Coupled Thermo-Electrochemical Modelling Framework for Predicting Lithium-ion Battery Performance and Degradation

Mechanical & Industrial Engineering
UNIVERSITY OF TORONTO

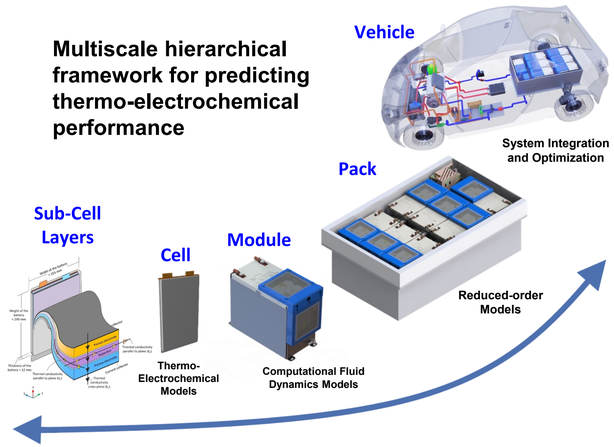
Oscar A. Alvarez[1], Mir A. Ali[1], Amador M. Guzman[1], Carlos M. Da Silva[1] , Cristina H. Amon[1,2]*

[1] Department of Mechanical and Industrial Engineering, University of Toronto
[2] Department of Chemical Engineering and Applied Chemistry, University of Toronto
**oscar.alvarez@mail.utoronto.ca*

atoms laboratory

Introduction

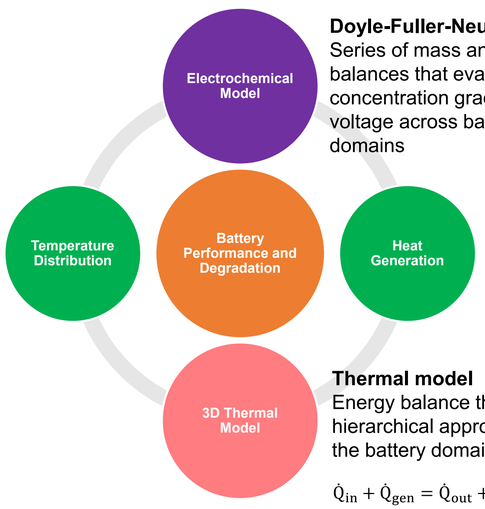
Multiscale hierarchical framework for predicting thermo-electrochemical performance



Objective

Develop a comprehensive numerical-experimental framework following a multiscale hierarchical approach for lithium-ion battery thermal management and lifecycle battery degradation analyses

Coupled Modelling Framework



Doyle-Fuller-Neumann (DFN)
Series of mass and charge balances that evaluate concentration gradients and voltage across battery domains

Thermal model
Energy balance through a hierarchical approach across the battery domains

$$\dot{Q}_{in} + \dot{Q}_{gen} = \dot{Q}_{out} + \dot{Q}_{acc}$$

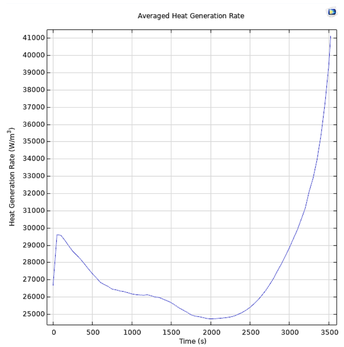
Preliminary Results

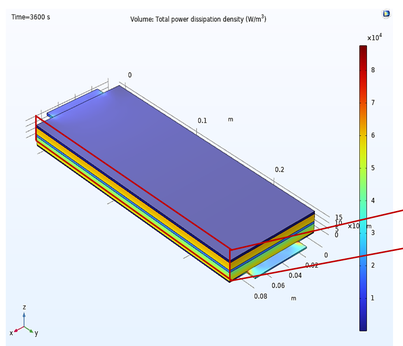
Heat generation rates

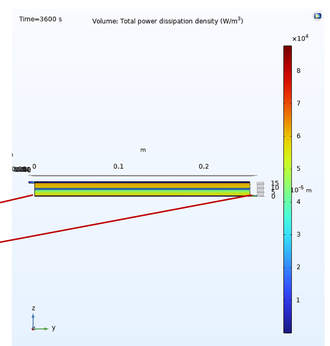
The battery heat generation rate is evaluated with DFN model using the following equation:

$$\dot{q} = \dot{q}_{ohm} + \dot{q}_{reac} + \dot{q}_{rev} = i_l \nabla \phi_l + i_s \nabla \phi_s + \sum_i a_i i_i \left(\eta_i + T \frac{\partial E_{Eq,i}}{\partial T} \right)$$

Volumetric heat generation rate [W/m^3] at 1C discharge rate:

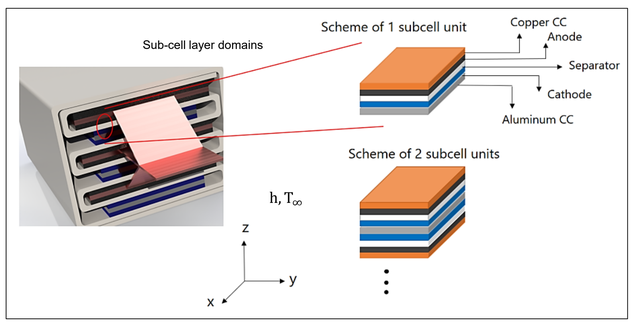




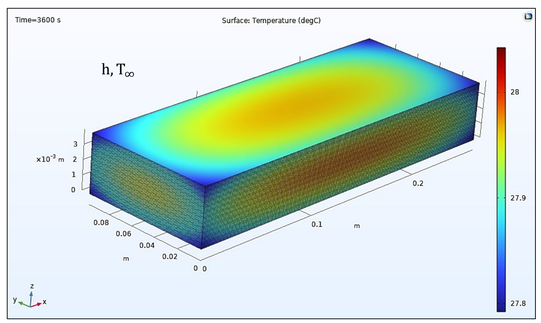


Effective thermophysical properties

Internal architecture of a pouch battery cell, composed of multiple sub-cell units



Temperature distribution at t = 3,600 s



$$k_{in-plane\ eff} = 28 \frac{W}{mK} \qquad k_{cross-plane\ eff} = 0.29 \frac{W}{mK} \qquad c_{p\ eff} = 928 \frac{W}{mK}$$

Conclusions

- Effective thermophysical properties can represent the entire battery as a homogeneous body, considering the heterogeneous and heat transport effects within the cell
- Heat generation rates are highly time and spatially dependent in large format pouch batteries
- Temperature gradients across lithium-ion batteries are also C-rate dependent
- Next steps involve investigating thermal responses at higher C-rates (2C, 3C), applying spatially distributed heat generation rates within the different sub-layer domains, incorporating degradation mechanisms into the thermo-electrochemical modelling framework, and validation/calibration activities in our upcoming TMS Laboratory (launching in Fall 2023)

Thermal management systems (TMS) Laboratory

Acknowledgements

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