Capacity fade modelling of lithium-ion battery under cyclic loading conditions

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HIGHLIGHTS

- Developed an electro-chemical battery model for ageing under cyclic loading condition.
- The capacity-power fade model considers temperature and variable porosity effects.
- This model links the battery performance with electrolyte partial molar concentration.
- Fast and robust algorithm with fully-implicit methods for high performance computing.

ARTICLE INFO

ABSTRACT

A pseudo two-dimensional (P2D) electro-chemical lithium-ion battery model is presented in this paper to study the capacity fade under cyclic charge-discharge conditions. The Newman model [1,2] has been modified to include a continuous solvent reduction reaction responsible for the capacity fade and power fade. The temperature variation inside the cell is accurately predicted using a distributed thermal model coupled with the internal chemical heat generation. The model is further improved by linking the porosity variation with the electrolyte partial molar concentration, thereby proving a stronger coupling between the battery performance and the chemical properties of electrolyte. The solid electrolyte interface (SEI) layer growth is estimated for different cut-off voltages and charging current rates. The results show that the convective heat transfer coefficient as well as the porosity variation influences the SEI layer growth and the battery life significantly. The choice of an electrolyte decides the conductivity and partial molar concentration, which is found to have a strong influence on the capacity fade of the battery. The present battery model integrates all essential electro-chemical processes inside a lithium-ion battery under a strong implicit algorithm, proving a useful tool for computationally fast battery monitoring system.

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1. Introduction

A battery management system (BMS) is an essential part of hybrid electric vehicles (HEV), plug-in electric vehicles (PEV), and also large-scale grid support systems. Also the demand for portable devices and electronic communication systems has accelerated the need for more focussed research in batteries and battery packs. The lithium-ion battery is a popular choice for battery packs due to its high energy density, relatively low self-discharge, low maintenance, and suitability for high current applications. The use of battery packs in grid support applications presents several challenges due to the rapid charge and discharge demanded by grid operation which may cause unexpected failure that can potentially lead to catastrophic damage to the batteries and bring the impact on to grid. A continuous monitoring of an individual battery is critical to the smooth grid operation and the estimation of remaining useful life (RUL) of the battery.

The success of a battery monitoring algorithm greatly depends on the accurate prediction of electro-chemical parameters, capacity fade and thermal characterisation. Capacity fade and the prediction of electro-chemical characteristics are linked to the battery operating conditions. The thermal heat generation is also highly complicated to characterise due to its dependency on multiple electro-chemical reactions. Electro-chemical modelling using partial differential equations can predict battery characteristics

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accurately, but with a high computational cost. This poses a main challenge for accurate battery modelling and emphasises the need to focus more on electro-chemistry as well as numerical schemes for an accurate and computationally fast monitoring system. This paper analyses the dependency of main factors such as temperature, depth of discharge (DoD) and the charging current rate on the SEI layer development. This study also improves the solution methods under an implicit algorithm to solve the electro-chemical effects in battery, making it as a useful tool for battery life monitoring.

There were early attempts to model the electro-chemical processes inside the battery by solving the governing equations using a pseudo two-dimensional model, known as the P2D model [1,2]. Later, Wang et al. [3] and Subramani et al. [4] approximated the concentration of solid particles of a P2D model using a second degree polynomial and improved the speed of calculation with an accuracy comparable to the P2D model. Dao et al. [5] and Bizeray et al. [6] modelled the basic electrochemistry inside the battery using mathematical simplification and reduction methods to improve the computational speed. These models enable a computationally fast solution of the problem, leading to an accurate estimation of battery parameters, which is extremely useful in battery monitoring systems. However, these mathematical methods are not accurate enough to predict the capacity fade coupled with thermal effects in a battery during multiple charge-discharge cycles.

Capacity fade modelling is very important for an accurate prediction of charge-discharge profiles in rechargeable battery RUL prediction. It has been observed that side reactions and degradation process in lithium-ion batteries may cause a number of undesirable effects, leading to capacity loss and the growth of the solid electrolyte interface (SEI) layer, which are normally salt degradation products of electrolyte and electrodes [7,8]. The loss of lithium ions contributes to the thickening of the SEI layer at the negative electrode, initially protecting the electrode against large voltage but eventually degrading the capacity. The actual process of capacity fade happens over hundreds of cycles while some batteries exhibit rapid degradation, strongly influenced by adverse operating conditions.

A detailed solvent diffusion model was proposed by Ploehn at al [8]. to evaluate the growth of the SEI layer in carbon anodes. Later, Ramadass et al. [9] developed a first principle based model to calculate the capacity fade effect by considering a continuous solvent reduction side reaction. Recently, Pinson and Bazant [10] showed that simple time dependent models were capable of predicting the capacity fade in electro-chemical batteries. The accuracy of these models depends on the numerical schemes and the calculation of heat generation inside the battery. Further improvement has been made to the battery modelling by Randall et al. [11] and by Tanim and Rahn [12].

An accurate thermal prediction is required to calculate capacity fade, since high heat generation is the main reason for accelerated capacity and power fade leading to uncontrollable side reactions. This also helps the engineers design a better battery cooling mechanism which enhances the battery life. Most of early thermal prediction studies were based on the lumped parameter approach, representing a battery as a large thermal mass without considering internal thermal conductivity [13]. Later, Wu et al. [14] extended the study of Smith and Wang [13] for a battery pack with interconnected resistance focusing on the load imbalance generated in automobile applications. In the lumped model, thermal properties are averaged, which reduces the accuracy of thermal prediction.

A distributed thermal model provides high accuracy thermal predictions at a high computational cost. One of the important attempts was made by Cai and White [15], extending the P2D model to include the thermal effect using COMSOL software. Attempts were made to improve the accuracy of distributed thermal model by extending it to multi-dimensions and length scales with the help of a reduced order model to limit the computational cost [16]. Ye et al. [17] experimentally determined accurate thermal modelling parameters and used it in simulation, and their results showed good agreement with test data.

Another notable study from our group on lithium-ion polymer battery was by Chacko and Chung [18] on thermal behaviour of cell during the combination of charge and discharge effect, using a three-dimensional fully coupled electro-chemical model. There is an experimental effort by Barai et al. [19] to characterise Li-ion batteries. Also other major contributions are by Yi et al. [20] and Kim et al. [21].

All the above studies point to the necessity of capturing three different effects such as electro-chemical reaction [13], capacity fade or power fade leading to ageing [9], and thermal effects that governs temperature distribution [15]. A strong and computationally fast battery life monitoring system also needs an accurate and fast numerical scheme or algorithm for solving the governing equations. Variable porosity also needs to be given importance above the three factors to accurately calculate the available specific area which directly affects the system of equations [22].

The present study predicts the basic electro chemistry inside the battery using a pseudo two-dimensional (P2D) model. This study also takes into account the heat generation inside the battery as well as the capacity fade and power fade due to solvent reduction reaction. A variable porosity model is introduced by linking the reactions with the partial molar volume. Hence this electrochemical model is an attempt to capture the electro-chemistry, capacity fade, and its coupled effects with temperature. The implementation of a computationally fast and robust algorithm makes this model suitable for BMS with high numerical accuracy. A finite volume based discretisation is adopted due to the inherent advantage that the boundary conditions can be applied non-invasively. An algorithm is proposed which sequentially solves the governing equations using an implicit method for time dependent discretisation, to evaluate the battery characteristics for multiple charge-discharge cycles.

2. Battery model

A Li-ion battery has typically three major components, namely, current collectors, porous electrodes and ionically conductive separator. This layout was first presented by Fuller et al. [23]. Later this modelling layout was widely adopted [9,13,15]. The negative composite electrode is made of active material of LiC_6 and the positive electrodes is made of metal oxide active material such as $LiMO_2$. The electrolyte is made of organic solvents or lithium salts such as $LiPF_6$ which promotes the ionic diffusion process. The P2D model assumes that the electrodes can be represented by the lattice of spherical particles of identical size. The surface concentration of each spherical particle is used to determine stoichiometry for calculating the open circuit potential (OCV).

During the discharge process, positive lithium ions from the negative electrode diffuse towards the positive electrode. The reverse electrochemical process occurs during the charge process, and the SEI layer consumes some of these lithium ions at the negative electrode leading to the thickening of the layer.

2.1. Governing equations

All governing equations and boundary conditions used in this study are given in this section. The basic electro-chemical battery model is based on Smith and Wang [13]. The capacity fade model