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A Summary of Analytical Model for Lithium-Ion Batteries

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Abstract: ***The high specific energy and energy density of commercial of lithium ion battery products makes them attractive for weight or volume sensitive applications. An overview of lithium-ion battery modeling researches was provided. The typical models for lithium-ion battery power management found in the literature were introduced, which included empirical model, numerical model and abstract model. Furthermore, the benchmarks of these modes were summarized. It could be seen that these models can be used in understanding battery behavior and can help system designers devise optimal battery management algorithms and operating strategy.***

Keywords: lithium-ion batteries; analytical model; empirical model; numerical model; abstract model

1. Introduction

Lithium-ion(Li-ion) batteries are a type of rechargeable battery which is comprised of cells that employ lithium intercalation compounds as the anode and cathode materials. The lithium ion moves from the anode to the cathode during discharge and from the cathode to the anode when charging.

The high specific energy and energy density of commercial of lithium ion battery products makes them attractive for weight or volume sensitive applications. Li-ion batteries allow a low self-discharge rate, long cycle life and a broad temperature range of operation [1], enable their utilization in a wide variety of applications. A wide array of sizes and shapes is now available from a variety of manufacturers. Single cells typically operate in the range of 2.5 to 4.2 V, approximately three times that of NiCd or NiMH cells, and thus require fewer cells for a battery of a given voltage. Li-ion batteries can offer high rate capability. In past decades, lithium ion batteries are one of the most popular types of battery for portable electronics with one of the best energy-to-weight ratios, no memory effect, and a slow loss of charge when not in use. Recently, lithium-ion batteries have been paid more and more attention to the popularity for electric vehicle(EV), hybrid electric vehicle(HEV), plug-in hybrid electric vehicle(PHEV) as well as aerospace applications, etc. due to their high input/output power, high energy density and large power capacity [1]. On all accounts, lithium-ion batteries are becoming the front-runner among rechargeable battery technologies. However, the massive commercialization of lithium-ion batteries for EV, HEV and PHEV applications has been hampered by high cell costs, safety concerns, limited cell life, and poor performance at low temperatures(e.g. below 0°C) [2]. Researches to overcome these limitations are being conducted on high-power lithium-ion cells where modeling is significantly important to assistant their advancement.

General analytical model for lithium ion battery power management are useful to select suitable batteries, to design products, to optimize battery management and operation when in researches in advanced EV, HEV, PHEV developments. It is valuable to incorporate actual battery state information into a power management model such as the effects of ambient temperature, self temperature fluctuation, degradation as well as the instant variation of remain capacity, etc., which are usually requires a mathematical model could captures the battery nonlinearities.

2. Overview of Lithium-Ion Battery Modeling Researches

Mathematical models are critical for lithium ion battery scientists and developers as they can help elucidate the processes within the cells, allow optimization of materials, cells, batteries, and systems, and support power management and control scheme. Mathematical models are perhaps more important for lithium battery development in EV/HEV/PHEV development than in other cases because of the relatively high complexity of EV/HEV/PHEV systems, and because of the difficulty in experimentally characterizing the inner workings of cells and batteries. The most important functions of a mathematical model may be:

- To focus experimental development efforts. Mathematical models can be used to instruct experiments and to improve interpolations and extrapolations of experimental data.
- To help understand the internal physical and chemical phenomenon inside the batteries. Since experimental characterization is usually difficult due to experimental technical limitations and difficulty in parameters independently control.
- To help system design and optimization and to evaluate the technical and economic performance of certain types of battery systems in practical applications. Models can be used to determine if one characteristic of battery is suitable in a certain application field and to evaluate overall scheme feasibility.
- To help select power management strategy and control algorithms. Due to of the complexity of battery systems, especially some types of hybrid systems, the fully dynamic models could be the basis for their control scheme development.

However, it should be noted that each of certain applications of battery models has a specific requirement in different level and different complexities. In many higher level applications, the predictive requirements are modest. For example, when only operational characteristics are focused, the relatively simple models are satisfactory and appropriate and it is possible to encapsulate the mass and energy balances and performance equations. On the other hand, if the understanding of the complex physical and chemical phenomena or optimization of cell geometries and flow patterns are needed, the models will be necessarily very sophisticated, and usually have intensive computational requirements.

To be convenient, the models in published literature commonly used in battery power management are divided into three types in this study. They are empirical model, numerical model and abstract model (with and without analytical insights). All of them will be discussed and compared in following sub sections.

3. Model Benchmarking

Typical models for lithium-ion battery power management found in the literature will be reviewed and benchmarked in this part. The models will include empirical model, numerical model and abstract model.

a. Empirical Models

Empirical models are the simplest models in the battery researches [1]. Although the empirical model is very convenient and with extremely low computational complexity, their accuracy is relatively low, and less physical insight was contained in them. The commonly used empirical models include Peukert's law model, battery efficiency model and Weibull fit model [3].

Peukert's law model presented by the German scientist W. Peukert in 1897[4], and is used to capture the non-ideal charge/discharge performance by using simple equations. The capacity, C, charged or discharged at a constant current, I , is expected as a power law relationship with lifetime t as,

$$C = I^k t$$

Where k is the Peukert constant and for an ideal battery, the constant k should be equal to 1, in this case the actual capacity would be independent of the current. The Peukert constant varies according to the age of the battery generally increasing with age. Application at low discharge rates must take into account the battery self-drain current[5]. In addition, Peukert's law could not account for dynamic varying load which is totally not appropriate for application in power management.

The battery efficiency model is beneficial to predict the ratio of actual capacity to theoretical capacity. The model could accounts for rate dependence and can handle the variable loads, and is useful to maximize the lifetime of battery systems as well as to be applied in scheduling real-time embedded systems. Some researchers used statistical methods to model the discharge behavior of lithium ion batteries**Error! Reference source not found.** for a fixed load and temperature. Then they fit a Weibull model with three coefficients to express the voltage at different state of discharge as a function of consumed capacity. It can be used in battery lifetime prediction.

b. Numerical Models

The numerical models are widely used in different fields in lithium ion battery research and development. The numerical models are commonly described by coupled partial differential equations (PDEs) to describe species and charge conservation in the solid and electrolyte phases, as well as energy conservation is also considered for the non-isothermal models. Numerical models are commonly used in evaluation of different cell and battery design and to help understand the impact of the operating conditions on battery performance and parameter distributions. By given a wide range of possible battery design considerations and operating parameters, the design could be examined and optimized. In fact, the numerical model is the most accurate and has great utility in lithium ion battery design and optimization models, and also could represent the detailed physico-chemical characteristics inside of the cells and batteries. However, they are the slowest to produce predictions and the hardest to configure, providing limited analytical insight for system designers [3]. In addition, the numerical model always needs much parameters and some of which are very difficult to be achieved by experiments or from published literature. Thus, model calibration and parameter estimation processes are usually needed.

Doyle, et al.[7,8] were the first to model the lithium ion cell using porous electrode and concentrated solution theories. Their 1D model captures relevant transport limitations and is general enough to adopt a wide range of active materials and electrolyte solutions with variable properties [9-13]. The 1D isothermal model was validated against a 525 mAh Sony cell phone battery [9]. The authors used a large Bruggeman exponent correcting for tortuosity in the negative electrode leading to the conclusion that the battery was electrolyte phase limited. They have developed the Dualfoil program(in Fortran languvage) to simulate lithium ion batteries. The program reads the load profile as a sequence of constant current steps, and the battery lifetime can be obtained from the output by reading off the time at which the cell potential drops below the cutoff voltage. Researchers have used Dualfoil to evaluate other battery models, and have extended the lithium/polymer/insertion cell model to include additional factors such as energy balance and capacity fading [13].

Fuller et. al. studied the practical consequence of these transient phenomena by modeling the effect of relaxation periods interspersed between discharge and charge cycles of various lithium ion cells. Voltage relaxation and the effect of repeated cycling were influenced very little by electrolyte concentration gradients and were primarily attributed to equalization of local state of charge across each electrode. Non uniform active material concentrations would relax via a redistribution process driven by the corresponding non-uniform open-circuit potentials across each electrode.

However, simulating a given lithium-ion battery can require much parameters based on knowledge of the structure, chemical composition, capacity, temperature, and other characteristics[3]. In addition, solving the model's interdependent partial differential equations requires using complex numerical techniques. In addition, simulating each load profile can take several hours or even days. Thus, the numerical model is hard to be applied in power management without appropriate simplifications.

c. Abstract Models

Instead of modeling discharge behavior either by describing the detailed electrochemical processes in the cell or by empirical approximation, abstract models attempt to provide an equivalent representation of a battery. Electrical-circuit and discrete-time models are particularly useful when compatible models of other system components. Although the number of parameters is not large, such models also employ lookup tables that require considerable effort to configure. In addition, despite acceptable accuracy and computational complexity, these models have limited utility for automated design space exploration because they lack analytical expressions for many variables of interest.

Gold has proposed equivalent circuits consisting of linear passive elements, voltage sources, and lookup tables to model lithium-ion batteries. In this approach, capacity fading is modeled by a capacitor whose capacitance decreases linearly with the number of cycles. The load current minus a rate-dependence offset flows through this capacitance. The voltage across the capacitance represents the ratio of delivered capacity to full charge capacity. This normalized state of charge is then converted via a lookup table. The temperature effect is modeled as a resistor capacitor circuit with two temperature-dependent sources. The main loop computes the cell voltage by superposing the effect of the state of charge, temperature, and cell internal resistance. Electrical-circuit models are inherently continuous-time and, while their simulation times are faster than those of numerical models except when the number of circuit is relatively large.

Usually, the simple equivalent circuit model comprising an electromotive force which can be formulated as a function of the state of charge, in series with internal resistance, which can be a function of SOC, temperature and cycle numbers. Such a model does not represent the dynamic behavior of the battery which is important for power management. A dynamic model of a battery normally contains a resistance-capacitance (RC) combination elements[14,15],. However, most of these models assume linearity even though the actual behavior of the battery is found to be significantly non-linear.

Some models combine a high-level representation of a battery for which experimental data determines the parameters with analytical expressions based on physical laws. For example, Daler et al. [15] developed a high-level analytical model that characterizes a battery using two constants, α and β, derived from the lifetime values for a series of constant load tests. Battery lifetime predictions using this model closely match both Dualfoil simulation results and experimental measurements. The simulation time is moderate, and the authors point out that it is possible to trade off accuracy with speed by reducing the number of terms in the summation and approximating the continuous-time load waveform $i(t)$ to an N-step staircase. However, the model does not account for the effect of temperature and capacity fading on the discharge characteristics.

Peng et al. recently proposed a high level battery model to estimate remaining capacity that considers both the temperature effect and capacity fading with successive cycles but assumes a constant current load. An expression for cell terminal voltage as a function of time are developed and, the effects of temperature are described by using the Arrhenius dependence on temperature of cell kinetics and transport phenomena, and then obtained an expression for the bulk properties of the active material as a function of the temperature. They also developed an expression for film thickness as a function of the temperature, discharge rate, and number of cycles. Using these quantities, they define state of charge as remaining capacity/full charge capacity and state of health as full charge capacity/full design capacity. The modeling results of capacity ratios agree well with Dualfoil simulation results with the same set of parameters, and the model could captures the effect of temperature and cycle aging on the battery state of charge. However, the model required more than 15 different parameters to set up the equivalent battery. In addition, the constant-load assumption limits the model's application in dynamic response simulation and optimizing with highly variable loads.

d. Remarks and summaries

It could be seen that above models can be used in understanding battery behavior and can help system designers devise optimal battery management algorithms and operating strategy. The benchmark of these modes can be summarized in Table 1.

Table 1: Model benchmarking

Model	*Accuracy*	*Dynamic response*	*Computational complexity*	*Physical insight*	*Model parameters*
Empirical	*Low*	*Difficult*	*Low*	*Less*	*Less*
Numerical	*High*	*Yes*	*High*	*High*	*Large number of model parameters. Some are very difficult to be achieved from experiments or published literature*
Abstract	*Medium, could be improved by induce physical formualtions*	*Yes*	*Relatively low, but depends on the circuit numbers and forms*	*Medium. Depends on if the elements are correlated with physical processes*	*Medium*

4. Conclusion

The high specific energy and energy density of commercial of lithium ion battery products makes them attractive for weight or volume sensitive applications. In this paper, the research developments of lithium-ion battery modeling researches were provided. The typical models for lithium-ion battery power management found in the literature were introduced, which included empirical model, numerical model and abstract model. Finally, the benchmarks of these modes were summarized. It could be seen that these models can be used in understanding battery behavior and can help system designers devise optimal battery management algorithms and operating strategy.

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Author Profile

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