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Modeling of lithium ion cells—A simple equivalent-circuit model approach

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Abstract

We present an equivalent-circuit-based battery model, capable of simulating charge and discharge behavior of lithium-ion batteries (LiB). The model, although simple in concept, can simulate complex discharge behavior with high fidelity, as validated by experimental results.

Keywords: Equivalent circuit model; Lithium-ion battery; Computer modeling and simulation

1. Introduction

Equivalent-circuit-based battery modeling is gaining popularity because this simple modeling technique can be used to successfully simulate battery performance for various chemistries, including valve-regulated lead-acid (VRLA) [1,2], nickel metal hydride (Ni-MH) [3], and LiB [4]. This approach reduces the need to understand detailed mechanisms and only requires a few parameters, which are easily obtainable from experiments, to reach high-fidelity predictions. Unlike first-principle-based modeling, this approach simplifies mathematical and numerical treatments to minimize or even avoid complicated and intensive computation requirements, so results can be quickly obtained.

Conventionally, electrochemical impedance spectroscopy (EIS) has been used to study transport and interfacial reaction kinetics in an electrochemical system. Analyses of complex impedance data rely on a framework that employs equivalent circuit diagrams to emulate the behavior of a series of elements in circuitry that represents the electrochemical system. Using the same framework, we can deploy a circuit of electrical elements in a proper configuration, based on our physical understanding of the cell configuration and chemistry, to construct an equivalent circuit model (ECM) to simulate cell performance and behavior.

An ECM may comprise three major parts: a static part representing the thermodynamic properties of the battery chemistry, such as the nominal capacity and open-circuit voltage (OCV) as a function of state-of-charge (SOC); a dynamic part that represents the kinetic aspects of the cell internal impedance behavior; and a source or load to complete the circuit for charge or discharge regimes; thus, allowing us to mimic the battery behavior and simulate its performance characteristics. As an example in Fig. 1, Yang and Liaw [5] show that, using a transmission-line ECM suggested by Barsoukov et al. [4], they were able to simulate the impedance response of an insertion electrode in a LiB cell by imposing the condition of a small voltage perturbation on the cell over a range of frequencies in MATLAB.

Our current interest is to use a more simplified model, with proper initial and boundary conditions, to simulate battery performance under dynamic charge or discharge conditions, and eventually, to predict life. The chemistry

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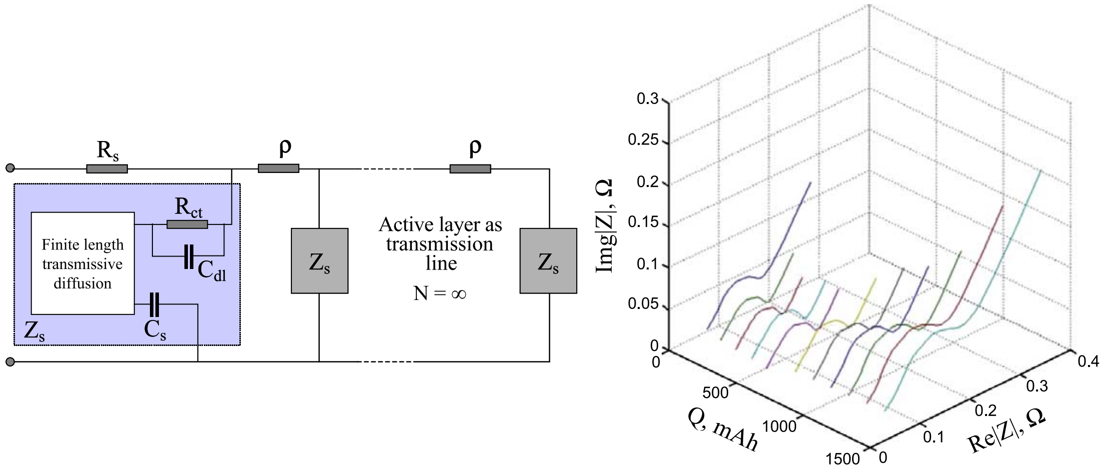

Fig. 1. (Left) A transmission-line equivalent circuit model describing the behavior of an insertion electrode in a lithium-ion battery under a small voltage perturbation, as proposed by Barsoukov et al. [4]. (Right) Simulated impedance spectra at different SOC for a Sony 18650 cell [5].

used in this work is currently under investigation by the U.S. Department of Energy (USDOE) Advanced Technology Development (ATD) program [6] for hybrid electric vehicle (HEV) applications.

2. Model description

A schematic of the model that we used for the remaining part of this paper is shown in Fig. 2, which resembles that used by Verbrugge and Conell [3] for Ni-MH cells. The unique feature we adopted in the model is the separation of (1) all Ohmic resistant components lumping into R_1, and (2) faradic non-linear components into the R_2C circuit. We favored this model over the transmission-line model shown in Fig. 1 due to its simplicity in describing behavior of an electrochemical system and the success we enjoyed in modeling a variety of chemistries. To develop this model for LiB, we first needed to incorporate the SOC-dependent OCV and resistance values (R_1 and R_2) into the model. Fig. 3 shows these SOC-dependent values of the LiB chemistry used in this work. The OCV values were obtained by discharging a fully charged cell at the C/25 rate, as reported in Ref. [7].

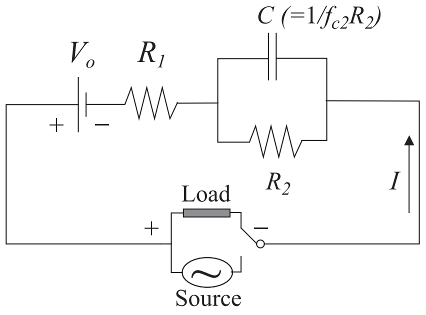

Fig. 2. The equivalent circuit model used in this work to simulate LiB performance for Gen 2 cells.

The resistance values were estimated from experimental data. A typical Nyquist plot of a cell is shown in Fig. 4, where the ac impedance spectra at 60% and 100% SOC are illustrated. R_1 was taken from the Nyquist plot, as shown in the figure, and assumed constant in the entire SOC range. This assumption is valid, since (1) we do not expect that the Ohmic resistance changes noticeably with SOC, and (2) the R_1 values at the two SOCs in the figure do coincide with each other at the real axis on the Nyquist plot. The SOC-dependent R_c (the cell total resistance R_1+R_2) values could be estimated from the difference in the voltage of the discharge curves determined at C/25 and C/1 rates, of which the experimental data are shown in Fig. 5. In the actual simulations, the R_c values were assumed to be a combination of two separate functions, R_c^o and R_c^s, as shown in Fig. 3, to adequately approximate the resistance change with SOC. The values of R_2 were obtained from subtracting R_1 from R_c. The capacitance, C, values can be calculated from the characteristic frequency, f_{c2}=1/R_2C, of the semicircle in the Nyquist plot that represents R_2C.

In this work, we will show how the cell voltage can be simulated from the ECM. Under a constant-current condition, Verbrugge and Conell [3] have derived the time-dependent cell voltage as

$$V(t) = \frac{Q(0)}{C} e^{-t/R_2C} + V_o - IR_1 - IR_2\left(1 - e^{-t/R_2C}\right), \quad (\text{where } I = \text{constant}) \qquad (1)$$

where $Q(0)$ is the nominal capacity, and V_o is the nominal SOC-dependent cell OCV. For any given time step, we estimate the charge passed, thus, deriving the SOC value at the end of the step. We use Eq. (1) to calculate the cell voltage change at various rates. Thus, a simulated voltage versus SOC (or time) discharge curve for a specific rate can be obtained. Fig. 5 shows a series of discharge curves at various rates, from C/25 to 10C, simulated from the ECM.

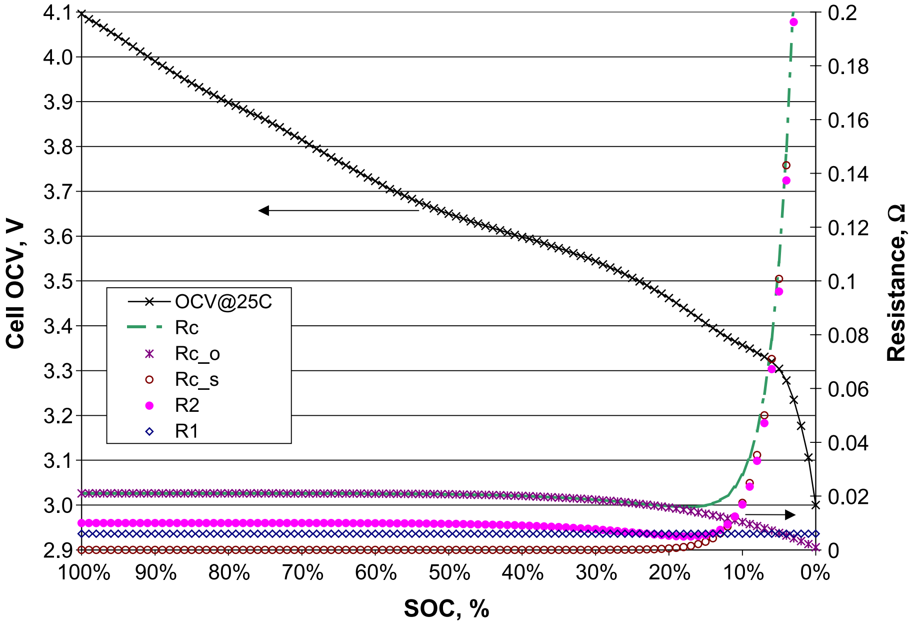

Fig. 3. The SOC-dependent OCV and resistance values for the total cell resistance (R_c and the two independent contributions R_c^o and R_c^s), R_1, and R_2 of the Gen 2 chemistry in the model.

The ability to simulate cell voltage under charge or discharge regimes is quite useful for battery research. For example, by imposing a suitable cut-off condition, we then calculate the amount of charge put in and released from the cell to yield the rate capacity, as well as charge efficiency. Furthermore, if the aging effects and degradation rates in the cell impedance are known, we can then perform simulations using various temperature and power conditions imposed on the cell to simulate the life performance. Other voltage or current versus time relationships, similar to that of Eq. (1), under different operating conditions can be derived accordingly for modeling other cell behaviors.

3. Experimental

The test cells (so called “Gen 2” cells) were received from Quallion (Sylmar, CA) as part of the USDOE ATD program efforts, and Sandia National Laboratories was commissioned to evaluate the cell performance to develop accelerated life tests. More detailed cell chemistry, configuration, test protocol; procedure, test result, and cell’s Arrhenius behavior from thermal aging can be found in Refs. [6–10] and will not be repeated here. This chemistry in a nominal 18650 cell consists of MAG-10 graphite-negative electrode, $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$-positive electrode, and 1.2 M $LiPF_6$ in ethyl carbonate/ethyl methyl carbonate (3:7

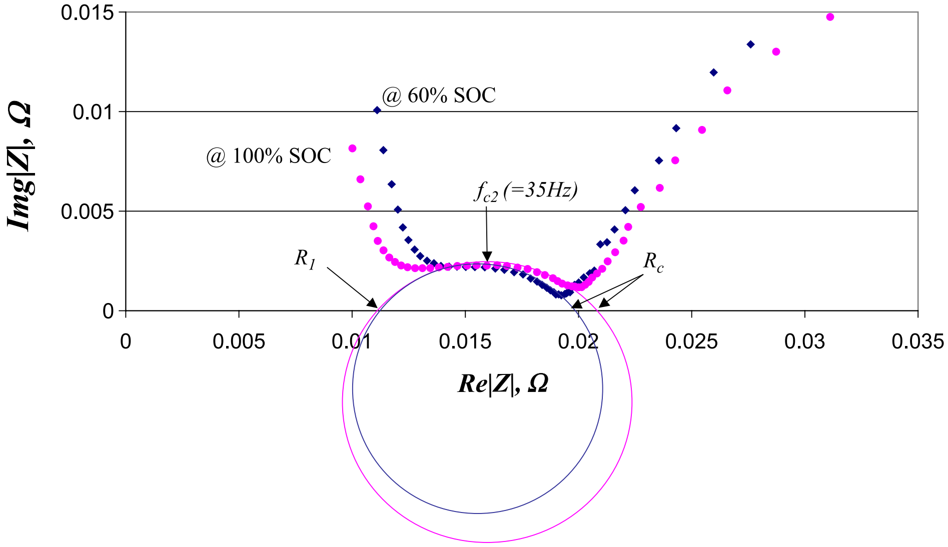

Fig. 4. A Nyquist plot showing the cell impedance change with frequency (0.01 to 10,000 Hz) and SOC in the Gen 2 cells.

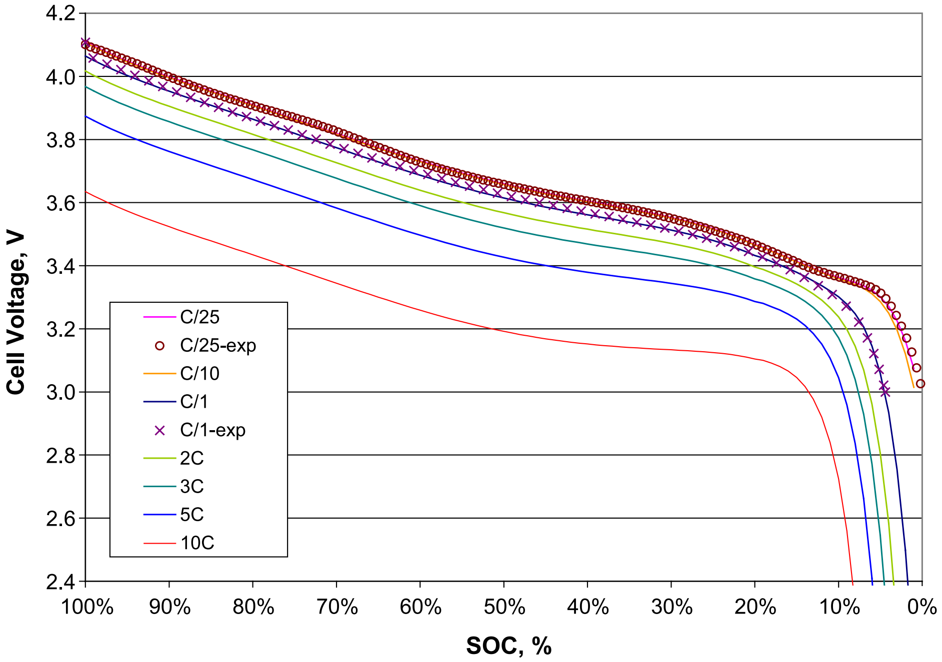

Fig. 5. Simulated discharge curves of cell voltage versus SOC at various rates and compared with experimental data collected at C/25 and C/1 rates for the Gen 2 cells.

wt.% ratio). The discharge curves at C/25 and C/1 and the complex impedance data of the Gen 2 cells generated in the tests were used in the development of the ECM and for validation.

4. Results and discussion

Barsoukov et al. [4] and Yang and Liaw [5] have previously shown that complex impedance responses of Sony 18650 cells could be simulated from a transmission-line model, as illustrated in Fig. 1. Fig. 1 illustrates a useful approach to simulate impedance response from the cell based on a transmission-line ECM. The synthesis of the Nyquist plot is significant for validation, since experimental data can be obtained from tests. The synthesis and validation with test results can assist us to enhance the understanding of the underpinning process related to aging and degradation. For example, we can hypothesize how the impedance would change with aging condition and synthesize the complex impedance response. By comparing with the test results, we can verify if such a hypothesis is correct or not. Through validation, the conformity with actual test results can then be used to simulate other cell performance characteristics. A greater conformity with other test results, such as power fade or capacity fade, can corroborate our quest for a better understanding of the degradation process to achieve a better life prediction.

Fig. 3 shows the OCV and resistance values determined from the experimental data as a function of SOC, which were used in the ECM described in Fig. 2 for the Gen 2 cells. Fig. 4 displays a typical Nyquist plot measured from one of the Gen 2 cells and the assignment of a few critical parameters such as the resistance values and the characteristic frequency used in the simulation. Fig. 5 shows a series of discharge curves of voltage versus SOC simulated at various rates for the Gen 2 cells. The simulation curves show a high degree of fidelity, as compared with experimental data collected at C/25 and C/1. In the simple ECM we used, we usually combine Ohmic-like contact resistance, including the electronic resistance of the leads, taps, and current collectors to the cell, into the serial resistance component R_1. For other non-linear, faradic behavior, including any semi-conducting path in the circuitry, and charge transfer or redox-related properties, we combine them into R_2. This simple treatment seems to work successfully so far.

In our current model, the behavior of R_c with SOC is quite intriguing, since it seems to be composed of at least two independent contributions. The contribution dominating in the higher SOC region seems to follow a power law, R_c^o=0.021–0.02(1-SOC)^6, while the other, becoming significant below 15% SOC, exhibits an exponential relationship, R_c^s=0.58[exp(−35*SOC)]. The emerging of these two contributions greatly impacts the shape of the discharge curves, thus, it is good for validation of the system. The origins of these contributions and their physical meanings are not clear at this moment. Additional efforts to investigate the impacts of these contributions to the cell performance, such as capacity and power fade, cycle and calendar life, are under way and will be reported elsewhere.

In all, the ECM approach shows simplicity, flexibility, and yet high fidelity in simulating battery performance characteristics, as illustrated in the accurate prediction of cell discharge behavior as shown in Fig. 5. With a set of carefully determined experimental data, such as OCV and resistance values as a function of SOC, we can construct an ECM with high fidelity to emulate cell performance and predict its characteristics via computer simulation.

5. Conclusion

A simple equivalent circuit model (ECM) can be used to express complicated lithium-ion battery performance via computer simulation, showing a high degree of agreement with the experimental data. Cell impedance response and discharge behavior can be simulated with this simple ECM approach. The validity of using this type of simple ECM approach exhibits great potential for battery research and development.

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