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An iterative computation method for interpreting and extending an analytical battery model*

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Abstract: Battery models are of great importance to develop portable computing systems, for whether the design of low power hardware architecture or the design of battery-aware scheduling policies. In this paper, we present a physically justified iterative computing method to illustrate the discharge, recovery and charge process of Li/Li-ion batteries. The discharge and recovery processes correspond well to an existing accurate analytical battery model: R-V-W's analytical model, and thus interpret this model algorithmically. Our method can also extend R-V-W's model easily to accommodate the charge process. The work will help the system designers to grasp the characteristics of R-V-W's battery model and also, enable to predict the battery behavior in the charge process in a uniform way as the discharge process and the recovery process. Experiments are performed to show the accuracy of the extended model by comparing the predicted charge times with those derived from the DUALFOIL simulations. Various profiles with different combinations of battery modes were tested. The experimental results show that the extended battery model preserves high accuracy in predicting the charge behavior.

Key words: Analytical battery model, Iterative computation method, Capacity response, Charge, Discharge
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INTRODUCTION

Batteries are the power providers for almost all portable computing devices. Due to finite capacity of the batteries, system lifetime has been the most important metric to judge the battery-powered computing systems. In order to design battery-optimal or energy-optimal architectures and applications with maximized battery lifetime, system designers require such design aided tools that implement a mathematical model, predict the battery behavior and thus help the designers search for the optimal schemes (Cai *et al.*, 2005; Zhuo and Chakrabarti, 2005; Zhuo *et al*., 2007).

Modeling the electrical and thermal properties of the battery is an active area of research in electrochemistry and electronic engineering. Many models are proposed, which are mainly classified into three types. One is based on the detailed electrochemical principles that can describe the internal dynamics of the batteries accurately (Doyle *et al.*, 1994; Song and Evans, 2000; Gu and Wang, 2000). These models consist of a series of complicated partial differential equations, usually proposed by chemical scientists and engineers. Subject to long simulation period and sophisticated parameters configuration, this type of models is generally not suitable for designing electronic systems. Battery models of the second type are those with high level at which batteries are represented by some abstract equivalent models, such as electrical circuits and stochastic processes (Gold, 1997; Chiasserini and Rao, 2001; Benini *et al.*, 2001).

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High-level abstract models have the advantages of considerable accuracy and only a few parameters. However, they are limited by lack of electrochemical basis and not general enough to represent the many characteristics of the battery, which lead to considerable large error. The third type of battery models seeks an intermediate approach. By capturing the major electrochemical principles, the intermediate approach achieves more accurate simulation results than the second type does (Rakhmatov *et al.*, 2003; Rong and Pedram, 2006). Besides the low computational complexity and small number of parameters, the third type of models has simple analytical expressions that can be used as the cost function to design battery-aware task scheduling policies. In (Rao *et al.*, 2003), the authors have extensively reviewed the battery models and related research fields.

The work presented here is to provide an algorithmic explanation to an existing battery model (Rakhmatov *et al.*, 2003) of the third type and extend this model to predict the charge behavior of the general lithium/lithium-ion battery. We assume that any load function of a battery can be approximated with step-wise current segments where each segment has a constant current. The current can be positive, negative or zero, indicating different modes (discharge, charge or recovery) of the battery. For each segment with current $i(t)$ and duration (t_s, t_e), there exists an internal diffusion process of the electroactive species in the battery. Based on the 1D Flick's laws and the Faraday's law, we can solve the diffusion partial equation and get the concentration distribution function of the electrochemical species and thus observe the components of the capacity "response" produced by any load segment (t_s, t_e). The initial condition of the diffusion equation at each step can be set as the ending concentration distribution function of the entire previous step. Similarly, the initial capacity of each step is set as the ending capacity of the entire previous step.

Therefore, this approach allows us to uniformly describe the battery behavior for any type of process (discharge, recovery or charge) iteratively. The discharge and recovery process correspond well to an existing accurate analytical battery model: R-V-W's battery model, and thus interprets this model algorithmically. Note that for a negative current in the BCs, the 1D diffusion equation can describe the charge process of the battery (Newman and Thomas, 2004). This method can therefore extend R-V-W's model easily to predict the behavior of charge processes, and can also be used to predict the behavior of battery with complicate process combinations. The accuracy of the extended model will be shown in the experiments.

The remainder of the paper is organized as follows. In Section 2, we introduce R-V-W's battery model, the existing analytical model that this paper aims to analyze. Then, the iterative computing approach is described in Section 3. In Section 4, we compare the results simulated by DUALFOIL with the experimental data predicted by the battery mode to verify the method. Finally, Section 5 concludes the work.

BACKGROUND

Rakhmatov *et al.*(2003) proposed their high-level battery model for predicting the lifetime and the behavior of the batteries in discharge and recovery processes. Their model attempts to describe the dynamics of the concentration at the surface of the electrode and thus gets the outer electrical characteristics of the battery.

Initially, the concentration of the electroactive species is identical anywhere in the electrolyte, which can be seen in Fig.1a. When the battery is connected to the circuit, the electrochemical reactions take place at the surface of the electrode that result in a concentration gradient across the electrolyte. Electrons flow into the external circuit and drive the computing devices. The battery is in its discharge process (Fig.1b).

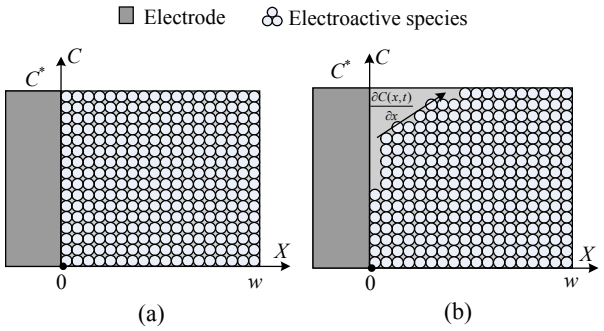


Fig.1 (a) Initial state of the battery with full capacity; (b) The battery in discharge process with a gradient of the concentration [adapted from Fig.2 in (Rao *et al.*, 2003)]

While the battery in the discharge process is disconnected from circuits, the concentration gradient will drive the electroactive species diffuse towards another equilibrium state so that the concentration is uniformly distributed again. This is the recovery process of the battery.

In contrast to the discharge process, a rechargeable battery is in the charge state while electrical energy is supplied for conversion into chemical energy. Reversed electrochemical reactions happen and the concentration of the species near the electrode rises. The charge process ends when the current through the battery declines to a steady low value (typically, the value is 2% of the capacity).

It is believed that 1D diffusion law can describe the behavior of the concentration gradient in the battery (Bard and Faulkner, 2000):

$$\frac{\partial C(x,t)}{\partial t}=D\frac{\partial^2 C(x,t)}{\partial^2 x}, \tag{1}$$

where, $C(x,t)$ is the concentration distribution function, representing the concentration of the electroactive species at distance x and time t. D is the diffusion coefficient. For simplicity, it is assumed that D is a constant, independent of the time and the distance.

Based on the Faraday's law, Rakhmatov *et al.*(2003) set the bound conditions (BCs) of the diffusion equation as follows:

$$\left.\frac{\partial C(x,t)}{\partial x}\right|_{x=0}=\frac{i(t)}{vFAD}, \tag{2}$$

$$\left.\frac{\partial C(x,t)}{\partial x}\right|_{x=w}=0, \tag{3}$$

where A denotes the area of the electrode, v is the number of reacting electrons and F is the Faraday's constant.

Suppose the discharge process begins at the initial full capacity state of the battery. The initial condition (IC) of the diffusion equation can be written as

$$C(x,0)=C^*. \tag{4}$$

With the conditions of Eqs.(2)~(4), they get the solution as

$$C(x,t)=C^*-\frac{1}{vFAw}\int_0^t i(\tau)\mathrm{d}\tau-\frac{2}{vFAw}\cdot\sum_{n=1}^{+\infty}\int_0^t i(\tau)\exp[-Dn^2\pi^2(t-\tau)/w^2]\mathrm{d}\tau. \tag{5}$$

It is assumed that when $C(0,t)$ is below the cut-off value C_{cutoff}, the battery fails and one can get the time-to-failure L. Let

$$\alpha=vFAw[C^*-C(0,L)], \tag{6}$$

$$\beta=\pi\sqrt{D}/w. \tag{7}$$

Then, Rakhmatov *et al.*(2003) get their battery model with two parameters (α, β) as follows:

$$\alpha=\int_0^L i(\tau)\mathrm{d}\tau+2\sum_{n=1}^{+\infty}\int_0^L i(\tau)\exp[-n^2\beta^2(L-\tau)]\mathrm{d}\tau, \tag{8}$$

$$l(t)=\int_0^t i(\tau)\mathrm{d}\tau, \tag{9}$$

$$u(t)=2\sum_{n=1}^{+\infty}\int_0^t i(\tau)\exp[-n^2\beta^2(L-\tau)]\mathrm{d}\tau, \tag{10}$$

$$\alpha(t)=l(t)+u(t), \tag{11}$$

where $\alpha(t)$ is the apparent lost capacity of the battery for the load profile $i(t)$, β is the parameter describing the nonlinear characteristics of the battery. Rao *et al.*(2005) gave the explanation of the two parts in the right hand side of Eq.(8). The first part, $l(t)$, is the capacity consumed by the external circuit, while the second part $u(t)$ is the "unavailable" charge during the discharge process due to the nonlinear feature of the battery itself. $u(t)$ can be recovered partially or totally if the battery is still not exhausted. Once the apparent lost capacity $\alpha(t)$ is larger than the initial capacity α, the battery will be cut off.

Suppose $i(t)$ is stepwise approximated as shown in Fig.2. For a load profile of period $(0, t_{m+1})$, the battery model (11) can be written as

$$\alpha(t_{m+1})=\sum_{k=1}^{m}I_k(t_{k+1}-t_k)+2\sum_{k=1}^{m}I_k\sum_{n=1}^{+\infty}\frac{1}{\beta^2n^2}\left\{\exp[-\beta^2n^2\cdot(t_{m+1}-t_{k+1})]-\exp[-\beta^2n^2(t_{m+1}-t_k)]\right\}. \tag{12}$$

Because the dynamic system given by Eqs.(1)~(4) considers the whole load profile $(0, t_{m+1})$, the battery model describes the total apparent capacity

"lost" during the period of (0, t_{m+1}). Both rate-capacity effect and recovery effect are well modeled (Rakhmatov *et al*., 2003; Rao *et al.*, 2005).

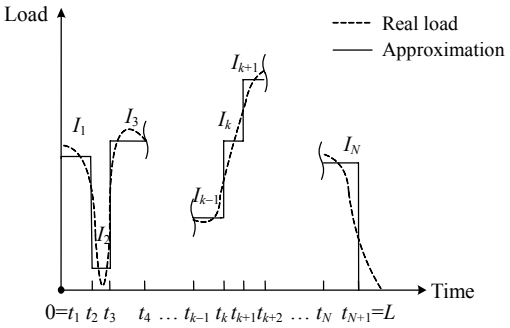


Fig.2 Stepwise approximation of current function *i*(*t*) [adapted from Fig.2 in (Rakhmatov *et al.*, 2003)]

ITERATIVE COMPUTING ILLUSTRATION AND EXTENSION FOR CHARGE BEHAVIOR

In this paper, we attempt to answer the following two questions:

Q1: Can we extend R-V-W's model to predict the behavior of the battery in the charge process accurately?

Q2: Can we grasp the capacity "response" produced by a load segment with any starting-time, any length and any type (charge, recovery or discharge)?

To answer the two questions, we solve the 1D diffusion equation with the boundary conditions of three types respectively.

For a load segment with current function $i(t)$ and duration (t_s, t_e), there exists an internal diffusion process of the electroactive species in the battery. Consequently, solving the diffusion equation with the corresponding BCs and ICs, we can observe the components of the capacity "response" produced by any load segment (t_s, t_e). Besides, with a negative current in the BCs, the 1D diffusion equation can describe the charge process of the battery (Newman and Thomas, 2004). It is practical to extend the battery model to predict the behavior of charge processes.

Based on the same electrochemical principles as that R-V-W's model refers to, our work provides some straightforward mathematical explanation for the iterative computing process of the model described by Eq.(12) and extends it to predict the charge process. In accordance with the three modes of the battery, the bound conditions (BCs) of the diffusion Eq.(1) can be set as:

Discharge: Eqs.(2) and (3);

Recovery: $\left.\dfrac{\partial C(x,t)}{\partial x}\right|_{x=0 \text{ or } w}=0;$

Charge: $\left.\dfrac{\partial C(x,t)}{\partial x}\right|_{x=0}=-\dfrac{i(t)}{vFAD},\ \left.\dfrac{\partial C(x,t)}{\partial x}\right|_{x=w}=0.$

And the initial conditions (ICs) for the partial differential Eq.(1) are the concentration distribution function at the initial instant of the current diffusion process. For example, as the process of duration (t_k,t_{k+1}), the initial condition can be written as

$$f(x)=C(x,\ t_k).$$

Solution of the diffusion process

The solution for Eq.(1) with the BCs of the discharge mode is described by the following equation. The details of how we derive this equation are omitted here due to the limited space. The technique can be found in (Polyanin, 2002):

$$C(x,t)=\frac{1}{w}\int_0^w f(\xi)\mathrm{d}\xi-\frac{1}{vFAw}\int_0^t i(\tau)\mathrm{d}\tau+\frac{2}{w}\sum_{n=1}^{+\infty}\int_0^w f(\xi)\cos\left(\frac{n\pi\xi}{w}\right)\mathrm{d}\xi\cos\left(\frac{n\pi x}{w}\right)\exp\left(-\frac{Dn^2\pi^2t}{w^2}\right)-\frac{2}{vFAw}\sum_{n=1}^{+\infty}\cos\left(\frac{n\pi x}{w}\right)\int_0^t i(\tau)\exp\left[\frac{-Dn^2\pi^2(t-\tau)}{w^2}\right]\mathrm{d}\tau. \tag{13}$$

As we can see, the concentration distribution function is the sum of the "response" of two input components: the initial concentration distribution function $f(x)$ and the current $i(t)$. The former depicts the result of the history load, while the latter represents the effect brought by the current diffusion process. Note that each response component has two parts where one part is related to the external circuit load and the other corresponds to the nonlinear feature of the battery.

Eq.(13) can be used to describe any mode of the battery process. We only need to associate a sign with the current. For discharge mode, the current is positive (the current is drawn from the battery). For the

charge mode, the current is negative (the current flows into the battery). And for the recovery mode, the solution can also be reduced as Eq.(14) by substituting $i(t)$ with zero in Eq.(13):

$$C(x,t)=\frac{1}{w}\int_0^w f(\xi)\mathrm{d}\xi+\sum_{n=1}^{+\infty}\left[\frac{2}{w}\int_0^w f(\xi)\cos\left(\frac{n\pi\xi}{w}\right)\mathrm{d}\xi\cdot\exp\left(\frac{-Dn^2\pi^2t}{w^2}\right)\cos\left(\frac{n\pi x}{w}\right)\right]. \tag{14}$$

Next, we will show how to compute $C(x,t)$ iteratively based on Eq.(13). Accordingly, the capacity function can be computed in a similar way. For any battery load function, we first approximate it as a step-wise load function, which has a number of segments where segment k has duration (t_k, t_{k+1}) and a constant current load I_k. I_k being positive, negative or zero correspond to discharge, charge or recovery process of the battery, respectively.

First two steps of the iteration

We discuss the first two steps of the iterative computation for a given load profile.

For the first segment (t_1=0, t_2) of discharge current load I_1, we can solve the diffusion Eq.(1) with its BCs [Eqs.(2) and (3)] and ICs [$f(x)=C^*$] [or we can get the solution directly by substituting the duration (t_1, t_2), load current I_1, and the initial condition $f(x)=C^*$ into Eq.(13)]. For the first segment of an initial full-capacity battery, only the discharge process is interested since a full-capacity battery does not need to be recovered or charged. The discharge process changes the equilibrium state of internal concentration distribution. The solution can be written as

$$C(x,t)=C^*-\frac{1}{vFAw}\int_0^t i(\tau)\mathrm{d}\tau-\frac{2}{vFAw}\cdot\sum_{n=1}^{+\infty}\cos\left(\frac{n\pi x}{w}\right)\int_0^t i(\tau)\exp\left[\frac{-Dn^2\pi^2(t-\tau)}{w^2}\right]\mathrm{d}\tau. \tag{15}$$

Let x=0 in Eq.(15), then we can get the same form as Eq.(5), the model of (Rakhmatov *et al*., 2003).

For the next segment (t_2, t_3), the IC of the diffusion equation should be set as the concentration distribution function of the end instant t_2:

$$f(x)=C(x,t)|_{t=t_2}=C^*-\frac{I_1(t_2-t_1)}{vFAw}-\frac{2I_1}{vFAw}\cdot\sum_{n=1}^{+\infty}\cos\left(\frac{n\pi x}{w}\right)\frac{w^2}{Dn^2\pi^2}\left[1-\exp\left(\frac{Dn^2\pi^2(t_2-t_1)}{w^2}\right)\right]. \tag{16}$$

Note that the initial condition for the second segment consists of two components: the constant $C^*-I_1(t_2-t_1)/(vFAw)$ and a Fourier cosine series.

The concentration function $C(x,t)$ for the second segment can then be written as Eq.(17) if the segment is at discharge mode:

$$C(x,t)=C^*-\frac{I_1t_2}{vFAw}-\frac{2I_1}{vFAw}\sum_{n=1}^{+\infty}\left\{\cos\left(\frac{n\pi x}{w}\right)\frac{w^2}{Dn^2\pi^2}\cdot\left[1-\exp\left(-\frac{Dn^2\pi^2t_2}{w^2}\right)\right]\exp\left(-\frac{Dn^2\pi^2t}{w^2}\right)\right\}-\frac{I_2(t-t_2)}{vFAw}-\frac{2I_2}{vFAw}\sum_{n=1}^{+\infty}\cos\left(\frac{n\pi x}{w}\right)\frac{w^2}{Dn^2\pi^2}\left[1-\exp\left(-\frac{Dn^2\pi^2(t-t_2)}{w^2}\right)\right]. \tag{17}$$

If the battery is being charged, the signs of the current in the last two items of Eq.(17) should be changed according to its BCs. That is

$$C(x,t)=C^*-\frac{I_1t_2}{vFAw}-\frac{2I_1}{vFAw}\sum_{n=1}^{+\infty}\left\{\cos\left(\frac{n\pi x}{w}\right)\frac{w^2}{Dn^2\pi^2}\cdot\left[1-\exp\left(-\frac{Dn^2\pi^2t_2}{w^2}\right)\right]\exp\left(-\frac{Dn^2\pi^2t}{w^2}\right)\right\}+\frac{I_2(t-t_2)}{vFAw}+\frac{2I_2}{vFAw}\sum_{n=1}^{+\infty}\cos\left(\frac{n\pi x}{w}\right)\frac{w^2}{Dn^2\pi^2}\left[1-\exp\left(-\frac{Dn^2\pi^2(t-t_2)}{w^2}\right)\right]. \tag{18}$$

Else, if the battery is in the recovery mode, the concentration function can be deduced as

$$C(x,t)=C^*-\frac{I_1(t_2-t_1)}{vFAw}-\frac{2I_1}{vFAw}\sum_{n=1}^{+\infty}\left\{\cos\left(\frac{n\pi x}{w}\right)\cdot\frac{w^2}{Dn^2\pi^2}\left[1-\exp\left(-\frac{Dn^2\pi^2t_2}{w^2}\right)\right]\exp\left(-\frac{Dn^2\pi^2t}{w^2}\right)\right\}. \tag{19}$$

Iterative form of the battery model

It is known that there is an orthogonal condition for the cosines which can be written as

$$\int_0^w \cos\left(\frac{n\pi x}{w}\right)\cos\left(\frac{m\pi x}{w}\right)\mathrm{d}x=\begin{cases}0, & m\neq n,\\ w/2, & m=n\neq 0,\\ w, & m=n=0.\end{cases}$$

This condition preserves the form of constant component and the Fourier cosine series in the iterative computation steps to derive the concentration function. We can get the iterative form of the function describing the concentration distribution dynamically as

$$C(x,t)\,|_{t_{m+1}\le t\le t_{m+2}}=C^*-\frac{1}{vFAw}\sum_{k=1}^{m}I_k(t_{k+1}-t_k)-\frac{2}{vFAw}\sum_{k=1}^{m}I_k\sum_{n=1}^{+\infty}\cos\left(\frac{n\pi x}{w}\right)\frac{1}{\beta^2n^2}\left\{1-\exp[-\beta^2n^2\cdot(t_{k+1}-t_k)]\right\}\exp\left[-\beta^2n^2(t-t_{k+1})\right]-\frac{I_{m+1}(t-t_{m+1})}{vFAw}-\frac{2I_{m+1}}{vFAw}\sum_{n=1}^{+\infty}\cos\left(\frac{n\pi x}{w}\right)\frac{1}{\beta^2n^2}\left\{1-\exp[-\beta^2n^2(t-t_m)]\right\}. \tag{20a}$$

Substitute the parameters α, β defined by Eqs.(6) and (7) into Eq.(20a), the iterative computing equation of the battery model is derived as

$$\alpha(t)\,|_{t_{m+1}\le t\le t_{m+2}}=\sum_{k=1}^{m}I_k(t_{k+1}-t_k)+2\sum_{k=1}^{m}I_k\sum_{n=1}^{+\infty}\left\{\left(\beta^2n^2\right)^{-1}\cdot\left\{1-\exp\left[-\beta^2n^2(t_{k+1}-t_k)\right]\right\}\exp\left[-\beta^2n^2(t-t_{k+1})\right]\right\}+I_{m+1}(t-t_{m+1})+2I_{m+1}\sum_{n=1}^{+\infty}\frac{1}{\beta^2n^2}\left\{1-\exp\left[-\beta^2n^2(t-t_{m+1})\right]\right\}. \tag{20b}$$

It can be observed from Eq.(20a) that the evaluation of the concentration function $C(x,t)$ for any t within (t_k, t_{k+1}) is composed of three parts:

(1) The constant C^* and the electrochemical species consumed by the external circuit in the m segments of constant current loads. In each iterative computation, this part is only changed by the new species concentration, "lost" or "input", of the current segment by $I_{m+1}\cdot(t-t_{m+1})$.

(2) The sum of the cosine series corresponding to the past (or history) segments. The only difference from the same part of the IC [e.g., one can observe that the instance of the IC from Eq.(16) lies in that from Eq.(20), the series has a factor of $\exp[-\beta^2n^2(t-t_{k+1})]$ on the amplitude. Intuitively, it can be illustrated as the decay factor of the "unavailable" concentration locked in the capacity by the corresponding past segments.

(3) The current segment with the load I_{m+1}. The signs of I_{m+1} are determined by the modes of the battery behavior: positive (discharge) or negative (charge).

For the load current profile, which is approximated by step-wise constant loads, the apparent capacity lost $\alpha(t)$ can be calculated in the same way as the concentration function $C(x,t)$. The orthogonal condition of the cosines makes the iterative computing process very simple. $\alpha(t)$ also has the features of the concentration function $C(x,t)$.

To write Eq.(20b) compactly, we can get the battery model with the condition $t=t_{m+1}$:

$$\alpha(t)\,|_{t=t_{m+1}}=\sum_{k=1}^{m}I_k(t_{k+1}-t_k)+2\sum_{k=1}^{m}I_k\sum_{n=1}^{+\infty}\left\{\left(\beta^2n^2\right)^{-1}\cdot\left\{\exp\left[-\beta^2n^2(t-t_{k+1})\right]-\exp\left[-\beta^2n^2(t-t_k)\right]\right\}\right\}.$$

The model has the same form as Eq.(12).

Properties with respect to iterative processes

The extending of the lifetime with the segment (t_m, t_{m+1}) will lead to the attenuating of the past "unavailable" capacity with the factor of $\exp[-\beta^2n^2(t_{m+1}-t_{k+1})]$, regardless of the battery mode of the current segment. The attenuation of the "unavailable" part brings different effect on the apparent capacity due to the sign of the current I_k ($k\le m$). For the segment of discharge load, it means that the "unavailable" charge locked in the battery is "released" or recovered, and the capacity "available" to the external circuit is increased by the same quantity accordingly. While in the case of the charge segment, the attenuation of the "unavailable" capacity cannot make any difference to the charge that can be drained by the external circuit. This phenomenon only changes the apparent capacity residual.

From Eq.(20b), we can observe that the apparent capacity, "lost" (discharge) or "input" (charge), for the current segment $[I_{m+1}, (t_{m+1}, t)]$ has the stable form as the third part of Eq.(20b):

$$\underbrace{I_{m+1}(t-t_{m+1})}_{\Delta l_{m+1}(t)}+\underbrace{2I_{m+1}\sum_{n=1}^{+\infty}\frac{1}{\beta^2n^2}\left\{1-\exp\left[-\beta^2n^2(t-t_{m+1})\right]\right\}}_{\Delta u_{m+1}(t)}.$$

1. *u*-*v* factor

Let us introduce a *u*-*v* factor $r_{m+1}(t)$ as the ratio of the capacity "unavailable", $\Delta u_{m+1}(t)$, vs. the actual capacity "lost" or "input" by external circuits, $\Delta l_{m+1}(t)$ for the load segment $[I_{m+1}, (t_{m+1}, t)]$.

$$\begin{aligned}r_{m+1}(t)&=\Delta u_{m+1}(t)/\Delta l_{m+1}(t)\\&=\frac{2I_{m+1}\sum_{n=1}^{+\infty}\frac{1}{\beta^2n^2}\left\{1-\exp\left[-\beta^2n^2(t-t_{m+1})\right]\right\}}{I_{m+1}(t-t_{m+1})}\\&=\frac{2}{t-t_{m+1}}\sum_{n=1}^{+\infty}\frac{1}{\beta^2n^2}\left\{1-\exp\left[-\beta^2n^2(t-t_{m+1})\right]\right\}.\end{aligned}$$

Note that the factor $r_{m+1}(t)$ is a function that has only one independent variable, the time t, with no respect to the current I_{m+1}. And the derivation of $r_{m+1}(t)$ with respect to t is always non-positive. That is, the factor is monotonically decreasing in t. Given a constant apparent α_{m+1} for the segment (t_{m+1}, t), the segment of the maximal $\Delta t=t-t_{m+1}$ achieves the largest actual capacity, $\Delta l_{m+1}(t)$, whether it is the discharge load or the charge process. For example, if the current iterative step is to charge a battery to the full-charged state from its cut-off state, the smaller charge current will "input" larger actual charge into the battery. Or, the less discharge current can drain more charge from a full-charged battery.

2. Critical instant

There also exists a critical instant $t_{cr}(\alpha_{m+1}, I_{m+1}, \hat{I}_{m+1})$ in the case of a constant apparent capacity α_{m+1} for the segment (t_{m+1}, t). Before the instant t_{cr}, the profile of larger charge current I_{m+1} holds the greater part of the actual capacity in the quantity of the constant α_{m+1}. Otherwise, the profile of the smaller current $\hat{I}_{m+1}$ occupies the actual capacity more. t_{cr} can be calculated as

$$t_{cr}(\alpha_{m+1}, I_{m+1}, \hat{I}_{m+1})=\frac{I_{m+1}}{\hat{I}_{m+1}}\cdot\Delta(\alpha_{m+1})+t_{m+1},$$

where $\Delta(\alpha_{m+1})$ is the cut-off time (either discharge or charge) with the current I_{m+1}. For a process charging the battery to a constant apparent capacity, if the duration of the process is longer than $t_{cr}-t_{m+1}$, we should choose the smaller charging current $\hat{I}_{m+1}$ for the higher actual capacity injected. Otherwise, I_{m+1} is the better choice as the charge current.

SIMULATION RESULTS

Firstly, we describe the case of full charge profiles. The battery is discharged to the cut-off state with a load of 222.7 mA and then the charge process begins. We simulate the charge profiles by the low-level battery model DUALFOIL (http://www.cchem.berkeley.edu/~jsngrp/fortran.html) for comparison. The battery is the same as that in (Rakhmatov *et al.*, 2003), which has the pair of the parameters α=40375 and β=0.273. The 59 parameters for DUALFOIL to simulate this battery can be referred basically to (Rakhmatov *et al.*, 2003). We have contacted the authors of DUALFOIL and modified the module of Version 3.0 to simulate the charge behavior of the battery.

When the voltage reaches 4.25 V for DUALFOIL or the capacity of the battery model arrives at 40375 mA·min, the charge process is terminated. Fig.3 illustrates the full charge curve with the charge current of 50 mA. The experiment data of the charge process are tabulated in Table 1, obtained from both the simulation module DUALFOIL and the battery model. The set of results is also shown in Fig.4. For all the charge currents, the predicted results fit the simulated data considerably well. The average prediction error is 5.03%. It is shown that the battery model preserves high accuracy in predicting the charge behavior.

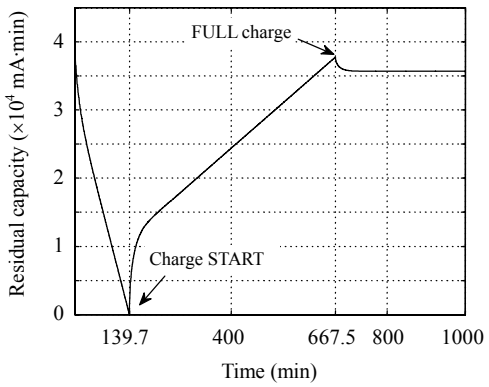


Fig.3 Predicted residual capacity of the battery in the case of FULL charged with current of 50 mA

Table 1 Fully charged time of simulation (DUALFOIL) and prediction (battery model)

Current (mA)	Time (min)		Error (%)
	Simulation	Prediction	
50	578.300	581.1	−0.48
100	270.833	269.8	0.38
150	160.267	166.0	−3.58
200	107.367	114.1	−6.27
230	87.183	93.9	−7.70
246.7	78.150	84.8	−8.51
350	52.417	48.6	7.28
400	41.083	38.6	6.04

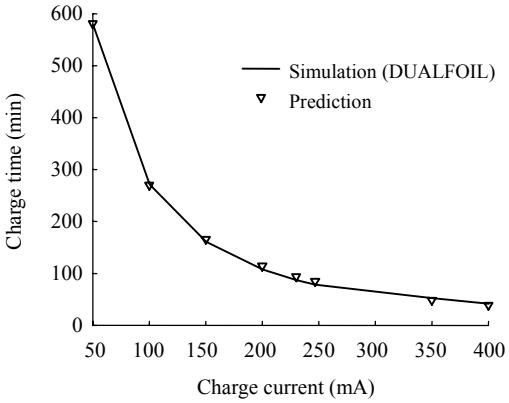


Fig.4 Simulation and predicted fully charged time

Fig.5 also shows the property discussed in subsection "Properties with respect to iterative processes". The battery is discharged to the cut-off state by 628.0 mA, and then fully charged with the currents of 50 mA and 150 mA, respectively. The charge process of 50 mA provides the battery with more actual capacity after the critical instant 236.8 min, shown by the dotted lines. And we can also find that the preceding discharge segment of 628.0 mA has a part of the capacity "unavailable" or "locked", marked as "u(26.5):628.0", where 26.5 min is the cut-off instant for the full-discharge process with the current of 628.0 mA. This part of charge is all recovered and conversed into the available charge. So, after t=450 min, the residual capacity is the sum of the actual capacity from the current charge segment and u(26.5):628.0.

We also conduct experiments on a series of complicate profiles. All the profiles are listed in Table 2. The profiles initiated with P have two types of battery modes: discharge and charge, while those profiles initiated with C have all the three modes:

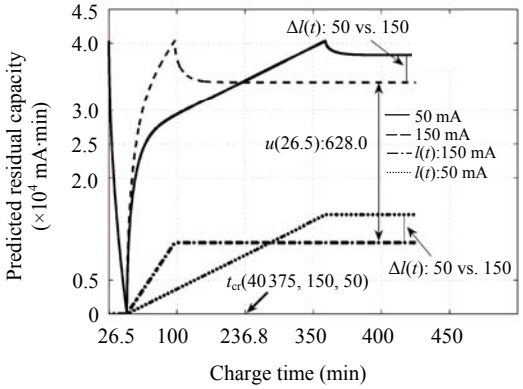
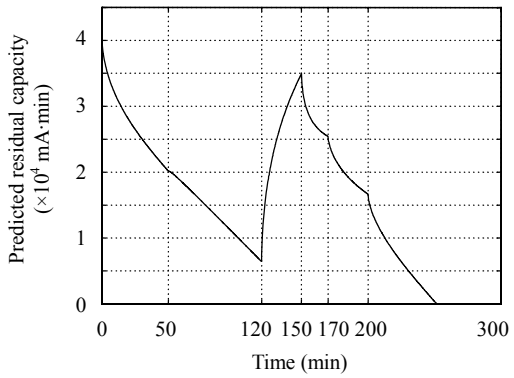


Fig.5 Curves of the charge processes with critical instant t_{cr}(40375, 150, 50). The actual capacity gap between charge processes 50 mA and 150 mA is denoted

Table 2 The set of complicated profiles

Profile	Current set I_k (mA)	Duration set, $t_{k+1}-t_k$ (min)
P1	(628.0, −100, 628.0)	(15, 30, 60)
P2	(494.7, −100, 494.7)	(25, 25, 100)
P3	(628.0, −200, 494.7)	(20, 30, 100)
P4	(222.7, 494.7, −200, 628.0)	(20, 20, 30, 100)
P5	(628.0, −200, 494.7, 222.7)	(20, 30, 20, 100)
P6	(628.0, −200, −100, 494.7)	(20, 15, 15, 100)
P7	(628.0, −200, 222.7, −50, 494.7)	(20, 20, 20, 20, 100)
P8	(222.7, −50, −200, −50, 494.7, −150, 628.0)	(50, 20, 10, 20, 15, 15, 100)
C1	(300, −220, 200, 0, −230)	(50, 50, 20, 40, 40)
C2	(250, −200, 0, 227)	(50, 20, 20, 300)
C3	(628, −200, 0, 628)	(15, 20, 20, 100)
C4	(494.7, −220, 0, 494.7)	(20, 15, 20, 200)
C5	(222.7, −200, 0, 222.7)	(50, 20, 20, 400)
C6	(222.7, 0, −200, 494.7)	(50, 20, 10, 300)
C7	(222.7, 204.5, −300, 0, 108.3, 222.7)	(50, 70, 30, 20, 30, 500)

discharge, recovery and charge. Each profile has the current set and its corresponding duration set labelling the duration. For example, the current set of C7 is (222.7, 204.5, −300, 0, 108.3, 222.7) and the starting time of the segment with the load of 222.7 mA from t=0 to 50 min. Then the battery is discharged at 204.5 mA for a period of 70 min till the instant t=120 min. The residual capacity predicted for the profile C7 and P8 are illustrated in Figs.6a and 6b, respectively. The 15 experimental results (cut-off time) of the profiles are shown in Table 3 and Fig.7. For the complicated profiles, the average prediction error is 2.1657%, and the maximum error does not exceed 6%.



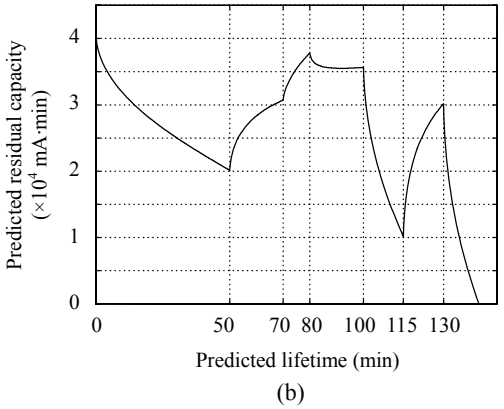


Fig.6 Residual capacity predicted for C7 (a) and P8 (b)

Table 3 Results of simulation and prediction with complicated profiles

Profile	Time (min)		Error (%)
	Simulation (DUALFOIL)	Prediction	
P1	64.300	65.3	1.53
P2	74.500	76.7	2.87
P3	80.200	82.7	3.02
P4	87.900	89.8	2.12
P5	135.700	135.5	0.15
P6	77.500	79.8	2.88
P7	101.200	104.2	2.88
P8	143.200	145.3	1.45
C1	168.750	159.7	5.36
C2	190.030	188.8	0.65
C3	76.650	75.1	2.02
C4	87.110	84.6	2.88
C5	198.583	197.6	0.50
C6	109.010	106.0	2.76
C7	254.020	251.5	0.99

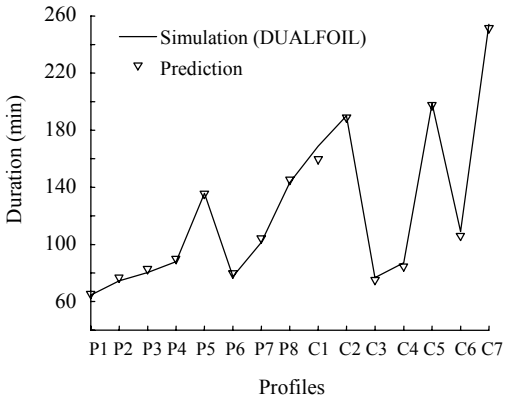


Fig.7 Cut-off time of 15 profiles: simulation vs. prediction

CONCLUSION

In this paper, we propose an iterative computing interpretation for a high-level battery model. By solving the 1D diffusion equation with the iterative initial conditions and the boundary conditions of three types (discharge, recovery and charge), we derive the iterative form of the battery model and thus extend it to predict the charge behavior. The predicted results fit the simulation data closely. It is demonstrated that the model can be used to evaluate the software and hardware schemes on complicate profiles, which may be composed of three types of battery working modes: discharge, recovery and charge. Experimental results show that the extended model preserves high accuracy in predicting the charge behavior.

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