Simplified Multiphysics Model for All-Solid State Microbatteries

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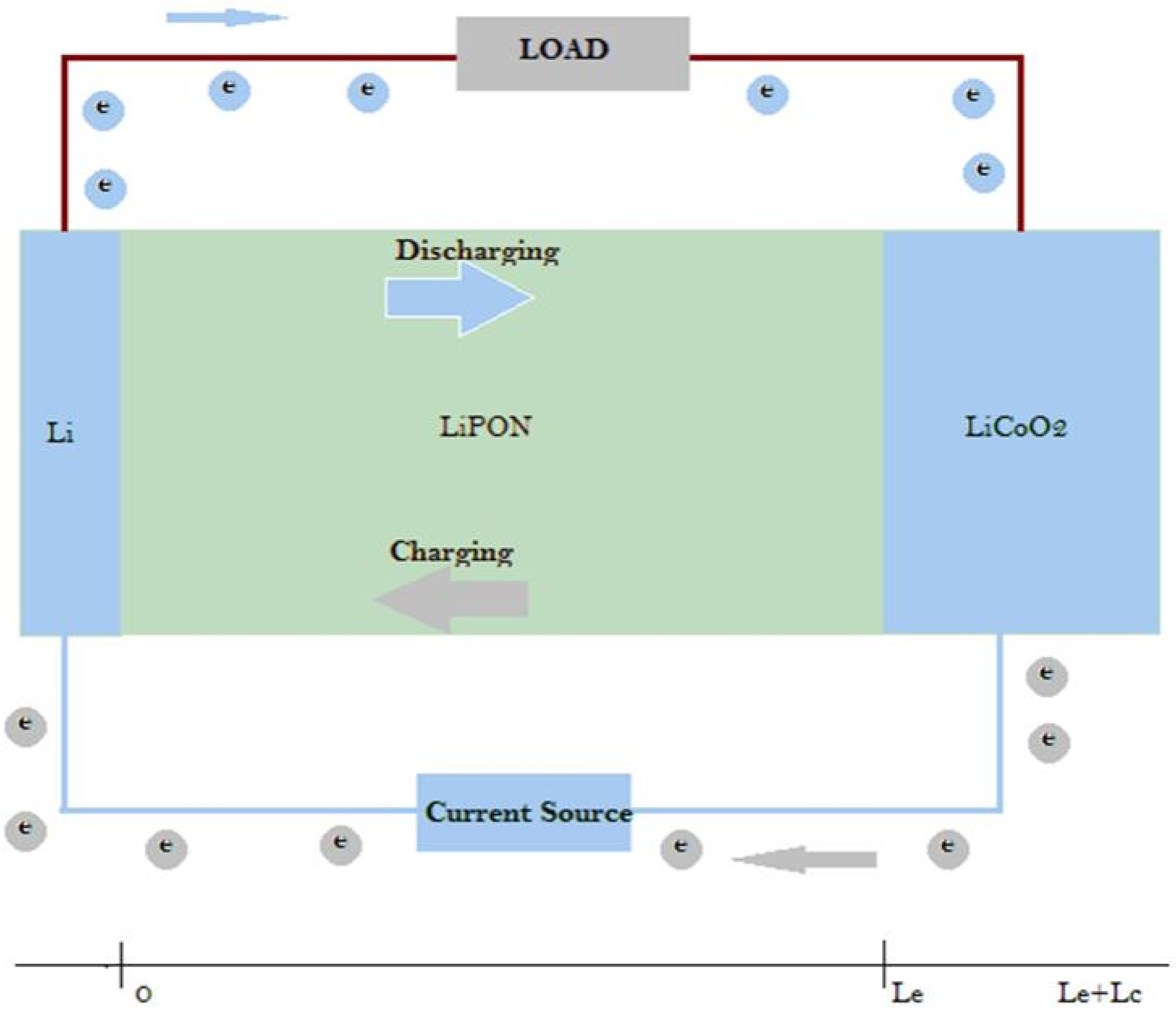
Introduction: We have developed a simplified partial-differential equation (PDE) model for a solid-state Li metal microbattery. The simplified PDE model was analyzed using both COMSOL Multiphysics and a finite-difference scheme implemented in Matlab. Results from the two approaches deviate by at most 2% from a full PDE model.



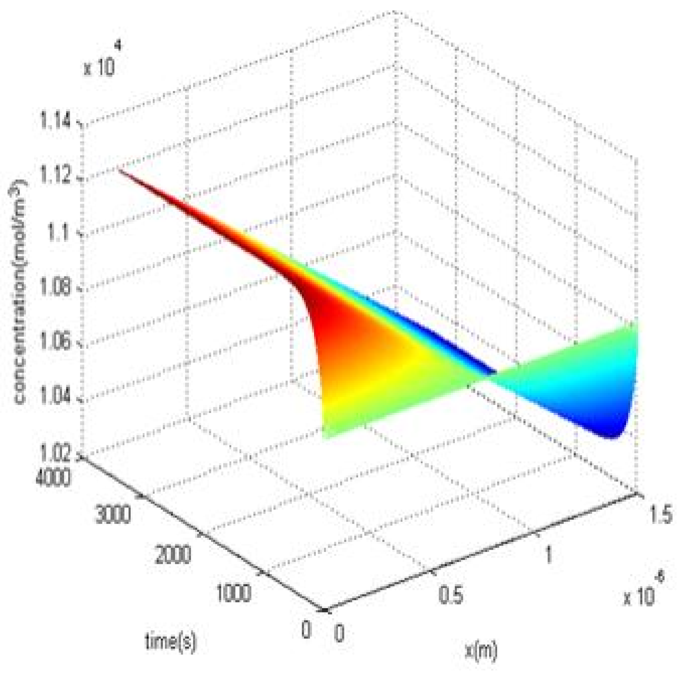
Planar solid-state Li microbattery

Modeling Approach: By assuming both local and global electro neutrality of the solid-state electrolyte we have reduced the nonlinear PDE describing both negative & lithium ions transport to a linear parabolic equation:

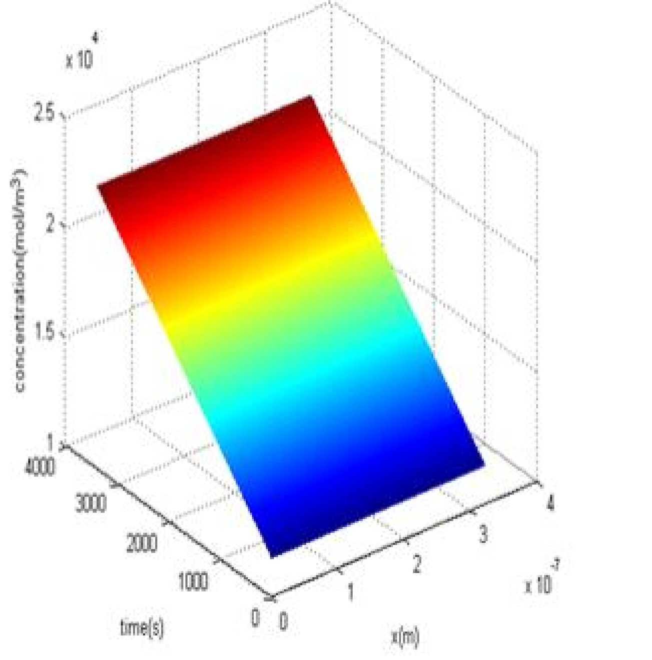
$$\frac{\partial c_i}{\partial t} = D_i \frac{\partial^2 c_i}{\partial x^2} - \frac{zF}{RT} D_i \left(c \frac{\partial E}{\partial x}\right) \Rightarrow \frac{\partial c}{\partial t} = \frac{D_1 D_2}{2(D_1 + D_2)} \frac{\partial^2 c}{\partial x^2}$$

where the nonlinear Nernst-Plank-Poisson equation [1], commonly used to model ion transport in electrochemical systems, is reduced to a linear diffusion equation [2]. This transformation makes the model ideal for further reduction and usage in embedded microbattery design and verification. Similar linear parabolic equation is used to describe the lithium transport inside the cathode. The model is first solved using COMSOL Multiphysics batteries and fuel cells module. It is further verified by applying a finite difference discretization and using Matlab ODE solver.

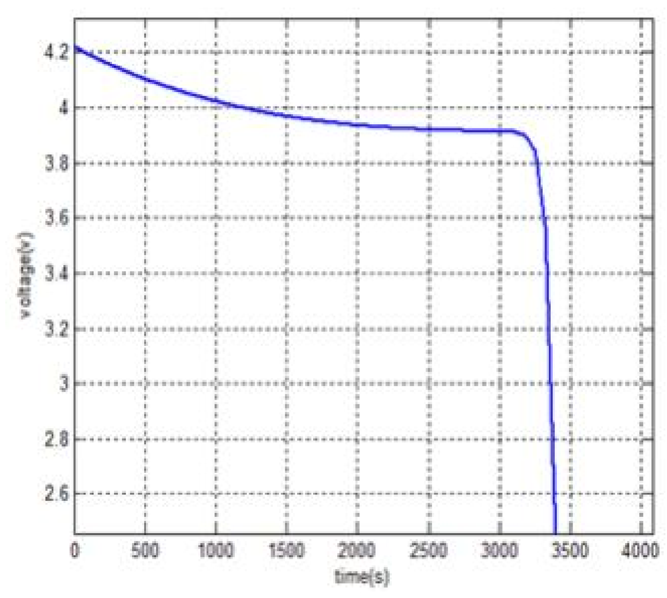
Results: The discrepancy between our model and the full nonlinear model is within 2% and runs six times faster than the nonlinear model. The figures below show the steady state Lithium concentration profiles in the electrolyte and cathode, respectively, for a discharge rate of C=1.



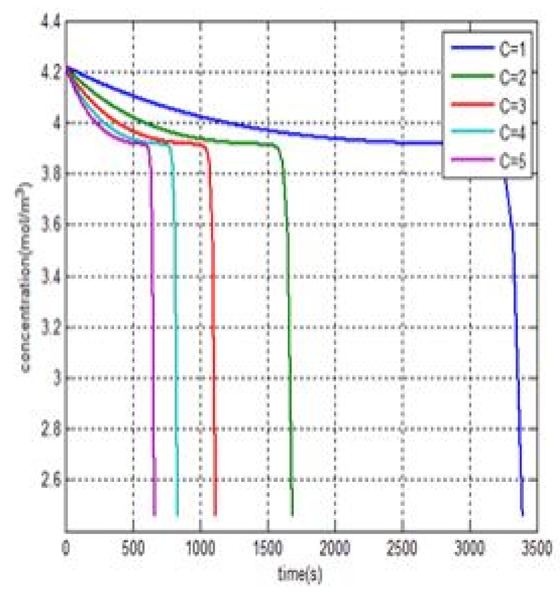
Electrolyte concentration



Cathode concentration



Comparing discharge profiles



Discharge profile predictions

The discharge profiles of the nonlinear and the simplified models are compared above. The model is also able to predict the discharge profile for discharge rates higher than C = 1.

Future Work: We plan to use the simplified model for generating compact micro battery models for usage in design, verification, and management flows of embedded battery subsystems.

References:

1. D.Danilov, R.A.H. Niessen, and P.H.L. Notten, Modeling All-Solid-State Li-Ion Batteries, *JES,* 58, A215-A222 (2011).
2. S. D. Fabre, D. Guy-Bouyssou, P. Bouillon, F. Le Cras, and C. Delacourt. Charge/Discharge Simulation of an All-Solid-State Thin-Film Battery Using a One-Dimensional Model, *JES,* 159, A104-A115 (2012).

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