# **State-of-Charge Estimation of Lithium-ion Battery Based on a Novel Reduced Order Electrochemical Model**

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On the basis of traditional single-particle model, an extended single-particle (ESP) electrochemical model that considers the influence of electrolyte phase potential on terminal voltage in the light of electrochemical characteristics of lithium ion battery is designed. The linear decreasing weight particle swarm algorithm is adopted to identify the key parameters of the ESP electrochemical model to reduce the effect of parameter identification error on the accuracy of state-of-charge (SOC) estimation. And an ESP-model-based extended Kalman filter (EKF) algorithm which can compensate the error caused by the simplified solution and random noise by feedback control is also proposed. The simulation results demonstrate that EKF algorithm reduce calculation errors, parameter measurement noises and increase accuracy of SOC estimation for lithium ion battery. Finally, the Charge/discharge test using 2300mAh LiFePO<sub>4</sub> battery is carried out at 3C FUDS and comparison of experimental and simulated results show that ESP-model-based EKF algorithm using for SOC estimation has good accuracy and robustness.

**Keywords:** Lithium-ion Battery; SOC Estimation Algorithm; Extended single-particle model; Model Errors

# **1. INTRODUCTION**

Nowadays, it is no exaggeration to say that power batteries have been the heart of new energy vehicles (NEVs), and play a significant role in the developing of new energy automobile industry. Lithium-ion battery has been widely used in NEVs due to its large specific capacity, high energy density, pollution-free and long driving mileage. In this respect, battery management system (BMS) is an essential module, which results in reliable power management, optimal power performance and safe vehicle that lead back for power optimization in NEVs. Considering the complex dynamic driving

conditions of NEVs, accurate SOC estimation of the battery can greatly prolong its service life, improve its efficiency and ensure its safety and reliability [1].

During the previous reported SOC estimation methods, the ampere hour integral method is dependent on the precise initial value of the integration, which may generate a great cumulative error due to sampling error and noise interference [2]. Another way for SOC estimation is the open circuit voltage method, which should be stationary for a long time in the open circuit voltage method. Thus, it is not suitable for real-time estimation of the battery. In recent years, the battery-model-based estimation method is attractive, which needs to establish a model which can accurately reflect the battery characteristics and indirectly estimate SOC by measuring the observable parameters, such as current, voltage and temperature [3]. In this respect, most of the researches focused on the equivalent circuit model and electrochemical model. The equivalent circuit model simulates the dynamic characteristics of a battery by means of circuit elements. The physical meaning of model could be easily understood and its calculation could be easily achieved. At present, there are many SOC estimation methods based on equivalent circuit model, including extended Kalman filter [4, 5], unscented Kalman filter [6] and other filtering algorithms, sliding mode observer [7], adaptive observer [8] and other non-linear observer. However, the equivalent circuit model cannot reflect the internal mechanism of the battery reaction, and the transient precision of the model is low. Using multiple linear regression method to identify the parameters of RC equivalent circuit model online can improve the accuracy of the model, but greatly increase the calculation amount of the estimation method.

The electrochemical model, based on the electrochemical principle, which reflects the microscopic mechanism of the battery and has higher precision, is of great significance to the research and the improvement of SOC estimation methods [9]. M. Doyle and T. Fuller, based on the concentration liquid theory and the porous electrode theory, established a pseudo-two-dimensional (P2D) model of a battery for the first time [10-12]. Although the model can accurately simulate the inside reaction of the battery, the amount of calculation was too many to achieve, especially for the online estimation in vehicle BMS. Therefore, a lot of work have been done for simplifying and reducing the P2D model.

Santhanagopalan [13] established a single particle (SP) model, in which both positive and negative electrodes were approximated by two spherical particles, and the concentration of Li<sup>+</sup> in the liquid phase was neglected. This model greatly improved the operation speed, and had good accuracy at small current rate. Subramanian [14] used volume averaging method and parabolic approximation to simplify the solid phase diffusion equation for solving the average and surface Li<sup>+</sup> concentration of solid phase. This method greatly reduces the computational complexity and maximum error was less than 5%. Compared with equivalent circuit model, electrochemical model is more complex. It is still a technically difficult to guarantee the accuracy, the effectiveness and stability of the SOC estimation algorithm.

In this paper, an extended single particle model (ESP) was established for improving the accuracy of the traditional single particle model. In the model, the influence of electrolyte phase potential on the battery terminal voltage was considered, and Parabolic approximation method and Padé approximation were used to simplify the  $Li^+$  solid phase and electrolyte phase diffusion equation.

Also, the key parameters were identified by linear decreasing weight particle swarm optimization, and the extended Kalman filter algorithm was used to modify the terminal voltage of the model for further improving the estimation accuracy of SOC. Finally, the effectiveness of the proposed algorithm was verified by simulation and experimental results.

#### 2. MODEL DEVELOPMENT

#### 2.1. Model simplification

Based on the P2D model theory, we assume that the  $Li^+$  solid phase diffusion process occurs in a typical spherical particle, neglecting the distribution of the solid phase  $Li^+$  concentration along the electrode direction. The internal reaction mechanism of the discharge process is shown in Figure 1. During the discharge process, it will produce a concentration difference, leading to the diffusion of the  $Li^+$  in the negative solid phase material from inside to outside, and then passes through the separator, following by insertion from the surface of the positive solid particles into the interior of the particles [15].



Figure 1. The internal reaction mechanism of the discharge process

Based on the above assumptions, instead of the local current volume density  $i_j(x)$ , the average current volume density  $\overline{i_j}$  is used throughout the cell, as shown in Eq. (1).

$$i_{j}(x) = \overline{i_{j}} = \frac{I}{Al_{j}}$$
(1)

Where, *I* is battery input current; *A*, electrode plate area;  $l_j$ , electrode thickness; in j = n, *sep*, *p*, *n*, *sep* and *p* represents negative electrode, separator and positive electrode of the lithium-ion battery respectively.

In comparison with the original SP model, the ESP model not only considers the influence of polarization over potential and open circuit voltage on model terminal voltage, but also the electrolyte

phase potential and Ohmic potential. Thus, the terminal voltage of the ESP electrochemical model can be expressed as the sum of the above potentials, as shown in Eq. (2) [11].

$$V_{t} = U_{p}(\theta_{s,p}(L)) - U_{n}(\theta_{s,n}(0)) + \phi_{e,p} - \phi_{e,n} + \eta_{p}(L) - \eta(0) + R_{f}I$$
(2)

Where,  $C_{s,j,surf}$  is surface concentration in the electrode particle;  $c_{s,j,max}$ , maximum solid phase concentration;  $U_p(\theta_{s,p}(L)) - U_n(\theta_{s,n}(0))$ , positive and negative open circuit voltage difference;  $\phi_{e,p} - \phi_{e,n}$ , electrolyte phase potential difference;  $\eta_p(L) - \eta(0)$ , polarization over potential;  $R_f I$ , Ohmic potential;  $\theta_{s,j}$ , particle surface electrode utilization, which can be obtained by Eq. (3).

$$\theta_{s,j} = \frac{c_{s,j,surf}}{c_{s,j,\max}} \tag{3}$$

#### 2.1.1. Solution of open circuit voltage

The most important thing to solve the positive and negative open circuit voltage is the solution of the solid diffusion equation. In the solid phase spherical active material, the distribution of  $Li^+$  concentration in spherical coordinates can be expressed by Fick's second law.

$$\frac{\partial c_{s,j}}{\partial t} = \frac{D_{s,j}}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial c_{s,j}}{\partial r} \right)$$
(4)

The initial boundary condition is

$$\begin{cases} D_{s,j} \frac{\partial c_{s,j}}{\partial t} \bigg|_{r=0} = 0 \\ D_{s,j} \frac{\partial c_{s,j}}{\partial t} \bigg|_{r=R_{s,j}} = -J_{j} \end{cases}$$

$$(5)$$

Where,  $c_{s,j}$  is solid phase concentration;  $D_{s,j}$ , solid phase diffusion coefficient;  $r \in (0, R_{s,j})$ , radial coordinate radius of electrode particles;  $R_{s,j}$ , electrode particle radius;  $J_j$ , pore wall flux of Lithium-ion on particle surface.

Based on the previous assumptions,  $J_j$  follows the Eq. (6).

$$J_{j} = \overline{J}_{j} = \pm \frac{\overline{i}_{j}}{a_{j}F} = \pm \frac{R_{s,j}\overline{i}_{j}}{3\varepsilon_{s,j}F}$$

$$\tag{6}$$

Where,  $a_j$  is active surface area per electrode unit volume;  $\mathcal{E}_{s,j}$ , active material volume fraction; F, Faraday constant.

The original solid phase  $Li^+$  diffusion equation is a partial differential equation with boundary conditions, and the solution is very complicated. Moreover, the estimation of the SOC requires only the surface concentration in the electrode particle. Therefore, in order to facilitate the implementation of the subsequent algorithm, the three parameter parabolic approximation method is adopted to simplify the solid lithium-ion diffusion equation [14]. The simplified concentration of solid phase can be expressed as Eq. (7).

$$c_{s,j} = a + b(\frac{r^2}{R_{s,j}^2}) + c\left(\frac{r^4}{R_{s,j}^4}\right)$$
(7)

Use the boundary conditions in Eq. (5) after substituting the parabolic approximation in Eq. (7) into Eq. (4).

$$\frac{d}{dt}\overline{c}_{s,j} = -3\frac{J_j}{R_{s,j}}$$
(8)

$$\frac{d}{dt}\bar{q}_{s,j} = -30\frac{D_{s,j}}{R_{s,j}^2}\bar{q}_{s,j} - \frac{45J_j}{2R_{s,j}^2}$$
(9)

$$c_{s,j,surf} = \overline{c}_{s,j} + \frac{8R_{s,j}}{35} \overline{q}_{s,j} - \frac{R_{s,j}}{35D_{s,j}} J_j$$
(10)

Where,  $\overline{c}_{s,j}$  is the average solid phase concentration;  $\overline{q}_{s,j}$ , the average solid phase flux. The boundary conditions have been known.

$$\begin{cases} \overline{q}_{s,j} \Big|_{t=0} = 0 \\ c_{s,j,surf} \Big|_{t=0} = c_{s,j,surf\,0} \end{cases}$$
(11)

Where,  $c_{s,j,surf\,0}$  is the initial solid phase concentration. This value directly affects the initial quantity of electric charge.

Use the boundary conditions Eq. (11) after substituting the parabolic approximation in Eq. (8, 9) into Eq. (10).

$$c_{s,j,surf}' = -\frac{48D_{s,j}}{7R_{s,j}} \left(-e^{-30\frac{D_{s,j}}{R_{s,j}^2}} \int J_j dt + e^{-30\frac{D_{s,j}}{R_{s,j}^2}t} \times \int J_j e^{30\frac{D_{s,j}}{R_{s,j}^2}t} dt\right) - \frac{57}{7}R_{s,j}J_j - \frac{R_{s,j}}{35D_{s,j}}J_j'$$
(12)

After the surface  $Li^+$  concentration is obtained, the positive and negative open circuit voltage can be obtained according to the expression of the open circuit voltage.

### 2.1.2. Solution of electrolyte phase potential

The original SP model assumes that the concentration of  $Li^+$  in the electrolyte is constant, neglecting the influence of the  $Li^+$  concentration in the solution on the potential energy change, which leads to the poor accuracy of the model under the large discharge current condition. In this work, based on the simplified the equation of electrode phase  $Li^+$  concentration distribution, electrolyte phase potential of the battery can be obtained *via* electrolyte phase potential equation. The  $Li^+$  concentration distribution of electrode phase can be expressed by the Fick's second law, as shown in Eq. (13).

$$\varepsilon_{e,j}\frac{\partial c_e}{\partial t} = D_{e,j}^{eff}\frac{\partial^2 c_e}{\partial x^2} + a_j \left(1 - t_+^0\right) J_j \tag{13}$$

The initial boundary condition is

$$\begin{cases} D_{e,n}^{eff} \frac{\partial c_e}{\partial x} \Big|_{x=l_n^-} = D_{e,sep}^{eff} \frac{\partial c_e}{\partial x} \Big|_{x=l_n^+} \\ c_e \Big|_{x=l_n^-} = c_e \Big|_{x=l_n^+} \\ D_{e,sep}^{eff} \frac{\partial c_e}{\partial x} \Big|_{x=(l_{sep}+l_n)^-} = D_{e,p}^{eff} \frac{\partial c_e}{\partial x} \Big|_{x=(l_{sep}+l_n)^+} \\ c_e \Big|_{x=(l_{sep}+l_n)^-} = c_e \Big|_{x=(l_{sep}+l_n)^+} \end{cases}$$
(14)

Where,  $\mathcal{E}_{e,j}$  is electrolyte phase volume fraction;  $D_{e,j}^{eff}$ , effective electrolyte phase diffusion coefficient;  $t_{+}^{0}$  is Li<sup>+</sup> electrolyte phase transference number.

The electrolyte phase lithium-ion diffusion equation is a set of parabolic partial differential equations with a large number of boundary conditions. For estimation and control applications, a more efficient approach to obtain an approximate solution can be formulated by taking the Laplace transform of Eq. (13).

$$sc_{e}(s) - D_{e,j}^{eff} \frac{d^{2}c_{e}(s)}{dx^{2}} - \beta \frac{I(s)}{Al_{i}a_{i}} = 0$$
(15)

Where,  $\beta = a_j(1-t_0^+)/F\varepsilon_e$ . When solving the battery electrolyte phase potential difference, we only need to know the electrolyte phase potential in electrode boundary (x = 0, x = L). It can obtain the transfer function that represents the effects of the electrolyte diffusion dynamics on the lithium-ion concentration at the electrode boundary (x = 0, x = L) via the Eq. (15). The two transfer functions are approximated and simplified by using the first order Padé approximation method and the linear expression of the Li<sup>+</sup> concentration in electrolyte phase can be obtained.

when x = 0

$$\frac{c_{e}(s)}{I(s)} = \frac{0.25\beta l_{n}}{AFD_{e,n}^{eff} \left(1 + 0.112 \frac{l^{2}}{D_{e,n}^{eff}}s\right)}$$
(16)

when x = L

$$\frac{c_{e}(s)}{I(s)} = \frac{0.33\beta l_{p}}{AFD_{e,p}^{eff} \left(1 + 0.092 \frac{l^{2}}{D_{e,p}^{eff}} s\right)}$$
(17)

By using the average current density and the boundary conditions at the interface, the Ohm's law of the electrode phase potential is simplified [16]. The potential difference between the anode and the cathode is given by

$$\phi_{e,n} - \phi_{e,p} = \phi_e(L) - \phi_e(0) = \frac{2RT(1 - t_+)}{F} \ln \frac{c_e(L)}{c_e(0)} - \frac{I(\delta_n + 2\delta_{sep} + \delta_p)}{2A\kappa^{eff}}$$
(18)

Where,  $\kappa_i^{eff}$  is effective electrolyte phase ionic conductivity.

### 2.1.3. Solution of polarization overpotential

The electrochemical reaction at the solid-liquid interface is described by the Bulter-Volmer dynamic equation. The relation between the  $Li^+$  pore wall flux and the surface polarization overpotential of solid particles can be obtained by this equation, and the Eq. (6) can be substituted into this equation.

$$\overline{J}_{j} = k_{j} c_{e}^{0.5} \left( c_{s,j,\max} - c_{s,j,surf} \right)^{0.5} c_{s,j,surf}^{0.5} \left[ \exp\left(\frac{\alpha F}{RT} \overline{\eta}_{j}\right) - \exp\left(\frac{-\alpha F}{RT} \overline{\eta}_{j}\right) \right]$$
(19)

Where,  $k_j$  is reaction rate constant,  $\overline{\eta}_j$ , average polarization overpotential,  $\alpha$ , electrode transfer coefficient, *R*, molar gas constant, *T*, battery operating temperature.

The average polarization overpotential can be obtained by solving the Eq. (19).

$$\overline{\eta}_{j} = \frac{RT}{\alpha F} \ln \left( \frac{J_{j}}{2j_{0}} + \sqrt{\left(\frac{J_{j}}{2j_{0}}\right)^{2} + 1} \right)$$
(20)

It follows from the discussion above, the final terminal voltage of ESP electrochemical model can be obtained by substituting the above solutions into Eq. (2).

$$V_{t} = U_{p} \left( \theta_{s,p} \left( L \right) \right) - U_{n} \left( \theta_{s,n} \left( 0 \right) \right) + (1 - t_{+}) \frac{2RT}{F} \ln \frac{c_{e}(L)}{c_{e}(0)} - \frac{I}{2A\kappa^{eff}} \left( \delta_{n} + 2\delta_{sep} + \delta_{p} \right) + \frac{RT}{\alpha F} \ln \frac{\xi_{p} + \sqrt{\xi_{p}^{2} + 1}}{\xi_{n} + \sqrt{\xi_{n}^{2} + 1}} + R_{f} I \quad (21)$$

#### 2.2. Model parameter identification

We use a cylindrical 2300mAh LiFePO<sub>4</sub> battery as the test cell. The battery electrochemical parameters are shown in Table 1, some of which are supplied by battery manufacturers and some from the literature [17]. In order to improve the accuracy of the model, the key electrochemical parameters are identified for the difficulty of obtaining directly. These parameters include positive and negative solid phase diffusion coefficient, positive and negative reaction rate constant, and initial positive and negative surface  $Li^+$  concentration.

Table 1. The electrochemical parameters of the LiFePO<sub>4</sub> battery

	$A/m^2$	<i>lj</i> / m	$R_j/m$	$D_{e,j}^{e\!f\!f}$ / $\mathrm{m}^2\cdot\mathrm{s}^{\text{-1}}$	$C_{s,j,\max} / \operatorname{mol} \cdot \mathrm{m}^{-3}$	$\mathcal{E}_{s,j}$	$\kappa_j^{e\!f\!f}$	$\mathcal{E}_{s,j}$	α
Negative electrode	0.1	50×10 <sup>-6</sup>	3.65×1 0 <sup>-8</sup>	4.97×10 <sup>-9</sup>	22806	0.6	0.18 3	0.3	0.5
Separator	0.1	$25.4 \times 1$ $0^{-6}$	_	9.19×10 <sup>-9</sup>	_	_	0.16 8	1	_
Positive electrode	0.1	36.4×1 0 <sup>-6</sup>	$3.5 \times 10^{-6}$	4.93×10 <sup>-9</sup>	31370	0.5	0.26 5	0.3	0.5

Notes:  $R = 8.314 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$ ,  $F = 96487 \text{ C} \cdot \text{mol}^{-1}$ , T = 298 K,  $t_{+}^{0} = 0.363$ ,  $R_{f} = 0.02 \Omega$ 

The expression of the open circuit voltage [20]:  $U_{p}(\theta_{s,p}) = 3.4323 - 0.8428 \exp[-80.2493(1-\theta_{s,p})^{1.3198}] - 3.2474 \times 10^{-6} \exp[20.2645(1-\theta_{s,p})^{3.8003}] + 3.2482 \times 10^{-6} \exp[20.2646(1-\theta_{s,p})^{3.7995}]$   $U_{n}(\theta_{s,n}) = 0.6379 + 0.5416 \exp(-305.5309\theta_{s,n}) + 0.044 \tanh(\frac{-(\theta_{s,n} - 0.1958)}{0.1088}) - 0.1978 \tanh(\frac{\theta_{s,n} - 1.0571}{0.0854}) - 0.6875 \tanh(\frac{\theta_{s,n} + 0.0117}{0.0529}) - 0.0175 \tanh(\frac{\theta_{s,n} - 0.5692}{0.0875})$ 

The terminal voltage data as the true value of the battery voltage was obtained by taking charge/discharge tests that were performed between 2.1 and 3.65V under a Land battery tester at various rates ranging from 0.1 to 2C at 25°C. And the linear decreasing weight particle swarm optimization (LDW-PSO), a highly intelligent bionic optimization algorithm, that can automatically adjust search strategy and accordingly has a large search space and speed at the initial stage of iteration and has strong local search ability in the final stage of the iteration [18], is used to identify the

unknown parameters in the ESP model. Therefore, adopting the ESP model to fit the terminal voltage of the test battery can minimize the error between the test terminal voltage and the model terminal voltage. The objective function of parameter identification is given by:

$$\begin{cases} \min\{J(\theta)\} \\ J(\theta) = \sum_{i=1}^{n} [V_i - f(I_i, \theta)]^2 \end{cases}$$
(22)

Where,  $V_i$  is the terminal voltage at the sampling point *i* of test battery,  $f(I_i, \theta)$  is the terminal voltage at the sampling point *i* of battery model,  $I_i$  is the current at the sampling point *i*,  $\theta = (D_{s,p}, D_{s,n}, k_p, k_n, C_{s,p,surf}, C_{s,n,surf})$  is the parameter vector to be identified in the ESP model.

According to the parameter selection principle of the particle swarm optimization [19], we need to determine the optimal region for each parameter of the LDW-PSO algorithm. The scale of particle swarm m is 20. Dimension of a particle swarm n is 6. Cognitive weight c1 and Social weight c2 are set to 2. The constraint factor r is set to 1. The number of iterations is 1000. The final parameter identification results are shown in Table 2. Figure 2 shows the trend of the fitness function values variation in the iterative process of parameter identification.

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	$D_{s,j}/\mathrm{m}^2\cdot\mathrm{s}^{-1}$	$k_j / \mathbf{A} \cdot \mathbf{m}^{2.5} \cdot \mathbf{mol}^{-1.5}$	$C_{s,j,surf0}/\mathrm{mol}\cdot\mathrm{m}^{-3}$
Positive electrode	6.13×10 <sup>-14</sup>	5.74×10 <sup>-11</sup>	1259
Negative electrode	1.12×10 <sup>-17</sup>	9.42×10 <sup>-12</sup>	18245



Figure 2. The trend of the fitness function values variation

#### 2.3. Extended kalman filter SOC estimation

Compared with the original SP model, the ESP model has higher precision. However, the uncertainty of the model is also increased because of using the average current volume density, simplifying Li<sup>+</sup> solid phase and electrolyte phase diffusion process, and affecting by other unmodeled factors and random disturbances. Therefore, this work adopts the extended Kalman filter algorithm (EKF) based on the established dynamic model, uses the voltage error between model output and measured to correct the estimated value in real time, so as to ensure the accuracy of the estimated value and system stability.

Extended Kalman filtering algorithm (EKF), an improved estimation algorithm for nonlinear systems based on the Kalman filtering algorithm, uses feedback control to estimate the process state and employ iterative loop method to achieve minimum variance estimation [21].

Based on the electrochemical model established above, define state variables  $x = [x_1, x_2] = [C_{s,p,surf}, C_{s,n,surf}]^T$ , input  $u = I_t$ , output  $y = V_t$ . Discrete nonlinear equations of state can be obtained:

$$\begin{cases} x(k+1) = Ax(k) + Bu(k) + W(k) \\ y(k) = V(x(k), u(k)) + U(k) \end{cases}$$
(23)

Where, *W* is the system noise; *U*, the observation noise. The system matrix *A* and the input matrix *B* can be directly obtained by Eq. (12). The nonlinear measurement function *V* is obtained by Eq. (21). The observation matrix *C* of the nonlinear equation can be obtained by taking the partial derivative of the state variable with the observation equation.

$$C = \partial V / \partial x \tag{24}$$

The recursive process of estimating SOC with EKF algorithm is as follows:

(1) The initialization phase: the initial value of state vector  $\hat{x}_{0|0}$  and the initial value of the error covariance of state variables  $P_{0|0}$  are given by

$$\hat{x}_{0|0} = E(x_0)$$

$$P_{0|0} = Var(x_0)$$
(25)

(2) The time updating phase: it includes the state vector prediction and the error covariance matrix prediction.

$$\begin{aligned} x_{k+1|k} &= A x_{k|k} + B u_k \\ P_{k+1|k} &= A P_{k|k} A^T + Q \end{aligned} \tag{26}$$

Where, Q is the system noise variance matrix, which is Gauss white noise (mean value is 0).

(3) The observation update phase: it includes calculation of the Kalman gain coefficient, updating of the state vector, and updating of the error covariance matrix:

$$K_{k+1} = P_{k+1|k} C^{T} (CP_{k+1|k} C^{T} + R)^{-1}$$

$$\hat{x}_{k+1|k+1} = \hat{x}_{k+1|k} + K_{k+1} \Big[ y_{k+1} - V(\hat{x}_{k+1|k}, u_{k+1}) \Big]$$

$$P_{k+1|k+1} = (I - K_{k+1}C)P_{k+1|k}$$
(27)

Where,  $R_k$  is observation noise variance matrix, which is Gauss white noise (mean value is 0).

The Forecast updating of the state vector and the error covariance matrix can be achieved by constantly circulating the above process. In the electrochemical model, the SOC of the lithium-ion battery can be directly expressed by the surface concentration of the  $Li^+$  the positive solid phase.

$$SOC = \frac{c_{s,p,surf} - c_{s,p,surf\,0\%}}{c_{s,p,surf\,100\%} - c_{s,p,surf\,0\%}}$$
(29)

Where,  $c_{s,p,surf0\%}$  and  $c_{s,p,surf100\%}$  are the surface concentration of lithium-ion on the positive solid phase when the battery is discharged or charged absolutely.

## **3. RESULTS AND DISCUSSION**

#### 3.1. Model verification



Figure 3. Terminal voltage of discharge curvesat 0.5C rate.



Figure 4. Terminal voltage error of discharge curvesat 0.5C rate.



Figure 5. Terminal voltage of discharge curvesat2C rate.



Figure 6. Terminal voltage error of discharge curve at 2C rate.

In order to verify the validity of the model under different magnification current conditions, the constant current discharge tests at 0.5C and 2C current rate are carried out to verify the accuracy of the ESP model with different currents after parameter identification. And The ESP model is also compared with the original SP model[13]. The comparison of the experimental results and the simulation results calculating from the original SP model and the ESP model at 0.5C are shown in Figure 3 and Figure 4. It can be seen that the accuracy of the extended single particle model is very high, which is comparable to the P2D model. The maximum error of the ESP model obtained by parameter identification and the experimental results is only 12mV, while the error of the SP model is 43mV.

When discharge at 2C rate (Figure 5-6), the results obtained by the SP model differ greatly from the experimental data with about 0.12V maximum error, indicating that the SP model is no longer applicable in the case of high current. By contrast, although the maximum error of the ESP model

established in the work is also increased to 50mV, the raised is relatively pretty and acceptable in the view of the engineering point. Therefore, The ESP model can effectively improve the accuracy of the original SP model at high current conditions.

In order to better reflecting the accuracy of the electrochemical model established in this work, it is summarized and compared the model performances of the ESP model and reported models as previous reported, such as with average model [22], parabolic polynomial (PP) model [23], simplified pseudo-two-dimensional (SP2D) model [24]. and terminal voltage errors comparison results are listed in Table 3. Therefore, it is show that the ESP model has been with higher accuracy compared with the most reported models .

Table 3. (	Comparison	of terminal	voltage	errors
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	Maximum error at 0.5C rate/ mV	Maximum error at 0.5C rate/ mV
This work	12	50
SP model[13]	43	120
Average model[22]	34	73
PP model[23]	23	83
SP2D model[24]	13	42

According to the results obtained, the ESP model can not only improve the accuracy precisely at low discharge rate, but also estimates effectively at high rate. This might be attributed to taking into account the potential energy difference, which is resulted from the distribution of the electrolyte phase potential within the battery, and using LDW-PSO algorithm to identify the key parameters of the model. Thus, the simulation and experiment results show that the ESP model established in our work can effectively improve the accuracy of the original SP model.

# 3.2. Algorithm verification



Figure 7. 3C FUDS current curve



**Figure 8.** Terminal voltage comparison of ESP, EKF and test at 3C FUDS. (a) Terminal voltage results; (b) Terminal voltage errors;

The federal urban driving schedule (FUDS), a typical dynamic condition, can simulate the actual situation of the vehicles traveling on the urban road. In our work, the FUDS charge-discharge test with 3C magnification is used to verify the accuracy of the ESP model and the ESP-model-based EKF algorithm under complex cyclic conditions. The terminal current curve is shown in Figure7.

To evaluate the effect of different models on the accuracy of SOC estimation, the terminal voltage estimation datum of the ESP model, the ESP-model-based EKF algorithm and the test values are compared in Figure 8. Under the complex dynamic driving conditions, ESP-model-based EKF algorithm can well simulate the terminal voltage characteristics of the batteries when the accuracy of the ESP model decreases.



**Figure 9.** Contrast curve between SOC estimation and test values.(a) SOC estimation result; (b) SOC estimation error

The terminal voltage errors of the ESP model and the ESP-model-based EKF algorithm are exhibited in Figure 8b. It can be seen that the maximum error of the ESP electrochemical model after the parameter identification of the LDW-PSO algorithm at 3C FUDS is 2.8%. Thus, the dynamic characteristics of lithium ion batteries would be finely reflected in this model. When the ESP-model-based EKF algorithm is used, the maximum error of the terminal voltage is only 0.9% and the RMS error is only 3.2 mV, showing that the EKF algorithm effectively reduces the interference of unmodeled factors and random noises, resulting in the low error.

Figure 9 is a comparison of SOC estimated values of the ampere hour integral method, the ESP model-based EKF algorithm and the test values of the batteries. It can be seen that when the value of SOC is very accurate at the initial stage, the precision of the ampere hour integral method is higher than the ESP-model-based EKF algorithm. However, with the increasing of charge-discharge time, the error of ampere hour integral method increases rapidly, because the ampere hour integral method uses the value of the last moment as the initial value. It will cause the small measurement error of current to accumulate gradually, resulting in more and more error. The error of ESP-model-based EKF algorithm fluctuates slightly when current changes are severe, but, as a whole, it is still stable in a small range. The results prove that the designed ESP-model-based EKF algorithm can eliminate the interference of system noise and observation noise and greatly narrow the error.

The detailed analysis of the SOC estimation errors is listed in Table 4. Under 3C FUDS dynamic conditions, the maximum SOC estimation error of the ESP-model-based EKF algorithm is 3.19% while that of the RMS is only 0.83%.

According to the results obtained, the ESP-model-based EKF algorithm exhibit excellent SOC estimation performance. The estimation error are lower than most of the reported methods which using the same battery parameters and cyclic conditions in the experimental process (as compared in Table 4)[25-29]. They might be related to their unique computational features in several aspects: (i) The ESP electrochemical model that considers the influence of electrolyte phase potential on terminal voltage in the light of electrochemical characteristics of lithium ion battery, which reflects the microscopic mechanism of the battery and has higher precision. (ii) the key parameters of the ESP model are identified by LDW-PSO algorithm which can automatically adjust search strategy, significantly increase search space and speed at the initial stage of iteration and has strong local search ability in the final stage of the iteration. (iii) EKF algorithm effectively reduces the interference of unmodeled factors and random noises, resulting in the low error.

	Maximum error/%	RMS error/%
This work	3.19	0.83
ampere hour integral method	7.25	3.26
SPM-based EKF algorithm[25]	4.32	1.32
AM-based EKF algorithm[26]	3.96	1.44
SPM-based UKF algorithm[27]	3.87	0.97
SPM-based output-injection observer[28]	4.28	1.06
P2D-model-based Luenberger observer[29]	3.11	1.31

 Table 4. Comparison of the SOC estimation errors

In order to verify the robustness of the algorithm, the SOC estimation curves of the ampere hour integral method and the ESP-model-based EKF algorithm are compared in Figure 10 in the case that there are large deviations in the initial SOC. As can be seen from the diagram, when the initial SOC error is 25%, the ESP-model-based EKF algorithm rapidly converges to the real value, showing excellent robustness.



Figure 10. Contrast curve between SOC estimation and test values when initial error exists

## 4. CONCLUSION

(1) On the basis of the SP model, by considering the influence of the electrolyte phase potential on the battery terminal voltage, the ESP electrochemical model of lithium-ion batteries is established, which improves the accuracy of the SP model under high magnification current condition. LDW-PSO algorithm is used to identify the key parameters of the model, and the accuracy of the model is verified by experiments and simulations. The maximum error is less than 50mV with a large current discharge rate of 2C.

(2) The ESP-model-based EKF algorithm is designed. By modifying the terminal model voltage, the EKF algorithm eliminates the interference of unmodeled factors and random noises, and the estimation accuracy of the SOC is improved. Simulation and experiment results show that the ESP-model-based EKF algorithm has good estimation accuracy in complex dynamic conditions, and the maximum estimation error is less than 3.19%.

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