

Influence of Electrode Kinetics on Lithium-ion Battery Characteristics

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Abstract

Introduction

The purpose of this work is to show whether an important difference in electrode potential and electrolyte concentration can be observed in a Lithium-ion battery model, when considering either the Butler-Volmer equation or the Tafel equation for describing the electrode kinetics (including a boundary layer between the electrolyte and the electrode particles). For this purpose, a mathematical model is composed describing the electro-chemical processes in a 2D Lithium-ion battery, inspired from the literature [1,2].

Use of COMSOL Multiphysics®

The mathematical model is solved for, using the Equations Based Model in COMSOL Multiphysics®. The 2D physical setup contains five domains: a negative electrode current collector (Cu), a negative porous electrode (Li_xC₆), a separator, a positive porous electrode (Li_yMn₂O₄) and a positive electrode current collector (Al). The electrode (present in the pores of the negative electrode, the separator and the positive electrode) consists of a solution of a lithium salt (LiPF₆) in a non-aqueous solvent (a 2:1 v/v mixture of ethylene carbonate (EC) and dimethylcarbonate (DMC)).

The current is considered to flow through the tabs on the top of the two electrodes. During discharge, the lithium ions insert into solid particles of the positive electrode and de-insert from the solid particles of the negative electrode. It is assumed that interfacial chemical equilibrium exists in the electrolyte phase due to a large value of the mass diffusivity of electrolyte. Also, interfacial electrical equilibrium is assumed to exist in both the electrolyte and solid active material phases due to either large values of their electronic conductivities or a small size of active material particles.

Results

The results are presented in Figures 1 to 4 and are taken along the top of the Lithium-ion battery. We can see clearly the differences in the results between using the Tafel equation and the Butler-Volmer equation. This implies that neglecting low overpotential is not to be suggested in Lithium-

ion batteries of the kind studied in this work.

Reference

- [1] W.B. Gu and C.Y. Wang, "Thermal-electrochemical modeling of battery systems," J. Electrochem. Soc., 147(8), 2910-2922 (2000).
[2] C.Y. Wang, W.B. Gu, and B.Y. Liaw, "Micro-Macroscopic Coupled Modeling of Batteries and Fuel Cells I. Model Development" J. Electrochem. Soc., 145, 3407-3417 (1998).

Figures used in the abstract

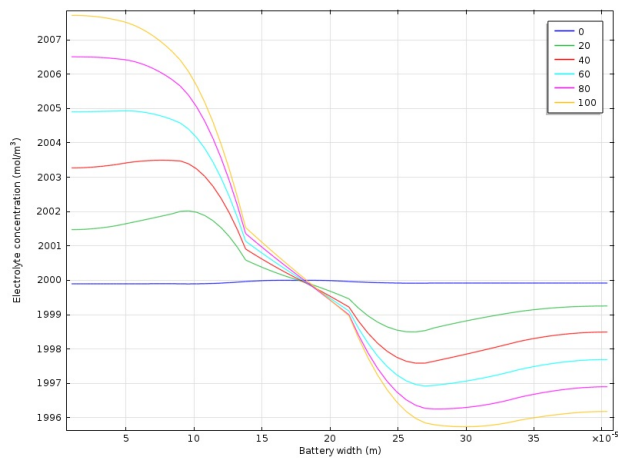


Figure 1: Electrolyte concentrations for Butler-Volmer kinetics; the legend shows the curves for different times in s.

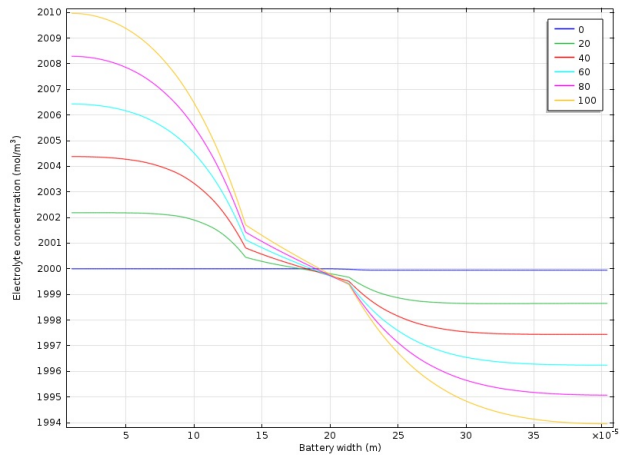


Figure 2: Electrolyte concentrations for Tafel kinetics; the legend shows the curves for different times in s.

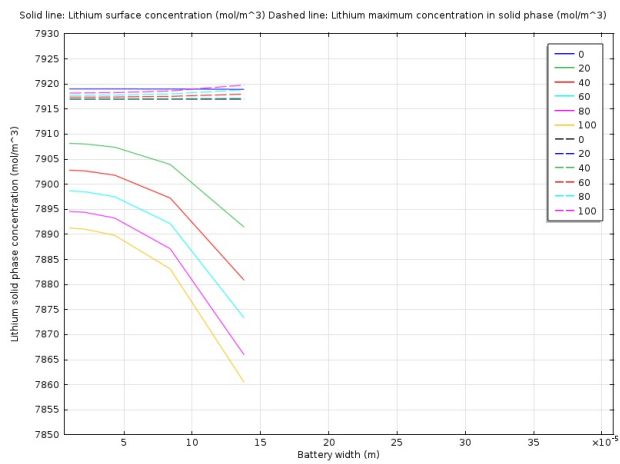


Figure 3: Lithium solid phase concentrations in the anode for Butler-Volmer kinetics; the legend shows the curves for different times in s.

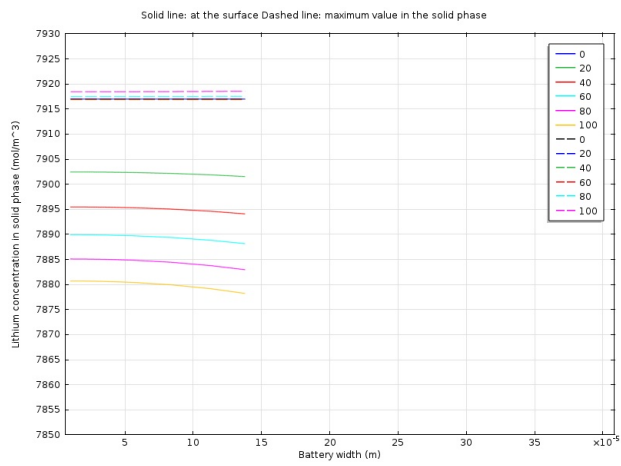


Figure 4: Lithium solid phase concentrations in the anode Tafel kinetics; the legend shows the curves for different times in s.