SOC Estimation of Lithium Battery Based on N-2RC Model in Electric Vehicle

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Abstract: The state-of-charge (SOC) of power batteries is one of the important parameters for electric vehicles, and an accurate battery model is the premise of improving the SOC estimation accuracy. Based on the Nernst electrochemical equation and second-order RC Thevenin equivalent circuit model, a novel battery modeling method is proposed in this paper. The electrochemical polarization voltage and concentration polarization voltage in the second-order RC Thevenin equivalent circuit model are added to the Nernst equation, and the improved Nernst equation is adopted to replace the electromotive force equation of second-order RC Thevenin equivalent circuit model , and the Nernst-second-order RC Thevenin equivalent circuit model(N-2RC) model is built. The parameters of this model can be obtained by nonlinear least square method. Because the electromotive force equation of this model is non-linear, unscented kalman filter (UKF) algorithm is adopted to estimate SOC. The simulation results verify the advantages of the proposed method.

Key Words: SOC, Nernst Equation, Equivalent Circuit Model, Unscented Kalman Filtering

1 INTRODUCTION

With the shortage of fossil fuels and serious environment problems, electric vehicles have gradually became the developmental direction of future automobiles due to their advantages of energy saving and environmental friendliness with zero emissions [1]. As one of the three key technologies of an electric vehicle, the battery management technologies are great significant to the normal operation of electric vehicle battery pack even electric vehicle. Among those technologies, the estimation of state-of-charge (SOC) is a core work in battery management technologies [2]. Accurate estimation of SOC can prevent battery from over charging or over discharging, reduce battery abuse and extend battery life. Therefore, accurate estimation of SOC is particularly important.

The ampere-hour integral method is a classic SOC estimation method. It is also called Coulomb counting, and is by far the most extensively used method in electric vehicle [3].Its principle is the definition of SOC.However, the ampere-hour integral method requires accurate initial value of SOC. When the electric vehicle starts running, the initial value of SOC cannot be acquired precisely. Therefore, there will be a certain errors between the estimated SOC and the actual SOC.The authors of [4] gave a neural network method that had an advantage in real-time online estimation. But this method requires a large amount of training data. Paper [5] adopted extended kalman filtering (EKF) algorithm to estimate SOC.The authors of [6] adopted particle filtering algorithm to estimate SOC. However, these methods all realized high accuracy estimation of SOC from improving filtering algorithm. According to the feedback mechanism, the accuracy of the filtering algorithm depends on the battery model whether can reflect the real battery characteristics. The existing models for lithium batteries mainly include equivalent circuit model and electrochemical model. The internal reactions of the battery are regarded as a series combination of voltage source, resistance and capacitance in the equivalent circuit model. Papers [7] [8] [9] gave some equivalent circuit models, such as Rint model, second-order Thevenin model and PNGV model. The equivalent internal resistances of the battery include ohm resistance, electrochemical polarization resistance and concentration polarization resistance. In second-order Thevenin model, one resistance stands for ohm polarization and the second-order RC loops depict the phenomenon of electrochemical polarization and concentration polarization [10]. Although these circuit models can well describe the volt-ampere characteristics of the battery, they cannot reflect the internal chemical reactions. The classic electrochemical Nernst model can directly obtain the relation between input and output variables through the chemical reaction equations, which can describe the relation between the electromotive force E and the activity of reactants. Moreover, the influencing factors of each parameter are clear and easy to be identified in Nernst model [11]. However, the classic Nernst model does not consider the effect of equivalent internal resistance. Ohm resistance was added to the Nernst model in paper [12]. Obviously, the modified Nernst equation still does not take into account the electrochemical and concentration polarization, which renders certain limitations of this model. On the contrary,

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the electrochemical and concentration polarization are well described in the second-order RC Thevenin model.

To address these issues, this paper proposes a novel modeling method. The voltage of the capacitances that describe the electrochemical polarization and concentration polarization in the equivalent circuit model are added to Nernst model. Terminal voltage equation in equivalent circuit model is replaced with the improved Nernst equation so that N-2RC model is built. Because the Nernst equation is non-linear, UKF algorithm is adopted to estimate SOC Finally, the accuracy of the proposed method is verified by simulation.

2 CLASSIC NERNST MODEL

Nernst equation has vital advantages in describing the electromotive force of battery. It can show the relation between electromotive force E and activity of internal reactants. There is internal redox reaction in any battery:

$$aA + bB \Leftrightarrow cC + dD \tag{1}$$

If C and D are reducible, A and B are oxidized, Nernst equation is as follows:

$$E = E_0 + \frac{RT_k}{nF} \ln \frac{[C]^c \cdot [D]^d}{[A]^a \cdot [B]^b} \tag{2}$$

Where T_k is the thermodynamic temperature, E_0 represents the standard electrode potential, it is also called Open circuit voltage at full charge, E stands for open circuit voltage that are usually represented by U_{oc} in the battery model, R and F are gas constant and Faraday constant, n represents the number of electrons gained or lost in the reaction of the electrode material,[A]−[D] denote the concentration (activity) of the substance, index a−d are the corresponding coefficient .The higher the index, the higher the activity of the reaction.

The electromotive force is produced by the reversible electrochemical reaction of battery, therefore, the voltage can be expressed as a function about the open circuit voltage at full charge and the activity of each participating reaction substance, the relevant parameters in the battery are expressed as the Nernst equation:

$$U_{oc} = E_0 + \frac{RT_k}{nF} \ln \frac{\alpha_{red}}{\alpha_{ox}} \tag{3}$$

α_{ox}, α_{red} respectively are the activity of high oxidation numbers ,low oxidation numbers of all the ions in electrode reaction.

The electrochemical reaction equations of lithium battery are as follows:

The positive response:

$$LiFePO_4 \Leftrightarrow Li_{1-x}FePO_4 + xLi^+ + xe^- \tag{4}$$

The cathode reaction:

$$xLi^+ + xe^- + 6C \Leftrightarrow Li_xC_6 \tag{5}$$

The overall reaction:

$$LiFePO_4 + 6xC \Leftrightarrow Li_{1-x}FePO_4 + Li_xC_6 \tag{6}$$

According to the reaction equations mentioned above, the formula (3) can be rewritten as:

$$U_{oc} = E_0 + \frac{RT_k}{nF} \ln \frac{\alpha_{Li^{x+}}}{\alpha_{Li_xC_6}} \tag{7}$$

Li_xC_6 is the pure solid, so that its activity is equal to 1. The activity of Li^+ can be described by the product of ionic activity coefficient and concentration.

$$\alpha_{Li^+} = C_{Li^+}\gamma_{Li^+} \tag{8}$$

Where C_{Li^+} is the concentration and γ_{Li^+} is the average activity coefficient of Li^+. There is not quantitative relation between C_{Li^+} and γ_{Li^+}. From empirical data, the higher the concentration, the lower the average activity coefficient.C_{Li^+} is the unreacted number of Li^+ ,it represents the capacity that has not been charged or the amount of power that has been released when the battery discharges. Based on the definition of SOC:

$$SOC = SOC_0 - \frac{1}{Q_0} \int_0^t \eta I d\tau \tag{9}$$

Where I and Q_0 respectively indicate the working current and the rated capacity, therefore, C_{Li^+} is associated with $1-SOC$, the larger C_{Li^+} , the larger $1 - SOC$. Because the bigger C_{Li^+} , the lower γ_{Li^+} , so γ_{Li^+} is associated with SOC. the larger γ_{Li^+} , the larger SOC . Therefore, equation (8) can be converted to:

$$\alpha_{Li^+} = (1 - SOC)^{\beta_1} SOC^{\beta_2} \tag{10}$$

Where β_1 is coefficient of relation between $1 - SOC$ and C_{Li^+} ,β_2 is coefficient of relation between SOC and γ_{Li^+} ,and they are positive. By taking (3)-(10) into account, the open circuit voltage expression can be gained:

$$U_{oc} = E_0 + \frac{RT_k\beta_1}{2F} \ln(1 - SOC) + \frac{RT_k\beta_2}{2F} \ln(SOC) \tag{11}$$

The variable temperature is not considered in this paper,so T_k is a constant. Finally, the above expression can be rewritten as:

$$U_{oc} = E_0 + K_1 \ln(1 - SOC) + K_2 \ln(SOC) \tag{12}$$

Where k_1, k_2 are constants.

During the charging process and discharging process of a lithium battery, the terminal voltage is not equal to the open circuit voltage, which is the reason why the battery has the equivalent internal resistance. There are three kinds of equivalent internal resistances: ohm resistance, electrochemical polarization resistance and concentration polarization resistance. It can be seen from hybrid pulse power characteristic(HPPC) test: the voltage changes instantaneously at the moment during the charging process and discharging process, which is caused by ohm resistance. The gradual change of voltage with time is caused by polarization resistances. Due to the simple calculation of ohm resistance, the influence of ohm resistance is usually added to the Nernst model called modified Nernst equation:

$$U_{oc} = E_0 + K_1 \ln(1 - SOC) + K_2 \ln(SOC) - IR_0 \tag{13}$$

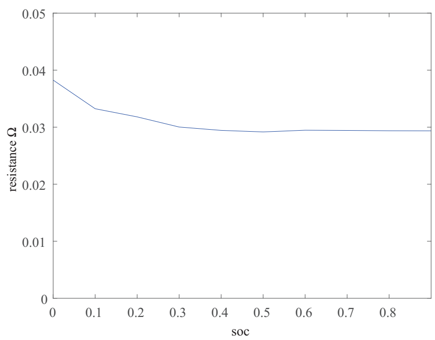

Figure 1: Identification Results of R_0

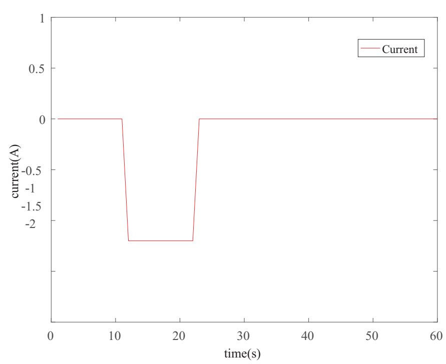

Figure 2: Current of HPPC Test

Where R_0 is ohm resistance, the value of R_0 could be calculated by using the value of instantaneous change voltage to divide the value of current. The identification results of R_0 are shown in Figure 1.

In order to obtain the values of parameters k_1 and k_2, curve fitting is performed on the formula (13). Because k_1 and k_2 are not directly related to SOC, the effect of SOC on its values can be neglected. So the parameters k_1 and k_2 are identified only when SOC is 0.9. The identification results are shown in the following table:

Table 1: Identification Results

SOC	k_1	k_2
0.9	0.719	-0.0027

Figure 2 shows the working current of HPPC test when SOC=0.9.The dynamic terminal voltage curve of the HPPC test and the simulated voltage curve of modified Nernst model are compared in Figure 3.

Because the modified Nernst model simply establishes the functional relation among the voltage, current, SOC and ohm resistance without polarization resistances, obviously it cannot describe the time-related gradient characteristic mentioned above.

It's worth noting that the effect of this gradient characteristic will exist whenever the battery's working current changes. Furthermore, when the battery in the state of intermittent discharge, the gradual change characteristic effect is very distinct. The difficulty in describing the gradient feature is the biggest drawback of this model, which greatly limits the application of this model.

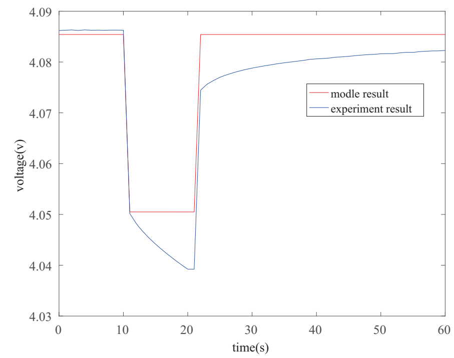

Figure 3: Terminal Voltage Comparison

3 EQUIVALENT CIRCUIT MODEL of LITHIUM BATTERY

The battery's charge-discharge characteristics are very similar to those of resistance and capacitance. Based on these characteristics, the battery's dynamic characteristics can be simulated with a circuit model composed of some circuit elements such as resistance, capacitance and constant voltage source .This is equivalent circuit model. Nowadays, the most popular equivalent circuit model is Thevenin model, it takes into account the similarity between characteristic of polarization resistance and capacitance, and that adds two RC loops to simulate the electrochemical polarization and concentration polarization in Thevenin model ,it usually be called second-order Thevenin equivalent circuit model shown in Figure 4.

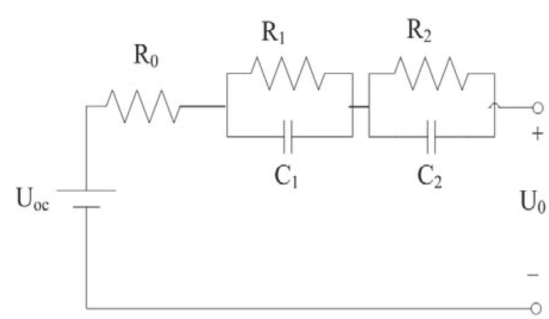

Figure 4: Second-Order Thevenin Equivalent Circuit Model

According to the basic principle of the circuit, the electrical equations of the model are as follows:

$$C_1 \times \frac{dU_1}{dt} + \frac{U_1}{R_1} = I \tag{14}$$

$$C_2 \times \frac{dU_2}{dt} + \frac{U_2}{dt} = I \tag{15}$$

Combined formula (14) - (15) with formula (9), the state-space model is gained as shown in formula (16):

Table 2: Identification Results

SOC	R_1	C_1	R_2	C_2
0.9	5.4	785.9	25.5	1581.9
0.8	8.6	478.5	19.7	1912.5
0.7	8.7	514.7	24.6	2054.9
0.6	5.2	928.2	55.8	1424.0
0.5	6.5	815.2	16.0	2327.7
0.4	2.9	959.4	16.9	1552.4
0.3	6.6	556.6	11.6	2303.2
0.2	4.0	833.5	21.1	1174.7
0.1	8.7	527.3	25.6	2253.1
0	12.3	360.3	44.0	1370.8

$$\begin{bmatrix} SOC \\ \overset{\bullet}{U_1} \\ \overset{\bullet}{U_2} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{R_1C_1} & 0 \\ 0 & 0 & -\frac{1}{R_2C_2} \end{bmatrix} \begin{bmatrix} SOC_0 \\ U_1 \\ U_2 \end{bmatrix} \tag{16}$$

$$+ \begin{bmatrix} -\frac{\eta\times T}{Q_0} \\ \frac{1}{C_1} \\ \frac{1}{C_2} \end{bmatrix} I$$

Where U_1 and U_2 respectively indicate voltage of R_1 and R_2, T indicates time.
The output equation is expressed as:

$$U_0 = U_{oc} - U_1 - U_2 - I \times R_0 \tag{17}$$

Where U_0 indicates terminal voltage.
As it's shown in Figure 3, the slowly rising phase of voltage after discharging is caused by polarization resistance, which can be regarded as a zero input response process, and its terminal voltage expression is expressed as:

$$U_0 = U_{0c} - U_{01}\exp\left(-\frac{t}{\tau_1}\right) - U_{02}\exp\left(-\frac{t}{\tau_2}\right) \tag{18}$$

Where U_{01} and U_{02} respectively indicate the initial voltage values of R_1 and R_2, τ is a time constant, and $\tau = RC$. During the discharging process, the voltage slowly decreases, which can be regarded as a zero state response process, and the terminal voltage is expressed as:

$$\begin{aligned} U_0 = U_{oc} - IR_1\left[1-\exp\left(-\frac{t}{\tau_1}\right)\right] \\ - IR_2\left[1-\exp\left(-\frac{t}{\tau_2}\right)\right] - IR_0 \end{aligned} \tag{19}$$

The nonlinear least square method is adopted to identify parameters, and the corresponding experimental data are fitted with CFTOOL, so the impedance parameters of the model can be obtained. In this paper, different SOC points are selected for identification accurate. The identification results are shown in Table 2:
Note that the unit of resistance and capacitance respectively are the mv and the pF in Table 2.
Although the equivalent circuit model can well describe the battery's volt-ampere characteristics, it cannot reflect the battery's internal problems from the electrochemical perspective.

4 ESTABILISHMENT of N-2RC MODEL

Based on the above analysis, this paper combines the equivalent circuit model and Nernst model to propose a novel power battery model – N-2RC model. The voltage of the capacitances and resistance of the second order Thevenin model are added to classic Nernst model, it's named improved Nernst model. And the formula (17) is replaced with the improved Nernst model. Therefore , the N-2RC model is determined as:
The state-space equation:

$$\begin{bmatrix} SOC \\ \overset{\bullet}{U_1} \\ \overset{\bullet}{U_2} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{R_1C_1} & 0 \\ 0 & 0 & -\frac{1}{R_2C_2} \end{bmatrix} \begin{bmatrix} SOC_0 \\ U_1 \\ U_2 \end{bmatrix} \tag{20}$$

$$+ \begin{bmatrix} -\frac{\eta\times T}{Q_0} \\ \frac{1}{C_1} \\ \frac{1}{C_2} \end{bmatrix} I$$

The output equation:

$$U = E_0 + K_1\ln(1-SOC) + K_2\ln(SOC) - IR_0 - U_1 - U_2 \tag{21}$$

5 SOC ESTIMATION BASED on UKF ALGORITHM

UKF algorithm is the combination of KF algorithm and UT transformation. The UKF algorithm is used for nonlinear systems, and it does not need to linearize the system equations, which is fundamentally different from the EKF algorithm. Therefore the system equation is more accurate [13].
The state-space equations and the measurement equations of the dynamic system are as follows:

$$\begin{cases} x_{k+1} = f(x_k, u_k) + w_k \\ y_k = g(x_k, u_k) + v_k \end{cases} \tag{22}$$

There are the state-space equation and the measurement equation established above for our N-2RC battery model, and the measurement equation is non-linear. where x_k denotes the state of the kth sampling period of the system, and y_k denotes the measured value, calculated by the measured equation of the state of the kth sampling period of the system. The function f denotes the state transition function, and g denotes the observation function.W_k is the system process noise, which can be regarded as $Gaussian$ white noise with variance Q_k, and V_k is measurement noise, which can be regarded as $Gaussian$ white noise with variance R_k.
The UKF algorithm is calculated as follows:
(1) Determine the initial value of the state variable, and the initial covariance matrix:

$$\begin{cases} \bar{x}_0 = E(x_0) \\ P_0 = E\left[(x_0-\bar{x}_0)(x_0-\bar{x}_0)^T\right] \end{cases} \tag{23}$$

(2)Select the sigma point and calculate the mean weight and covariance weight for each sample point:

$$x_{k|k}(i)=\begin{cases}\bar{x}_k, & i=1\\ \bar{x}_k+\sqrt{(n+\lambda)P_{k|k}}, & i=2,...n+1\\ \bar{x}_k-\sqrt{(n+\lambda)P_{k|k}}, & i=n+2,...2n+1\end{cases} \tag{24}$$

$$W_k(0)=\frac{\lambda}{n+\lambda} \tag{25}$$

$$W_c(0)=\frac{\lambda}{n+\lambda}+(1-\alpha^2+\beta) \tag{26}$$

$$W_k(i)=\frac{1}{2(n+\lambda)}, i=1,2,...2n \tag{27}$$

$$W_c(i)=\frac{1}{2(n+\lambda)}, i=1,2,...2n \tag{28}$$

Where n is the dimension of the state variable.$\lambda=\alpha^2(n+k)-n$,$\alpha\in[0,1]$ describes the distance between the sampling point and the mean point. In the normal distribution, β= 2, and $k=0$ is the ratio factor.

(3) The first estimate of the system state matrix is:

$$\begin{cases} x_{k+1|k}(i)=f\left(x_{k|k}(i),u_{k+1}\right)\\ \bar{x}_{k+1|k}=\sum_{i=1}^{2n+1}W_k(i)\,x_{k+1|k}(i)\end{cases} \tag{29}$$

(4)The first estimation of covariance of state variables matrix is:

$$P_{k+1|k}=\sum_{i=1}^{2n}W_c(i)\,(x_{k+1|k}(i)-\bar{x}_{k+1|k})(x_{k+1|k}(i)-\bar{x}_{k+1|k})' + Q_{k+1} \tag{30}$$

(5) The estimation of measured variables is given by:

$$\begin{cases} y_{k+1|k}(i)=g\left(x_{k|k}(i),u_{k+1}\right)\\ \bar{y}_{k+1|k}=\sum_{i=1}^{2n+1}W_k(i)\,y_{k+1|k}(i)\end{cases} \tag{31}$$

(6) The estimation of the covariance of the measured variables, the covariance between the measured variables and the state variables, and the UKF gain is:

$$\begin{cases} P_{yy}=\sum_{i=1}^{2n+1}W_c(i)\left(y_{k+1|k}(i)-\bar{y}_{k+1|k}\right)\\ \quad\times\left(y_{k+1|k}(i)-\bar{y}_{k+1|k}\right)^T+R_{k+1}\\ P_{xy}=\sum_{i=1}^{2n+1}W_c(i)\left(x_{k+1|k}(i)-\bar{x}_{k+1|k}\right)\\ \quad\times\left(y_{k+1|k}(i)-\bar{y}_{k+1|k}\right)^T\\ K_{k+1}=P_{xy}P_{yy}^{-1}\end{cases} \tag{32}$$

(7) The second update of the state matrix and the covariance of the state variables and return to the next iteration calculation as follows:

$$\begin{cases} x_{k+1|k+1}=\bar{x}_{k+1|k}+K_{k+1}\left(y_{k+1}-\bar{y}_{k+1|k}\right)\\ P_{k+1|k+1}=P_{k+1|k}-K_{k+1}P_{yy}K_{k+1}^T\end{cases} \tag{33}$$

In this paper, SOC and the voltage U_1 and U_2 are selected as state variables, the battery terminal voltage U_k is selected as the measurement variable, and the working current I_k is selected as the input variable, then discretize formula (20) and (21), according to the process of UKF algorithm described above estimate SOC.

6 SIMULATION RESULTS and ANALYSIS

In order to validate the accuracy of the proposed model, MATLAB is used for simulation to establish mathematical model of SOC according to formula(20) and (21). The rated capacity of lithium battery is 2.4 Ah.The rated voltag is 3.7V. The test current is shown in Figure 5, the simulation results are compared with the classic Nernst model in Figure 6, and the error curves are shown in Figure 7.

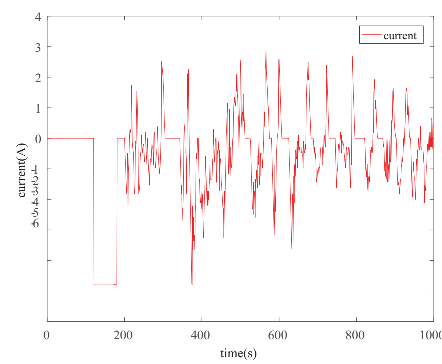

Figure 5: Current of UDDS

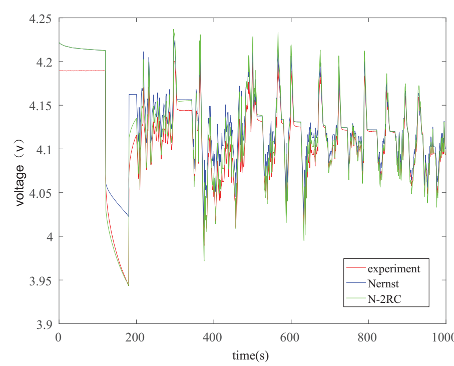

Figure 6: Terminal Voltage Contrast

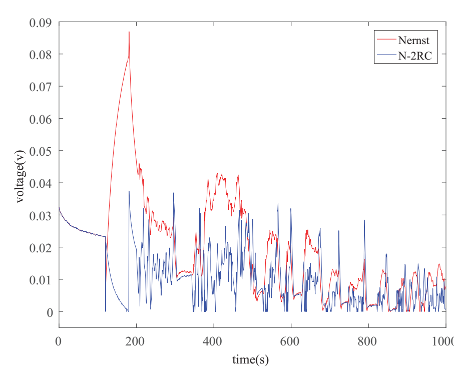

Figure 7: Error Conparison

Based on the basic process of UKF algorithm, let α=0.7,β=2,k=2 , then, start UKF to estimate SOC.The estimation result curve of SOC is shown in Figure 8. In addition, this result is compared with that of ampere-hour integral method and the estimated error is shown in Figure 8. The estimated error of SOC is controlled below 2% in Figure 9. It demostrates the SOC estimation method proposed in this paper can guarantee the accuracy.

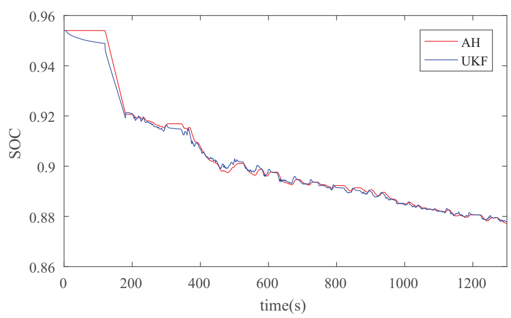

Figure 8: Comparison of SOC Estimation

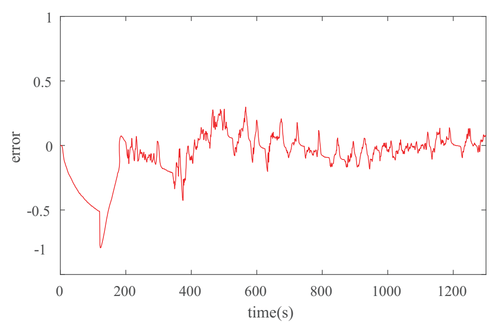

Figure 9: Error of Estimation

7 CONCLUSION

As an essential parameter for the energy control of an electric vehicle, the state-of-charge (SOC) of power lithium battery needs to be accurately estimated to improve battery life and vehicle performance. In this paper, the advantages and disadvantages of the equivalent circuit model and the Nernst model are analyzed,and that the N-2RC model is established by combining the advantages of the above mentioned models. UKF algorithm is adopted to estimate SOC based on the N-2RC model. Compared with ampere-hour integral method, the error curve shows the superiority of the proposed model .Besides, the proposed algorithm is simple in structure, easy to implement in engineering, and has strong practicability.The influence of temperature on the battery model has not been considered in this paper, and relevant studies will be carried out in the future.

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