Development of a Mathematical Model for Spiral-wound Li-ion Batteries

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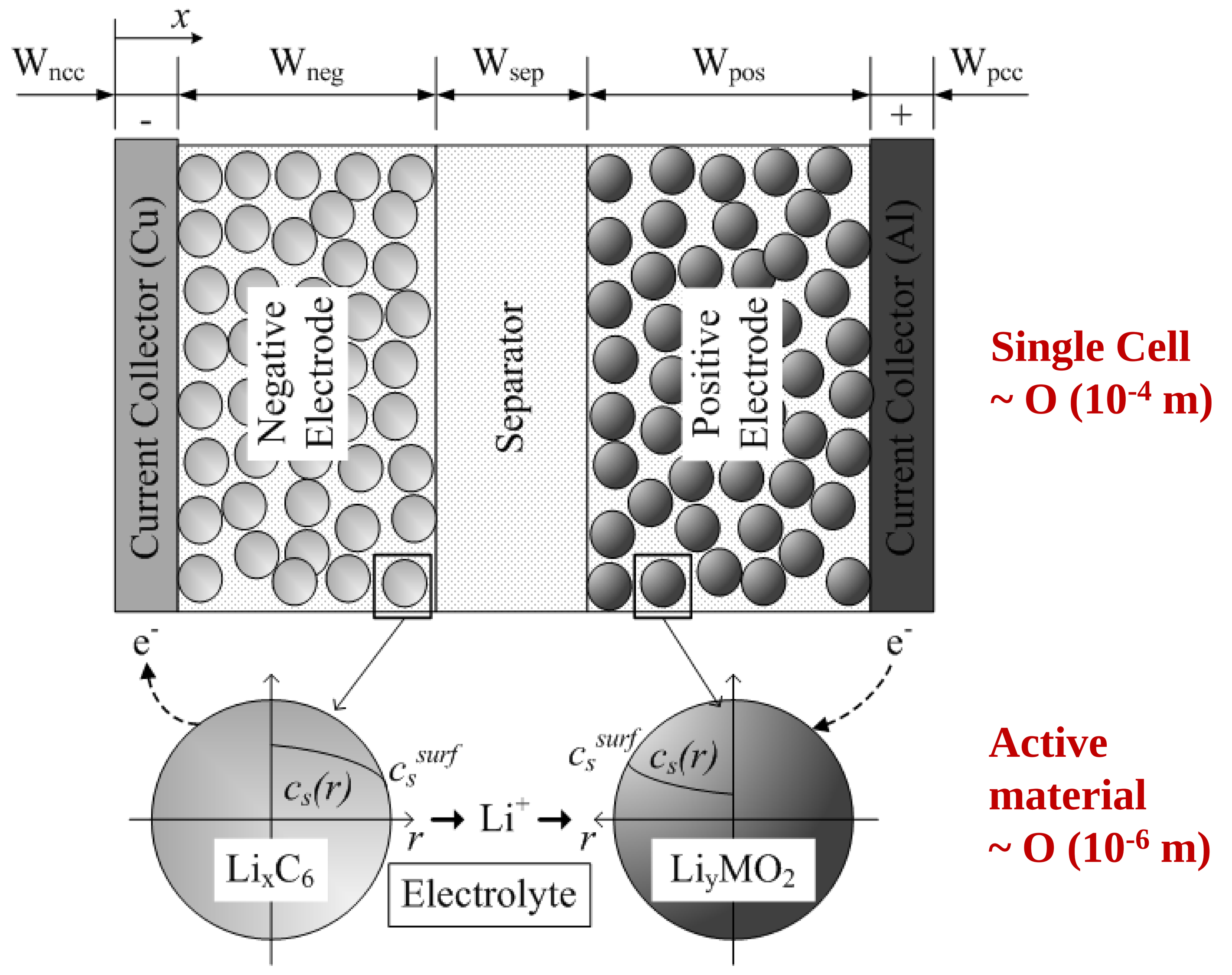
Introduction

- Lithium-ion batteries can be found in a range of form factors: for example, cylindrical, prismatic, and coin cells, where the cylindrical and prismatic cells are mostly of spiral-wound construction.
- The shape and size, in turn, affect the thermal envelope of the batteries as well as the overall performance since the electrochemical reactions are temperature dependent -- in fact, elevated temperatures can give rise to thermal runaway with catastrophic consequences.
- One way to study and explore various "what-if-scenarios" for a lithium-ion battery is through mathematical modeling coupled with a numerical solver for the resulting non-linear partial differential equations that describe transport as well as heat generation.
- Existing mathematical models for lithium-ion batteries -- most are one-dimensional and only consider single-way coupling between the electrochemical and thermal behavior.
- This work aims to give a detailed description of a two-dimensional (2D) multiscale mathematical model for a cylindrical (18650) spiral-wound lithium-ion battery (can be applied to spiral-wound prismatic cells as well) capturing the micro as well as the macroscale effects.
- The model couples the electrochemical and thermal behavior through the heat generation arising from reversible, irreversible and ohmic heating effects and the temperature-dependent transport and electrochemical parameters.

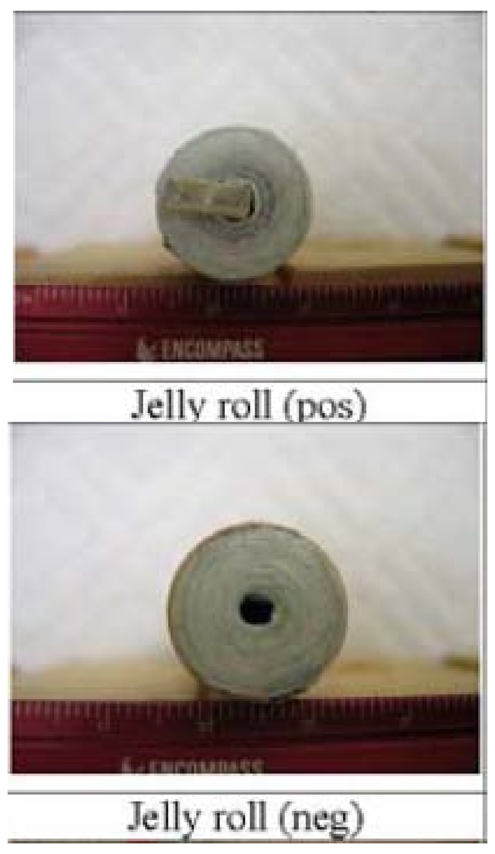


Schematic of a single cell representing various functional layers and illustrating the multiscales involved in modeling

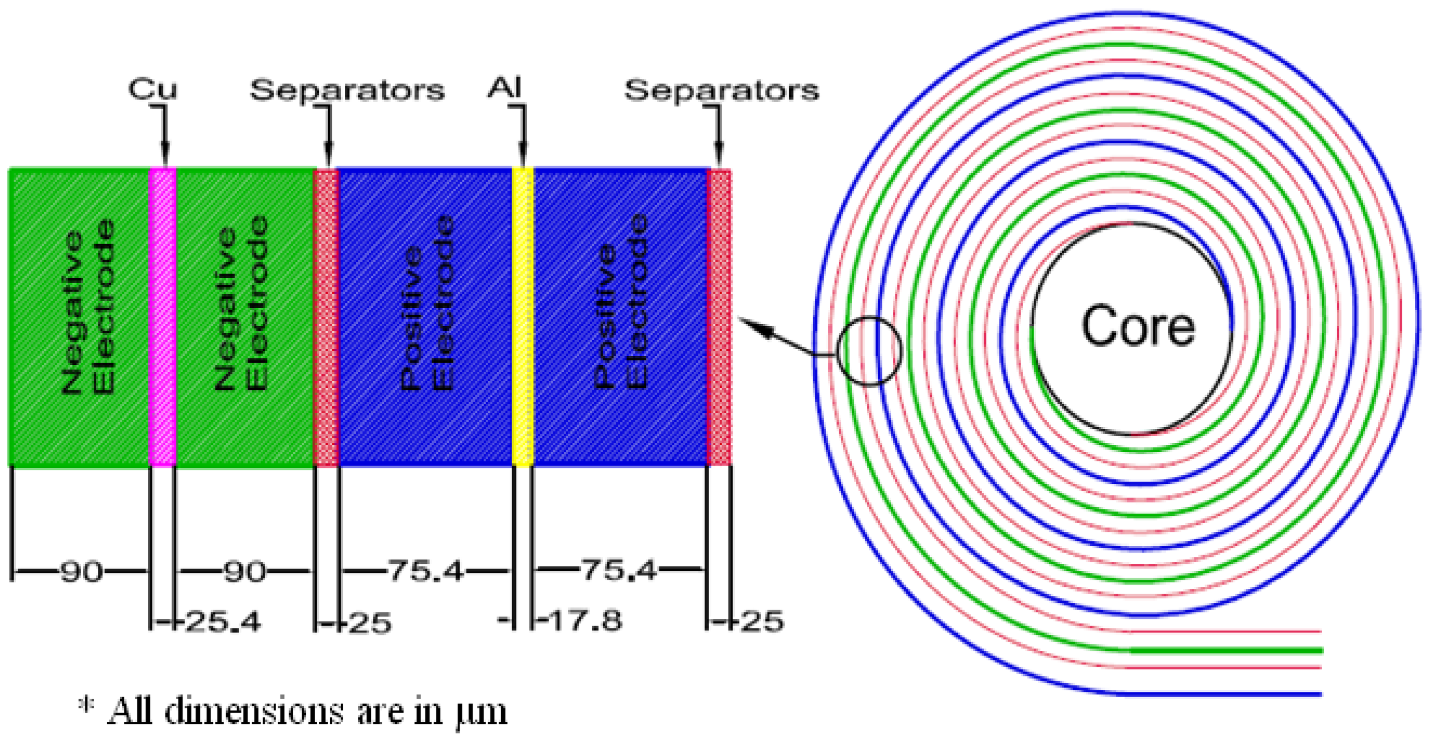
2D Model

~ O (10^{-3} m)

Bare spiral wound cylindrical cell



Jelly Roll inside the cell

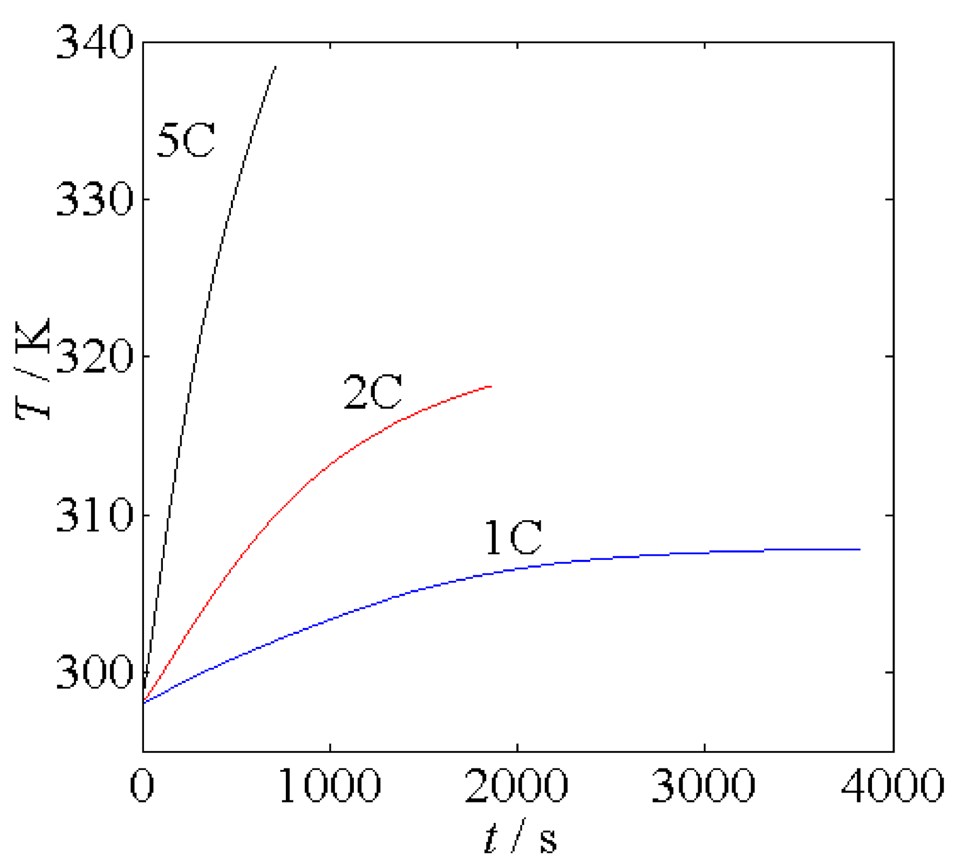


Two dimensional schematic of a Li-ion battery showing various functional layers with their respective thicknesses

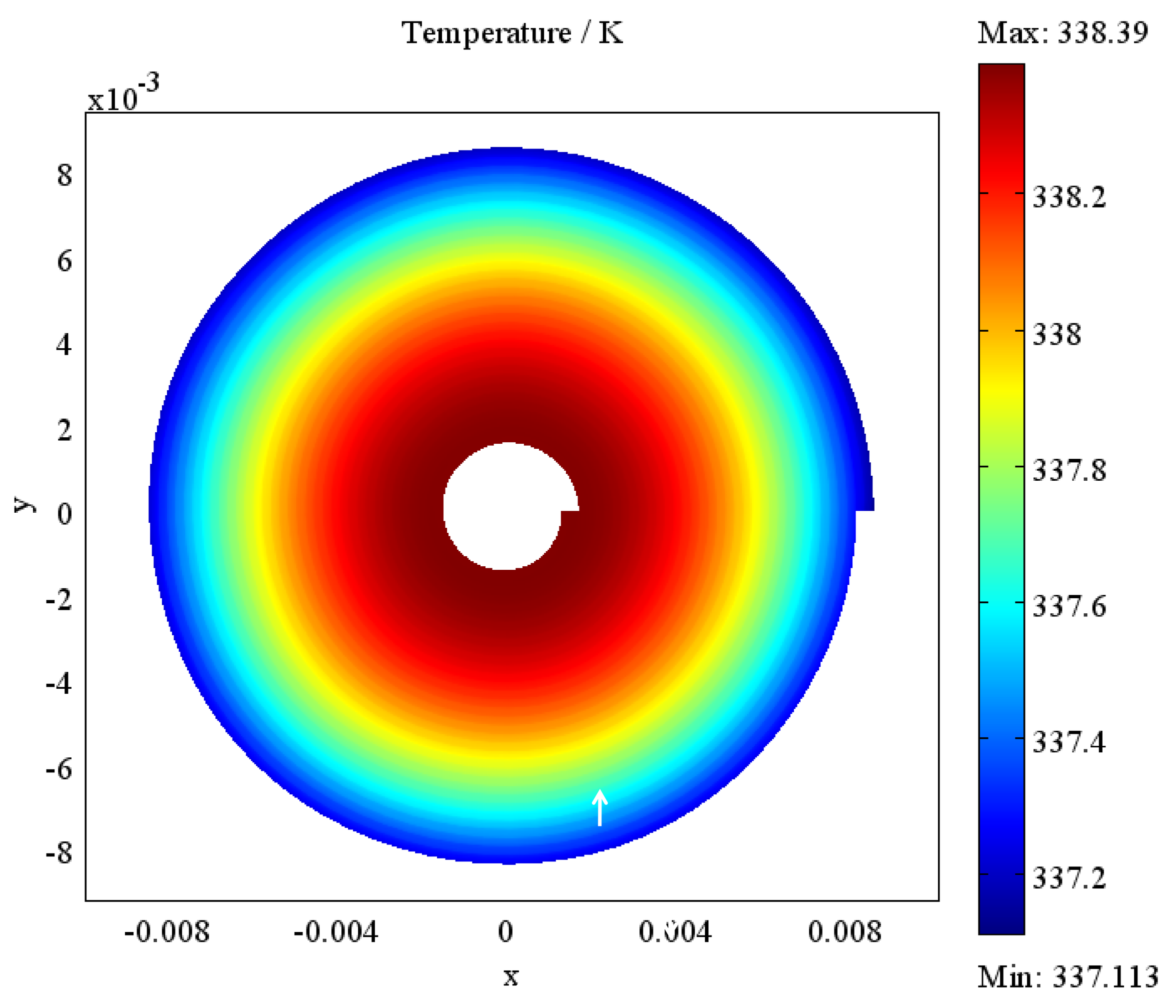
Model equations and assumptions

- Conservation of charge, species and energy – Multiscale model
- Narrow gap approximation leads to a 2D model from a 3D model.
- Natural convection on outside to 25°C ambient and insulated at inside (worst case scenario considered inside).
- Negative electrode – Li_xC_6, positive electrode – $LiMn_2O_4$ coated on both sides of Copper and Aluminium current collectors.
- Outer can of the 18650 cell is not considered, size of the inner core is assumed to be 3.6mm.
- Numerical solver – Comsol Multiphysics 3.5a

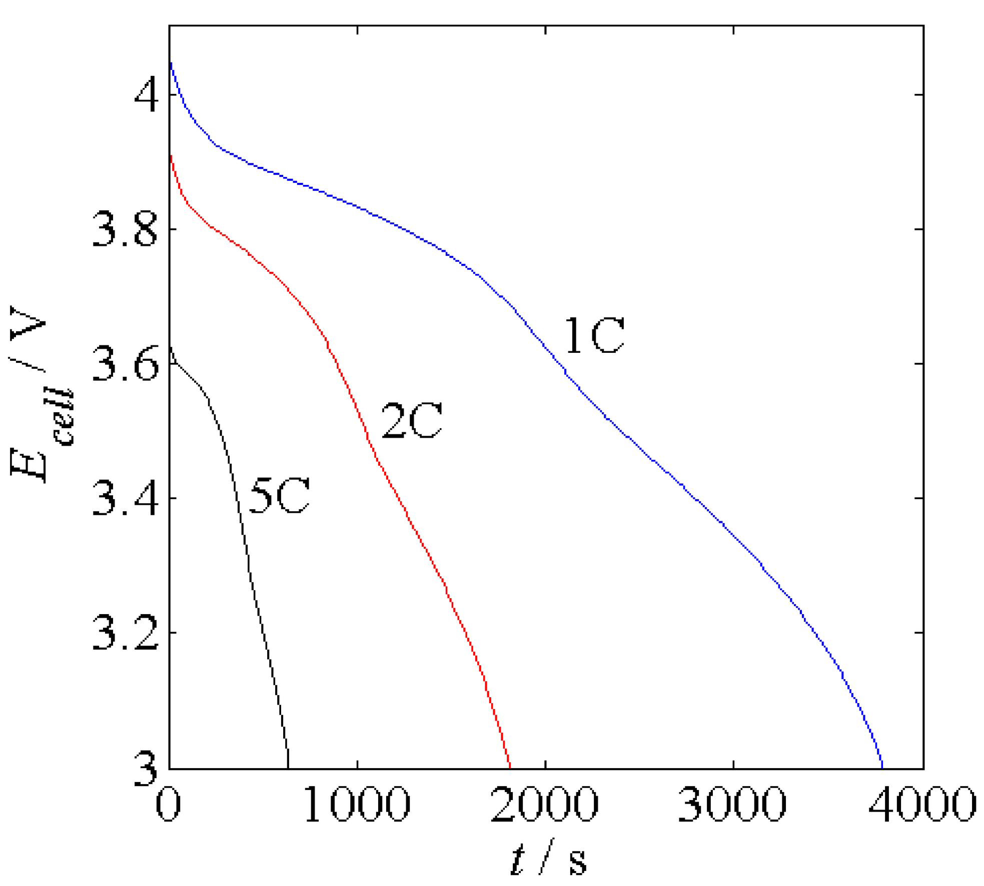
Results and Discussion



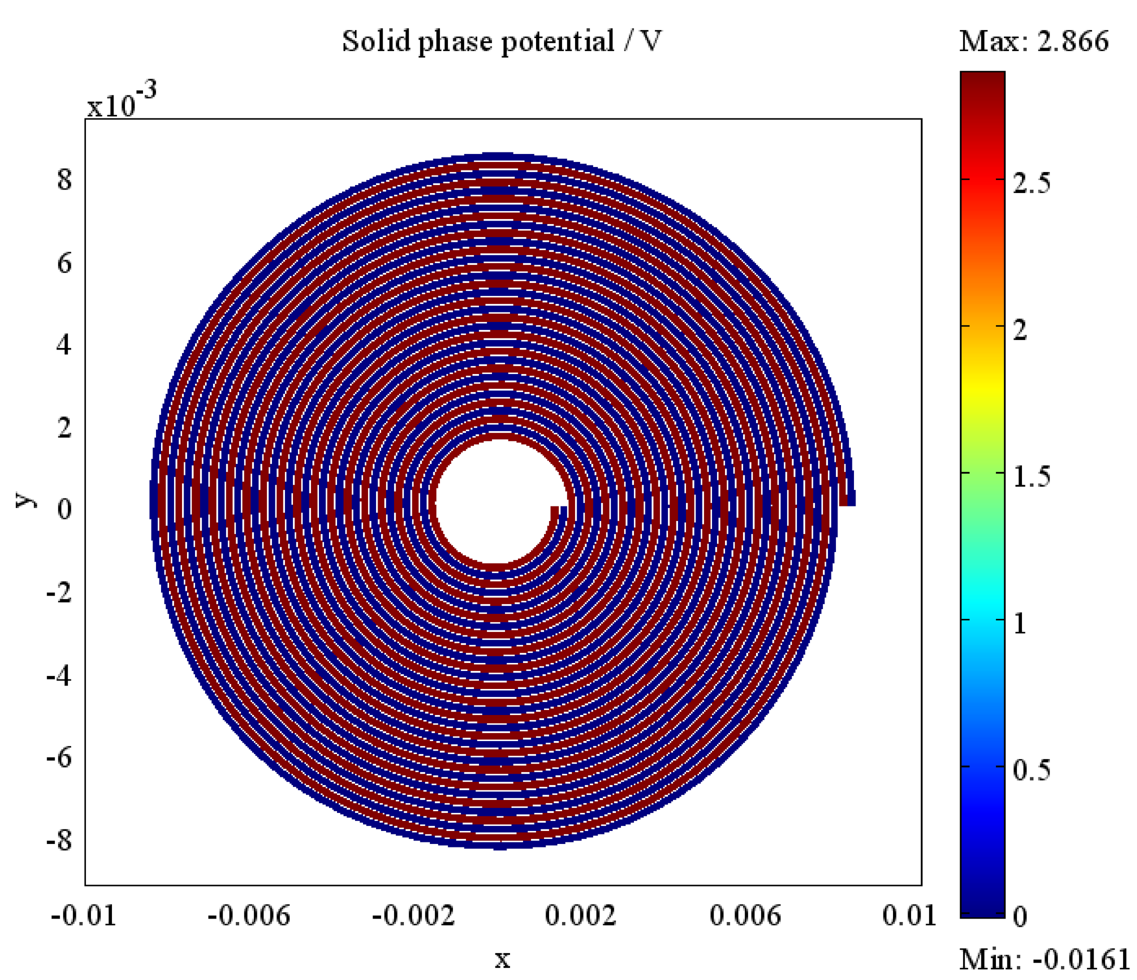
Temperature vs. time at the innermost point of the spiral wound cell at different discharge rates



Temperature profile at the end of discharge at 5C rate



Cell voltage vs. time at different discharge rates



Solid phase potential distribution at the end of discharge at 5C rate

- Higher discharge rates – Faster heat generation and higher temperature rise, lower capacity as indicated.
- No appreciable temperature gradient within the jelly roll from the centre to the outer – max. of 1.3°C at 5C rate. Lumped heat approach will be useful to get quick results but not for thermal runaway cases that requires the use of detailed model.
- Discharge at higher C rates as well as at higher ambient temperature may lead to thermal runaway and hence necessity of a thermal management system.
- Thermal runaway can be simulated by introducing Arrhenius relationships for the reaction rates
- Uniform potential distribution in the electrodes – In reality, the distribution of active materials is not uniform that will lead to non-uniform potential distribution and hence non-uniform temperature distribution as well. Therefore, there will be hot spots inside that could be identified by the 2D model.

Summary

- A 2D multiscale mathematical model for the transport phenomena inside the spiral wound cylindrical Lithium-ion battery is presented.
- The model couples the electrochemical and thermal behavior through the heat generation and the temperature dependent properties.
- Spatial non-uniformity of battery physics is captured by the model.
- Temperature difference within the jelly roll is relatively small but the temperature rise is significant at higher discharge rate that necessitates a thermal management system in place of high power applications.