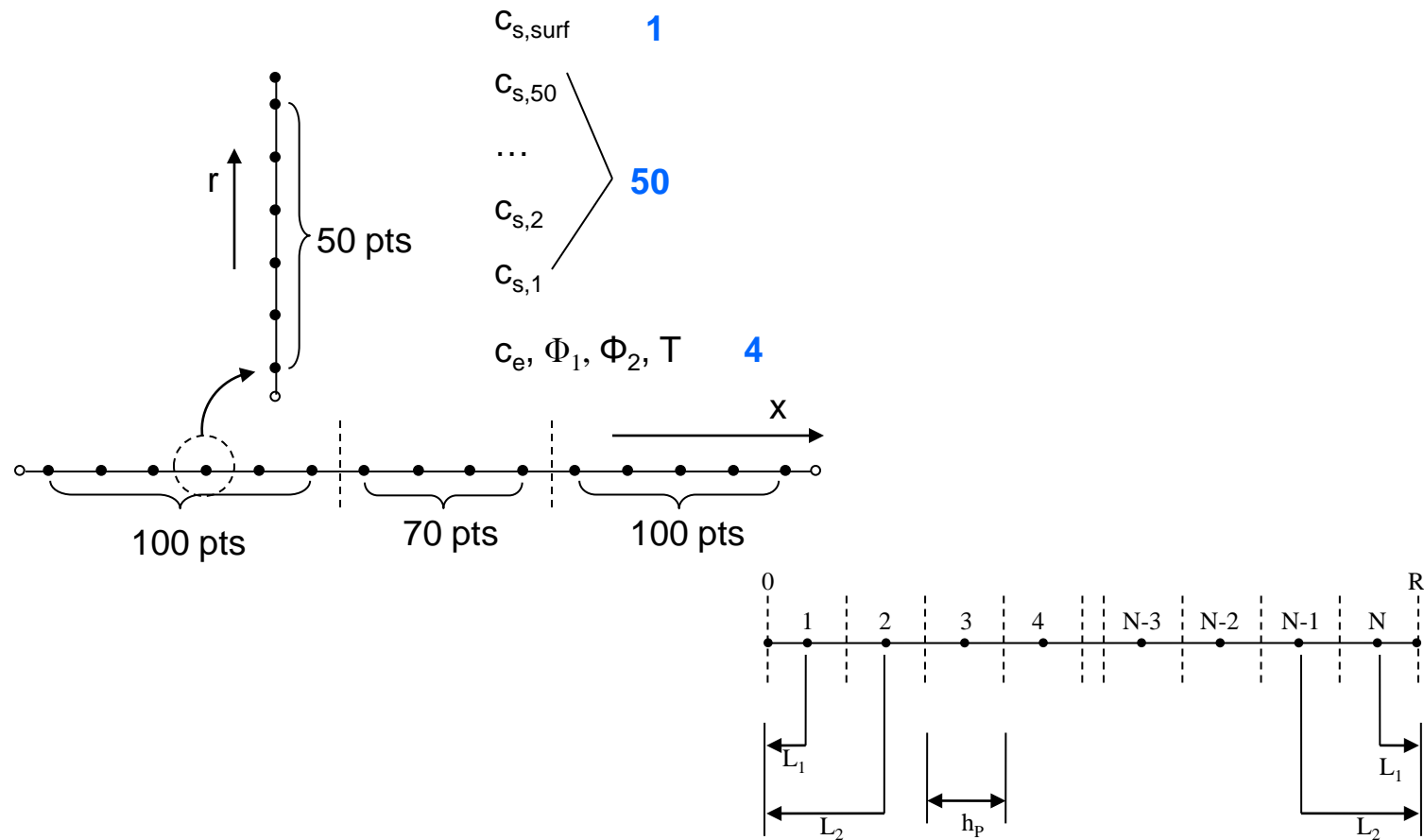


The top 1D geometry consists of three segments which denote the positive electrode, the separator and the negative electrode. The bottom two rectangles represent the solid phases in the positive electrode and the negative electrode, respectively. The pore wall flux is extracted from the 1D geometry and projected to the top boundary of the 2D geometry. The concentration of Li ions on the top boundary of the 2D geometry is projected to the 1D domain as the surface concentration of the solid particles.



# Model Validation

- Discretization Scheme in FORTRAN (Finite Volume Method)

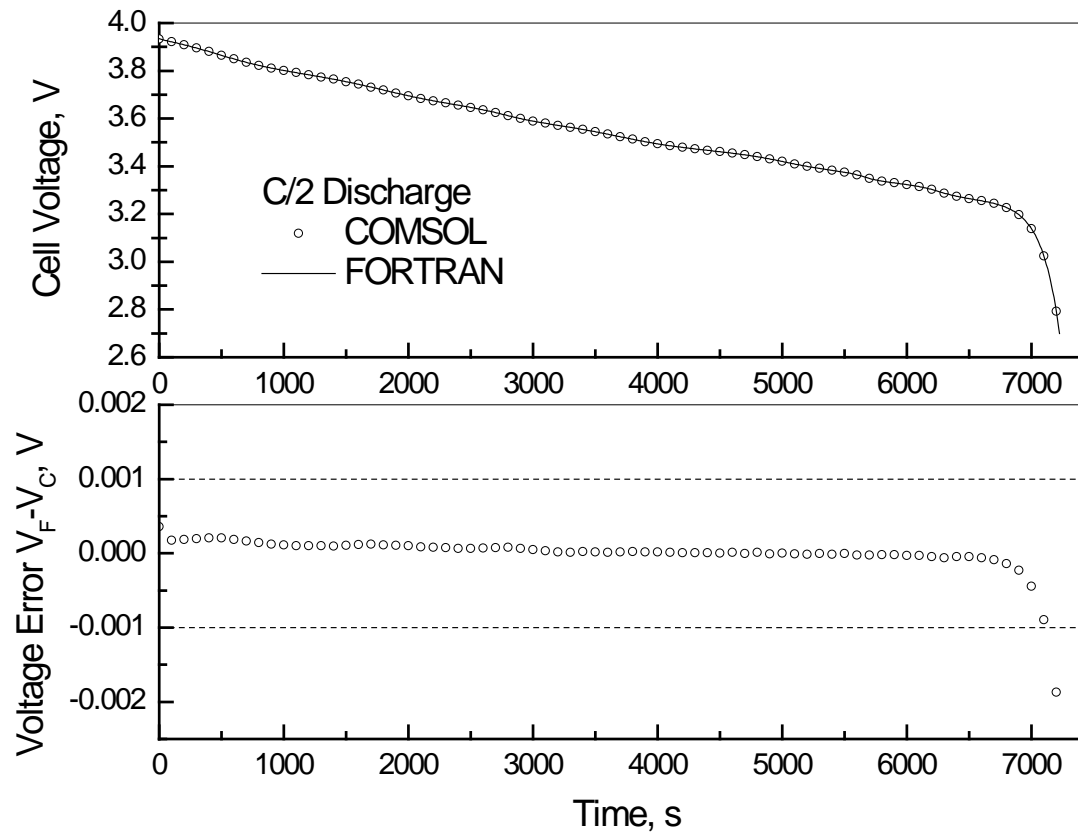






# Model Validation

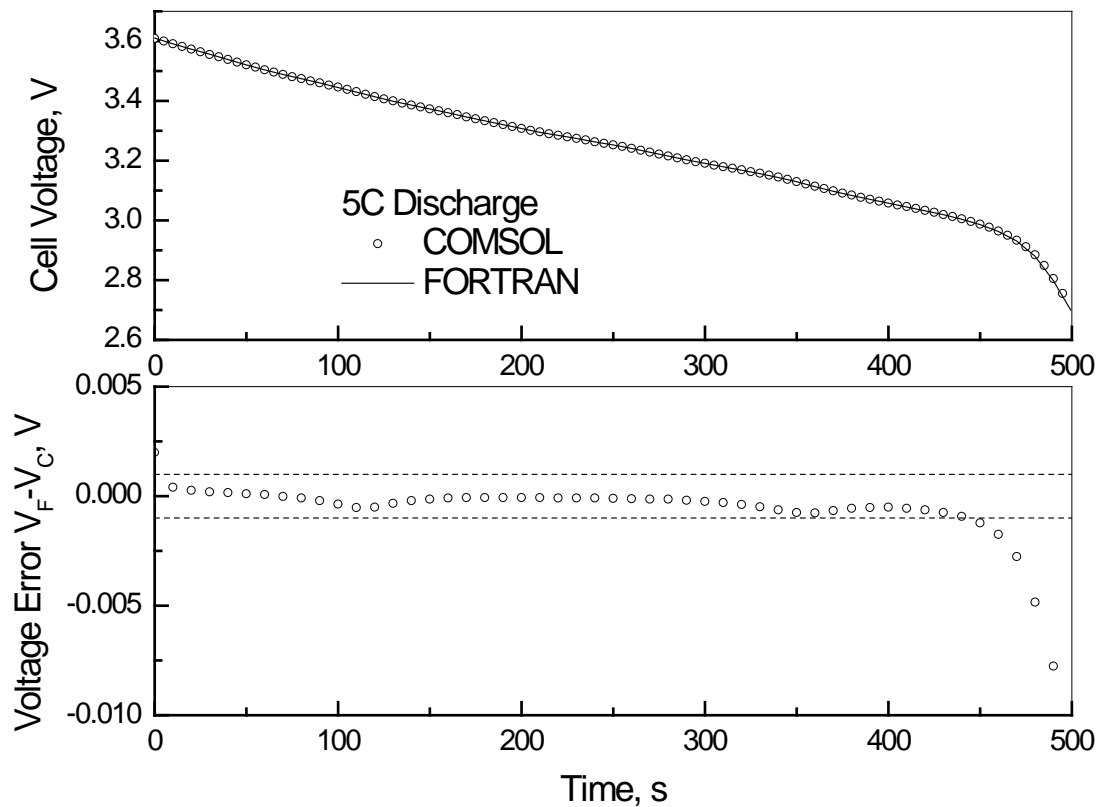
- Comparison of the Simulated Cell Voltage under Low Current Rate





# Model Validation

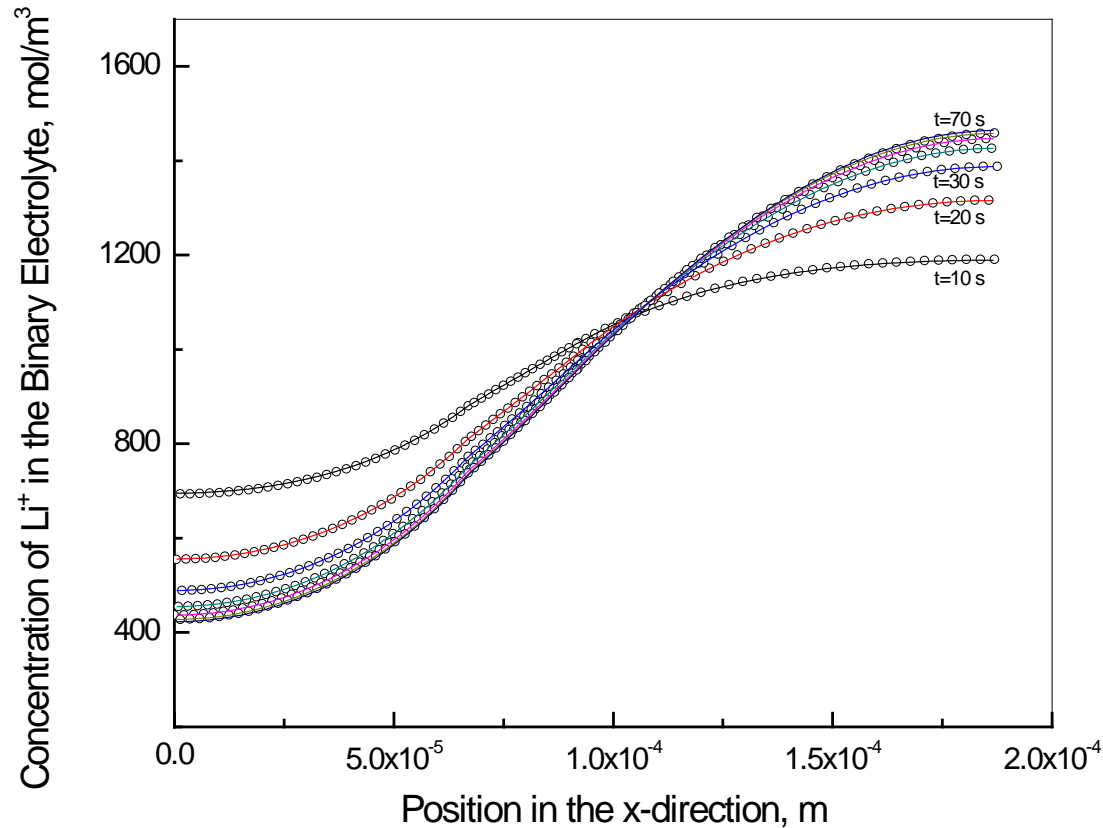
- Comparison of the Simulated Cell Voltage under High Current Rate



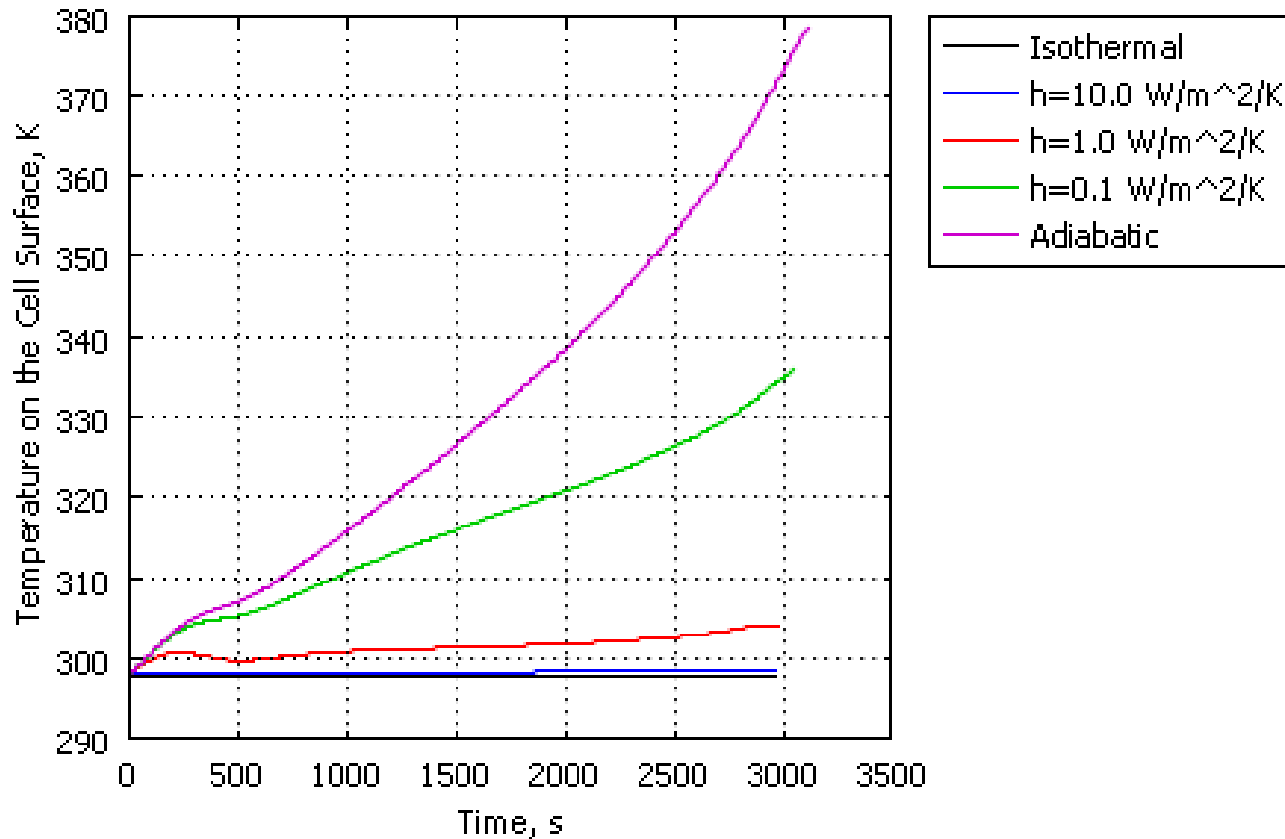


# Model Validation

- Comparison of the Profiles of the Concentration of the Binary Electrolyte



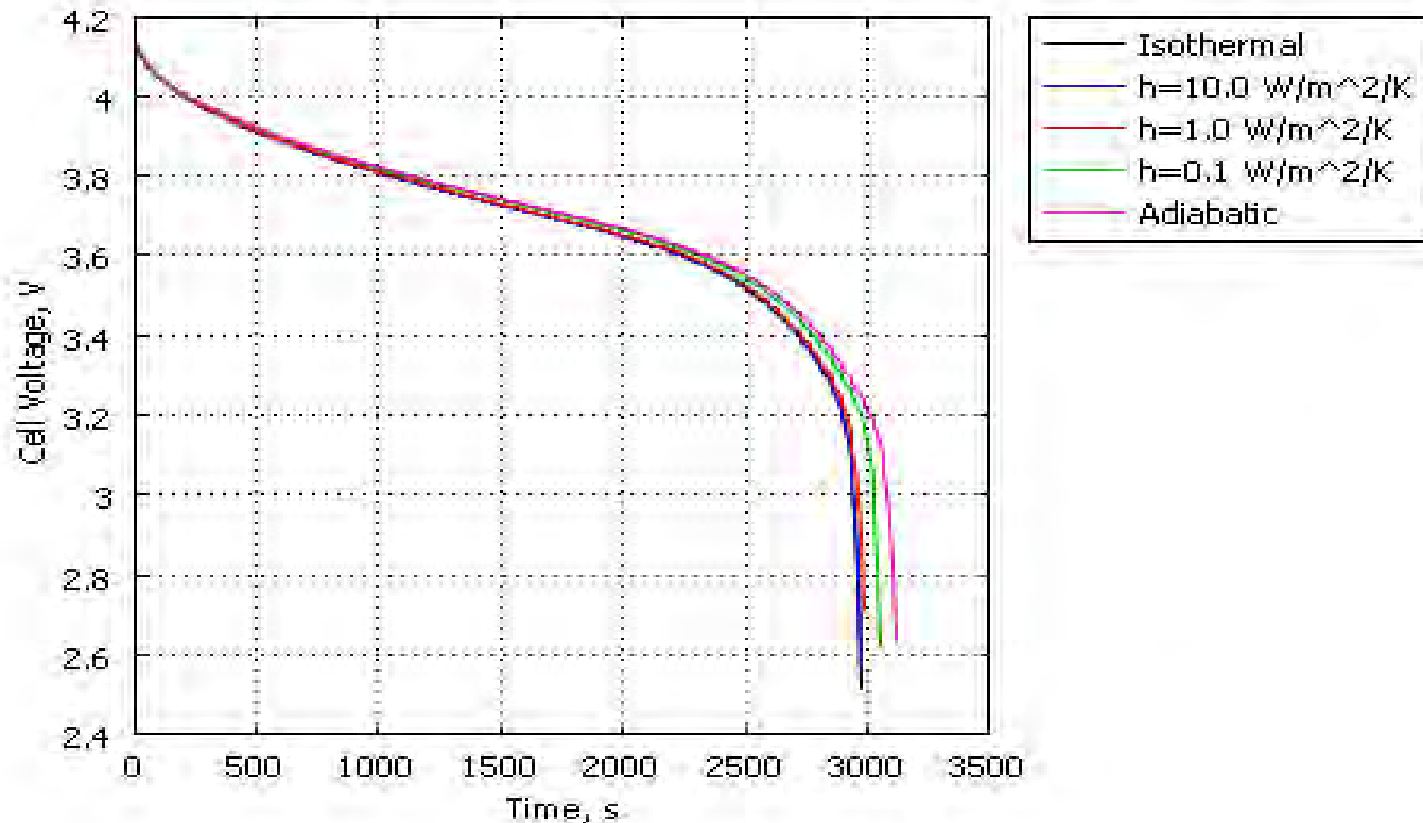
# Simulation Results in COMSOL MP



The temperature on the cell surface at 1C discharge process under three different cooling conditions where the heat transfer coefficient is 10.0, 1.0 and 0.1 W/m<sup>2</sup>/K, respectively, and two limiting conditions: the isothermal condition and the adiabatic condition.

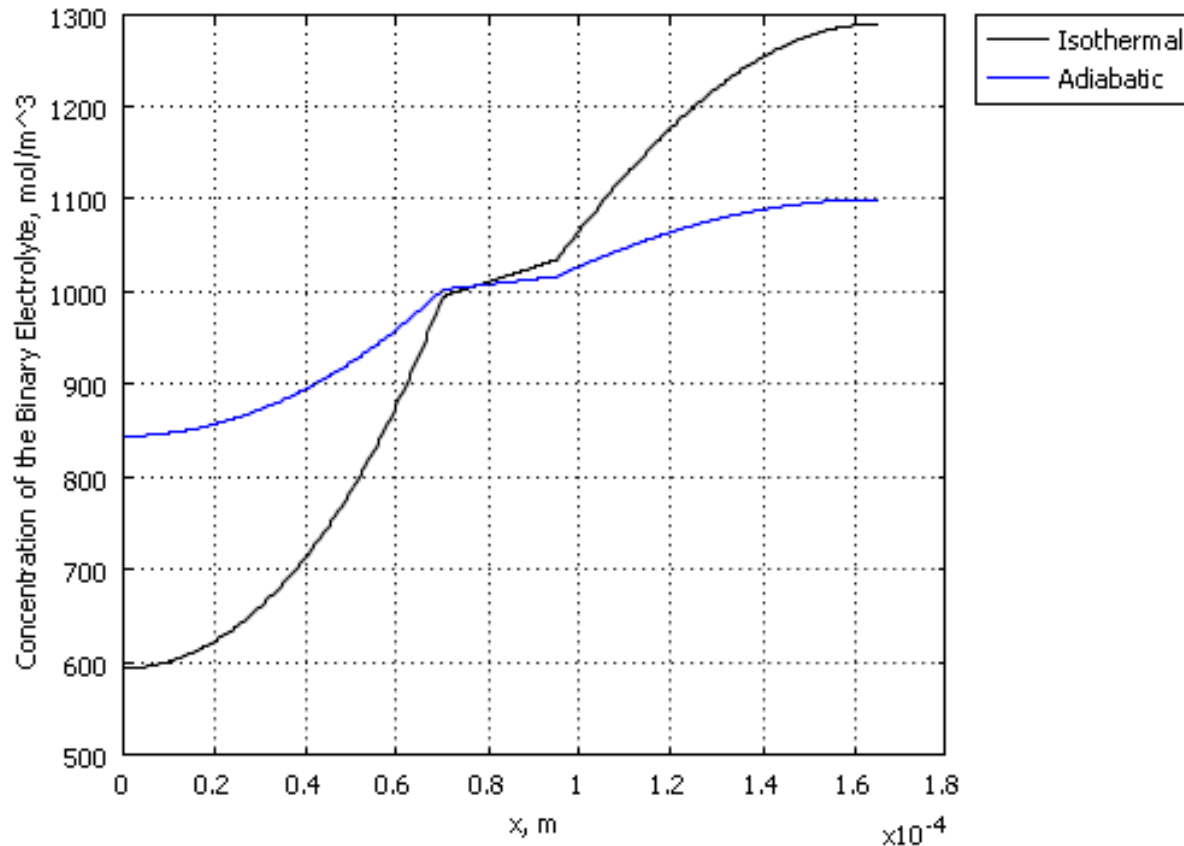


# Simulation Results in COMSOL MP



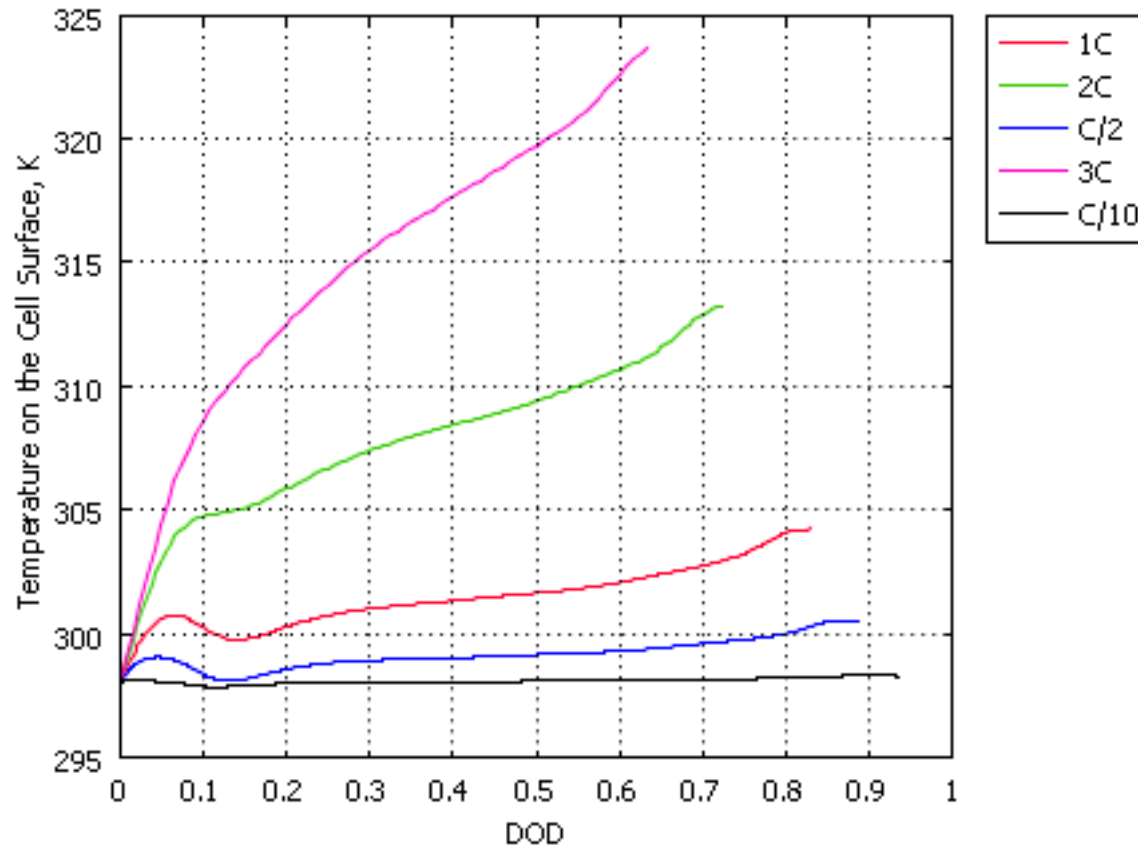
The cell provides more discharge capacity when it is placed in a better heat isolation environment (i.e. adiabatic condition). In a better isolated environment, the cell temperature increases faster during the 1C discharge process which results in the higher diffusion coefficient for the binary electrolyte and reduces the diffusion limitations.

# Simulation Results in COMSOL MP



The concentration profile under the adiabatic condition is flatter than that in the isothermal case, which indicates a better diffusion property in the electrolyte under the adiabatic condition than under the isothermal condition.

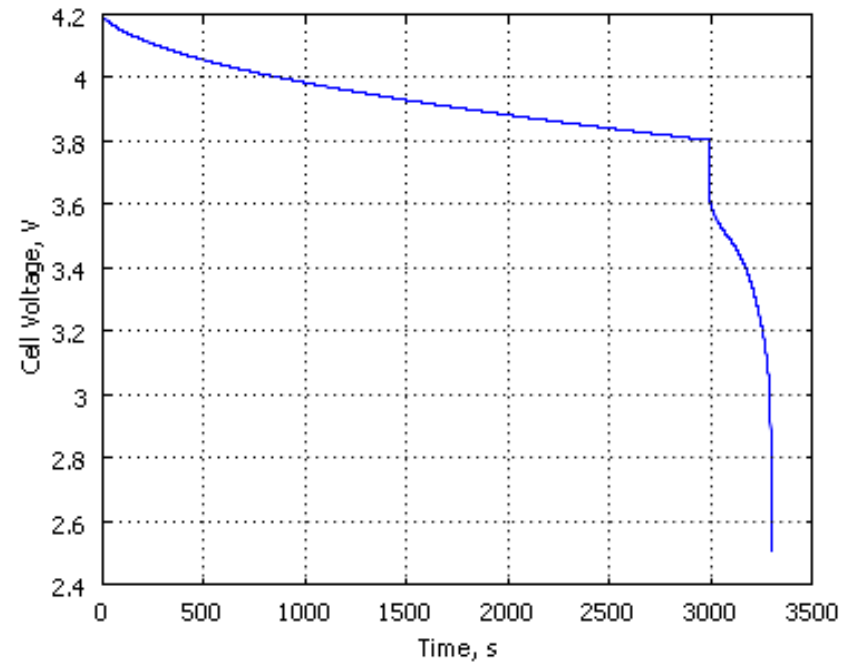
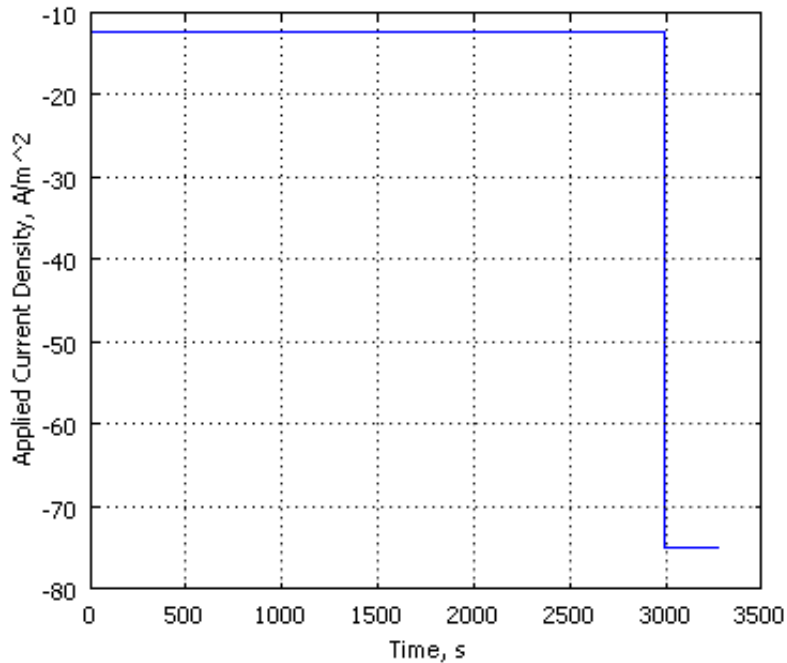
# Simulation Results in COMSOL MP



Temperature on the cell surface during discharge process under different current rates while the heat transfer coefficient  $h=1.0 \text{ W/m}^2/\text{K}$  where the DOD is defined as:  
 $\text{DOD} = \text{time} * \text{C rate} / 3600.$



# Simulation Results with Pulse Discharge

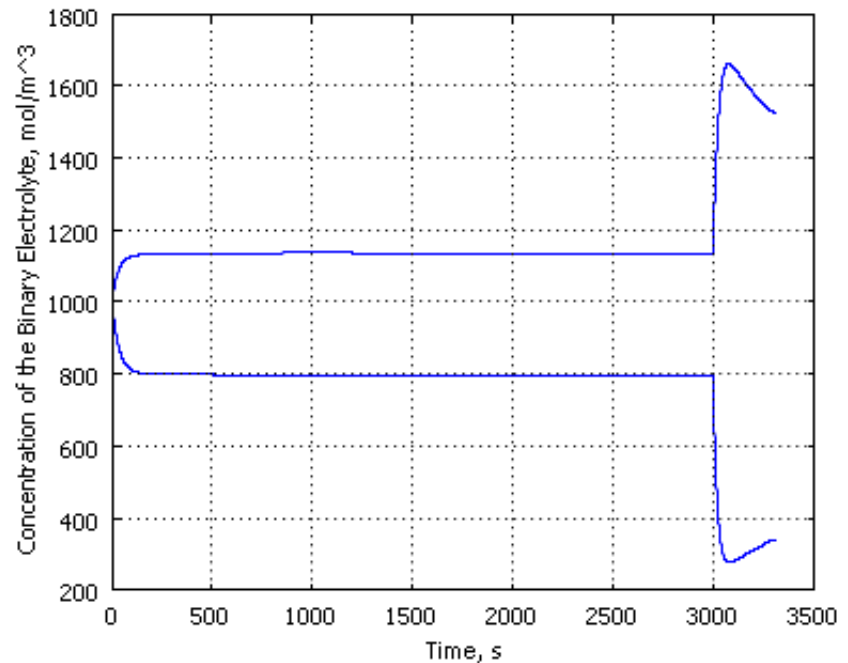
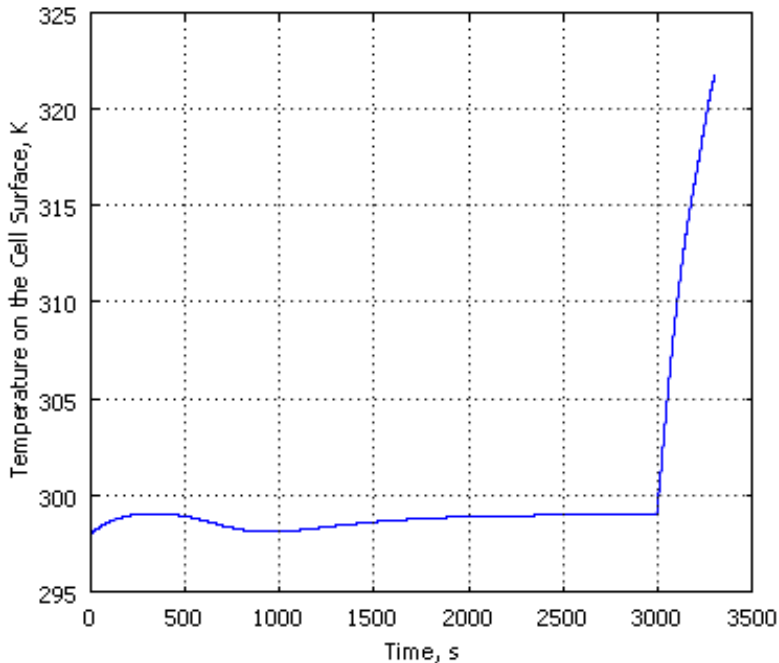


Test protocol: the cell voltage during the C/2 discharge for 3000s followed by a 3C pulse discharge until the cell voltage drops to 2.5V.





# Simulation Results with Pulse Discharge



The corresponding temperature on the surface of the cell is also plotted in the figure on the left. The surface temperature at the end of the 3C pulse is slightly less than that in the pure 3C discharge process.

Figure on the right shows the concentration of the binary electrolyte at the two ends of the cell during the pulse discharge process. At the beginning of the pulse, the concentration of the electrolyte changes extremely, after that it relaxes and tend to a stable value.



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Thank you for your Attention!

Questions?

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