

Modeling of Li-ion Battery Performance in Hybrid Electric Vehicles

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ABSTRACT

Considerable improvements can be obtained in battery performance for hybrid electric vehicles (HEVs) by employing an electrochemistry-transport model based on a multi-physics modeling framework and ultrafast numerical algorithms. One important advantage of this approach over the lumped equivalent circuit (or look-up table) approach is the ability of the former to adapt to changes in design and control. In this work, we present mathematical and numerical details of our approach, and demonstrate the robustness of this battery model in simulation of short-pulse charge/discharge characteristic of HEV driving cycles under room and low temperatures.

INTRODUCTION

Hybrid electric vehicles (HEVs), using a battery system in conjunction with a small combustion engine, play a critical role in future automobiles due to their intrinsic advantages of increasing fuel efficiency and reducing carbon dioxide emission. The Li-ion battery is expected to find widespread application in the next generation HEVs by replacing currently used nickel-metal hydride batteries as the Li-ion battery offers 40-50% battery weight reduction and 20-30% volume reduction as well as some margin of efficiency improvement [1]. To realize it, both experimental and modeling efforts should be made to understand the fundamental mechanisms

governing the performance of Li-ion battery under HEV conditions.

As compared to experimental studies, only minor progress has been made on computer modeling of the Li-ion battery. Early attempts were made by Newman and his co-workers, who develop a general 1D model using porous electrode and concentrated solution theories [2,3]. More recent contributions were due to Wang and his co-workers to account for solid-state diffusion and thermal behaviors [4-7].

Compared to the lumped equivalent circuit (or look-up table) approach, an electrochemistry-transport model is more advantageous and offers more insight for battery design and application to HEVs. Furthermore, by adding side reactions into the model, these electrochemistry-transport-degradation models [8-14] have the potential to evaluate and predict cell aging. Therefore, in this work we aim to develop a comprehensive Li-ion battery model based on our previous work [4-7]. The performance model to be presented in this work will be used in the future for studying Li-ion battery degradation by adding specific side reactions. Besides the voltage prediction during constant current charge/discharge under room temperatures as most electrochemistry-transport models do, our model was also validated against experimental data from tests designed for HEV cells under both room and low temperatures.

BACKGROUND

A typical Li-ion cell consists of negative electrode (or anode), electrolyte, separator and positive electrode (or cathode); the two electrodes are separated by the separator and the separator and electrodes are filled with electrolyte as shown in Figure 1. The electrolyte, often a good ionic conductor but an electronic insulator, provides a transport-medium for Li-ions to travel between the two electrodes and keeps electrons in the external circuit.

The simulation carried out in this study is for an 18650 experimental cell consisting of lithium nickel-manganese-cobalt oxide ($\text{Li}(\text{Ni},\text{Mn},\text{Co})\text{O}_2$) positive electrode and graphite negative electrode. During a charge process, Li-ions de-insert from lithium nickel-manganese-cobalt oxide solid particles, and travel through the electrolyte solution to intercalate into Li_xC_6 . Electrons are forced to follow an opposite path through an external circuit. During a discharge process, Li-ions and electrons then travel in reverse. The electrode reactions are:

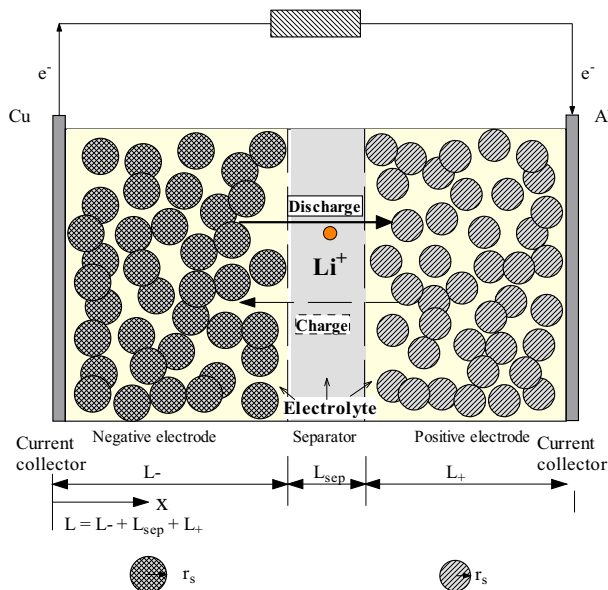


Figure 1: Schematic of 1D (x-direction) Li-ion cell model with coupled 1D (r-direction) solid-diffusion submodel.

MATHEMATICAL MODEL

1D MODEL - The basic assumptions of the proposed transient model based on computational fluid dynamics (CFD) are listed below:

1. No gas phase is present.
2. Concentrated binary electrolyte is assumed [2].
3. Charge transfer kinetics follows Butler-Volmer equation.
4. Ionic species transport in the electrolyte is by migration and diffusion only.
5. The active electrode materials are made up of spherical particles of uniform size.
6. Volume change during cell operation is neglected, resulting in constant electrode porosities.
7. The transport of lithium inside the solid active material particles is by diffusion with constant diffusion coefficient.
8. The entire cell is assumed to have temperature spatially uniform and not varying with time.

Porous electrode theory is adopted in modeling the composite electrodes consisting of active material and electrolyte solution. The solid and electrolyte phases are treated as superimposed continua with each phase having its own volume fraction, while the microstructure of each phase is not considered. Therefore, the material balances should be averaged in a volume large enough to treat electrochemical reaction as a homogeneous volumetric term but small compared to the overall dimension of the electrode. To account for tortuosity effects, electrolyte diffusion coefficient and ionic conductivity are corrected using Bruggeman relationships, $D_e^{eff} = D_e \epsilon_e^{eff}$ and $\kappa^{eff} = \kappa \epsilon_e^p$, respectively, where p is the Bruggeman exponent. And electronic conductivity is corrected as $\sigma^{eff} = \sigma \epsilon_s^p$, for each electrode. Here, ϵ_e and ϵ_s are electrolyte and solid phase volume fractions, respectively.

An electrochemical Li-ion battery model can be derived with the above assumptions. The final governing equations are summarized as follows. For more details about the general modeling approach, please refer to Ref. [2-4].

CHARGE COSERVATION EQUATIONS - From the simple Ohm's law, the current in solid phase, i_s , is related to the potential in solid phase, ϕ_s , as

$$i_s = \sigma^{eff} \frac{\partial \phi_s}{\partial x} \quad (3)$$

Through the electrode, due to the insertion and de-insertion reactions at the electrode/electrolyte interface, the current in solid phase changes as follows