Model for Efficient Optimization of Thick Lithium-Ion Battery Electrodes

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While the use of thick electrodes in Li-ion batteries provides an appealing pathway to increase the energy density and reduce the cost of inactive components, it faces a critical challenge of poor rate performance due to kinetic limitation on mass transport. A thorough understanding of the trade-off between the power and energy density for thick electrodes is currently lacking, which impedes the efforts in the design and optimization of electrode structures for specific applications. To address problem, we developed an analytical model to provide very efficient and yet accurate prediction of the discharge performance of thick battery electrodes. Compared to the widely used numerical simulations based on the porous electrode theory, this model offers a more transparent understanding of the limiting factors on the rate performance of thick electrodes and the effects of structural parameters. A significant advantage of the model is that it incurs negligible computation cost compared to the pseudo-2D battery simulations, and thus provides a powerful tool for the efficient optimization of thick electrodes within the multi-dimensional design space.

Our model is derived based on the fact that the capacity utilization of thick electrodes is limited by electrolyte transport and a pseudo-steady state of electrolyte transport is established after a transient period during discharge. These two observations allow us to arrive at an analytical expression for the discharge capacity at termination based on the steady-state assumption and mass conservation in electrolyte. As shown in Figure 1a, the predicted distribution of Li ion concentration in electrolyte agrees very well with the numerical simulation. The depth of discharge (DoD) calculated from the model provides excellent approximations to the simulation results without any adjustable parameters, see Figure 1b. This model is generally applicable to electrodes that display solid-solution intercalation behavior such as the layer oxide cathodes paired with the graphite anode at low to moderately high discharge rates.

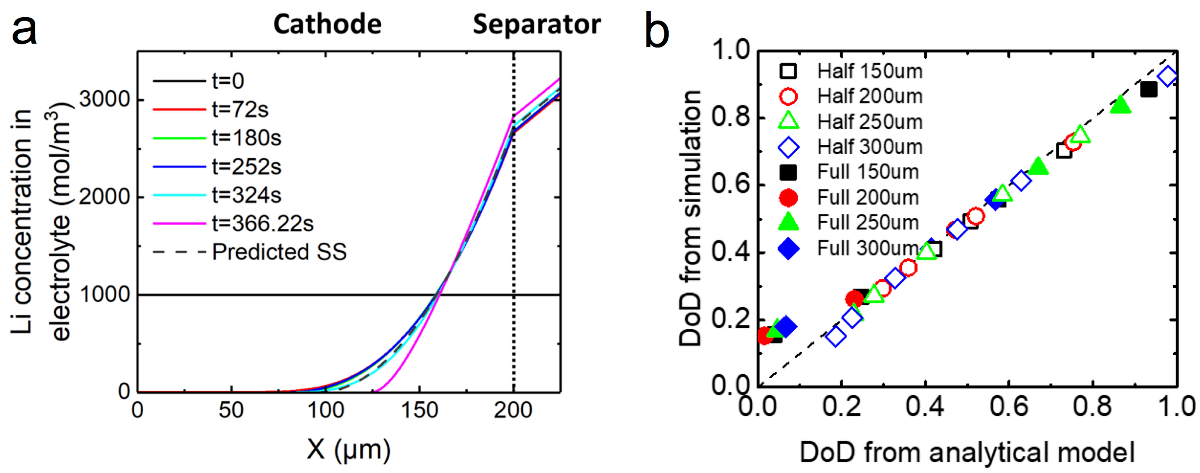

Figure 1 (a) Li concentration distribution in electrolyte across cathode thickness in a NMC/graphite cell calculated from the pseudo-2D simulation (solid lines) and the analytical model (dashed line). (b) Comparison of DoD predicted by pseudo-2D simulation and analytical model for various electrode thickness in half or full cell configurations.