Solid State Diffusion in Insertion Electrodes

Venkat R. Subramanian, James A. Ritter
and Ralph E. White
Center for Electrochemical Engineering,
Department of Chemical Engineering
University of South Carolina
Columbia, SC 29208

Insertion electrodes are preferred because of reversibility, high energy density and large range of selection of materials. Solid/liquid phase potential and electrolyte concentration in insertion electrodes (e.g., lithium/polymer/insertion cell) are governed by the concentrated solution theory[1]. The transport of intercalating species in the solid phase is governed by diffusion. The solid phase diffusion is related to the transport in the electrolyte through the continuity of pore wall flux at the particle surface.

Doyle *et al.*[1] applied Duhamel's superposition theorem to this pore wall flux and performed the integration numerically. This approach cannot be used for concentration dependent diffusivity[2-5] (figure 1), which is especially important for predicting the temperature rise of the lithium-ion cell[6]. Botte and White[6] solved this pseudo two dimensional problem by solving numerically both in the electrolyte and inside the particle. Numerical simulations are computationally intensive and extension to pseudo three-dimensions and to a cell stack seem out of reach.

Parabolic profile approximations commonly used in adsorption models[7] has been extended for the use in the modeling of solid-state diffusion in the spherical electrode particles (figure 2). A quantitative criterion for the validity of these approximate models will be presented. This approach reduces the partial differential equation to two coupled ordinary differential equations and saves the computation time drastically. Application to pseudo two and three dimensional modeling of lithium-ion batteries will also be discussed.

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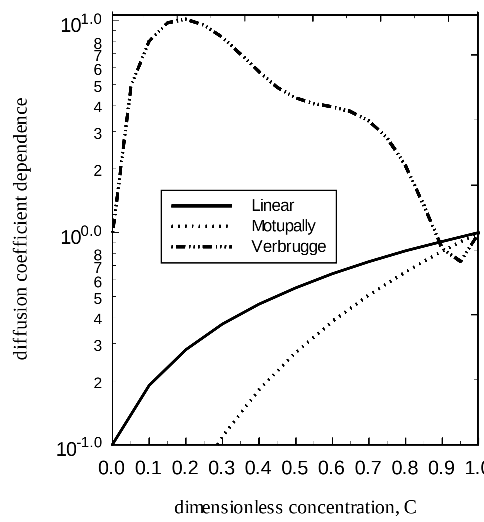

Figure 1: Variable Diffusivity

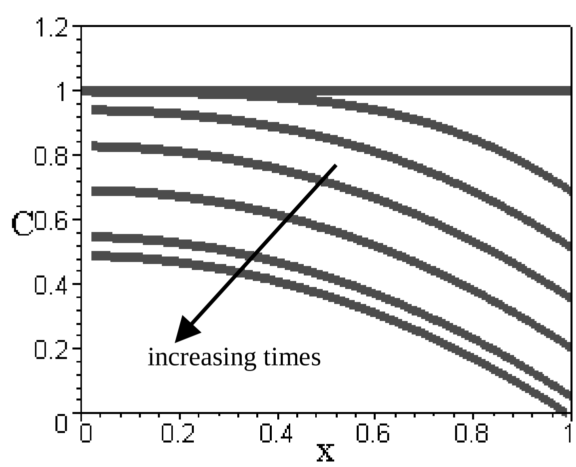

Figure 2: Concentration Profiles inside a spherical particle.