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Numerical Simulation of Pressure Management Strategies for Lithium-ion Pouch Cells

Reza Behrou, Dept. Civil, Environmental & Architectural Eng., University of Colorado Boulder, reza.behrou@colorado.edu
Kurt Maute, Dept. Aerospace Eng., University of Colorado Boulder, kurt.maute@colorado.edu
Kandler Smith, Center for Transportation Technologies and Systems, NREL, kandler.smith@nrel.gov

Multi-scale modeling of lithium-ion batteries We study the influence of internally/externally induced mechanical stresses on the electrochemical performance of lithium-ion batteries. We focus on the dependence of the ion transport in the separator on the stress state. Internally induced stresses are caused by intercalation of Li ions into active particles in the electrodes which leads to swelling of the particles and expansion of the electrodes. In addition, application of external pressure on the battery also results in stresses. Peabody and Arnold [1] observed that compressive external pressure and/or intercalation-induced expansion of electrodes lead to a significant decrease of the ionic conductivity in separator. Experimental results suggest a nonlinear relationship between ionic conductivity and internally/externally induced stresses. To gain further insight into this relationship and it consequences on the overall performance of the battery, we present a numerical model that accounts for multi-physics coupling phenomena across multiple scales and captures the dependency of the ionic conductivity on the stress state via a simple model.

In order to characterize the effect of internal/external pressure on the ionic conductivity of separator, we build upon a 3D finite element model which considers the fully coupled electrochemical-thermal-mechanical response of battery at both cell and particle levels. To accurately capture the mechanical response of the individual layers, we introduce a state-of-the-art solid shell finite element formulation into our finite element model. To account for the interaction between different phenomena at different computational scales we distinguish three different length scales in our multi-scale modeling: at the $macro-scale$, the electrochemical and mechanical performance of the entire battery are characterized through the Li^+ ion concentration, c_l, the electric potential in solid phase, ϕ_1, the electric potential in liquid phase, ϕ_2, and the macroscopic displacement, $\mathbf{u}$; at the $micro-scale$, the performance of single active particle is investigated through the lithium concentration in the particle, c_s, the microscopic displacement, u, and the hydrostatic stress field, σ_h; and at the $meso-scale$, the interaction between macro- and micro-scales are related through homogenization methods. The micro-scale phenomena are captured at the macro-scale through introducing an effective porewall flux, j_{eff}, and electrochemical eigenstrains, $\mathbf{e}^{ch}$ [2]. Each length scale is characterized by specific governing and constitutive equations and the relationship with other length scales. The macro- and micro-scales governing equations are summarized in Tables. 1, where ε is the liquid volume fraction of the electrode or porosity, F is Faraday's constant, t_+^0 is lithium ion transference number, $\mathbf{b}$ is the body force, BV is Butler-Volmer equation, and j_s is the micro-scale porewall flux. For further details, we refer the readers to the work by Golmon et al. [2, 3, 4].

The above model is augmented to account for the dependence of the ionic conductivity in the separator on the stress state. Following the work by Peabody and Arnold [1], we describe the ionic conductivity as a function of the hydrostatic stress through the following model:

$$\kappa_\infty(\sigma_h) = \kappa_{\infty_0} e^{-\beta\sigma_h}, \qquad 0.01 \leq \beta \leq 0.1 \tag{1}$$

where κ_{∞_0} is the initial ionic conductivity and β is the decay rate.

Table 1. Governing equations in multi-scale modeling of lithium-ion battery [2].

Equation type	Macro-scale equations	Micro-scale equations
Diffusion-migration	$\varepsilon \frac{\partial c_l}{\partial t} + \nabla.\mathbf{N} + \frac{1}{F}\frac{\partial t_+^0}{\partial c_l}\mathbf{i_2}.\nabla c_l - (1-t_+^0)j_{\text{eff}} = 0$	$\frac{\partial c_s}{\partial t} + \nabla.\mathbf{J} = 0$
Current in solid phase	$\nabla.\mathbf{i_1} + F j_{\text{eff}} = 0$	–
Current in liquid phase	$\nabla.\mathbf{i_2} - F j_{\text{eff}} = 0$	–
Mechanical deformation	$\nabla.\sigma + \mathbf{b} = 0$	$\nabla.\sigma = 0$
Reaction kinetics	–	$BV(c_l, \phi_1, \phi_2, c_s) - F j_s = 0$

Numerical simulation We study the effect of internally/externally induced stresses on the ionic conductivity of separator with the numerical model outlined above. While our computational framework can be readily used to study the thermal effects, we neglect such effects in the current study. We discharge the battery at different magnitudes of the external pressure and analyze the response of the battery during a full discharge process. Figure 1 shows the effect of external pressure on the electrochemical performance of the battery. Comparison of the discharge curves for the unstressed and stressed cell shows that there is a significant capacity fade and reduction in discharge time as the external pressure increases. These results are in agreement with one reported by Peabody and Arnold [1].

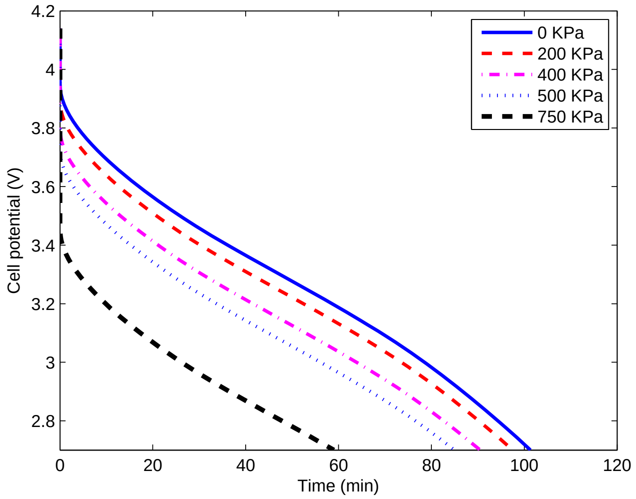

Figure 1. Variation of cell potential with time during full discharge process at different external pressure.

References

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