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ORIGINAL RESEARCH

Construction and simulation analysis of lithium-ion batteries thermoelectric coupling model based on digital twin

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Abstract

With the rapid development of energy storage technology, it is significant to evaluate the operating status of lithium-ion batteries efficiently and accurately, so as to ensure their safe operation and reduce the probability of accidents. For the problems of long simulation time and low accuracy in existing models, this paper proposes a construction method of lithium-ion batteries thermoelectric coupling model based on digital twin. First, the digital twin structure system of lithium-ion batteries is proposed. Second, considering the coupling effects of the thermodynamic model and the equivalent circuit model, the thermoelectric coupling model is constructed based on the digital twin platform ANSYS TwinBuilder. The thermodynamic model is reduced in order and the simulation time is reduced to second level, which improves the simulation efficiency and meets the real time simulation requirements of the digital twin. Furthermore, considering that the operating parameters of lithium-ion batteries are variable, the parameters of the equivalent circuit model are identified online based on the variable forgetting factor recursive least squares algorithm. It updates parameters of the model and improves the simulation accuracy. Finally, the efficiency and accuracy of the model are verified through simulation analysis.

1 | INTRODUCTION

Under the background of dual carbon, the traditional power system is transforming into the power system with new energy as the main body. New energy has the characteristics of large randomness and strong volatility. A high proportion of new energy connected to the grid will affect the power system stability [1, 2]. The coordinated scheduling of lithium-ion batteries and new energy plays an important role in promoting the new power systems construction. However, lithium-ion batteries safety accidents such as fires and explosions occur frequently around the world. Thermoelectric conditions are the key factors affecting their safe operation. Considering the thermoelectric coupling of lithium-ion batteries, it is of great significance to evaluate the operating conditions such as temperature and voltage quickly and accurately. According to the evaluation results, operators can take corresponding measures to reduce the probability of accidents [3, 4].

The concept of digital twin was first proposed by Professor Grieves in 2003. It was defined as a three-dimensional model, including physical entity, digital counterpart and a link mechanism between them [5]. At present, digital twin has carried out a large number of exploratory research and demonstration applications in aviation, ocean, forestry, transportation and other fields [6, 7]. However, digital twin research in the field of batteries is still in its infancy. Research on batteries digital twin technology can bring new solutions to accurately assess the operating status and then manage batteries. At present, there is still a lack of systematic modeling theory, evaluation methods and application scope for batteries digital twin. Therefore, research on the construction method of lithium-ion batteries thermoelectric coupling model based on digital twin has reference significance for the development of batteries digital twin technology.

For the lithium-ion batteries thermoelectric coupling research, there are mainly two types: electrochemical-thermal coupling model [8, 9] and electric-thermal coupling model [10–12]. The electrochemical-thermal coupling model describes the electrochemical process inside batteries through partial differential equations. Differential equations contain many

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unknown variables and are complex. Identifying parameters and solving equations are difficult. The electrochemical-thermal coupling model is usually used in the fields of batteries structure and parameters design. However, it is rarely used in engineering [10]. For the electric-thermal coupling model, ref. [13] established a batteries thermal model based on the mathematical principles of heat conduction and surface heat convection heat dissipation. It was coupled with an equivalent circuit model to build the coupled thermoelectric model. The model parameters were identified offline to estimate temperature and voltage. Ref. [14] established a thermal mathematical model based on the mathematical principles of thermal transfer and thermal generation. Considering the temperature influence on the changes of equivalent circuit model parameters, a thermoelectric coupling model was established. The charging strategy was optimized based on the improved particle swarm optimization algorithm and the temperature during the charging process was estimated. Ref. [15] used the circuit form to build the lithium-ion batteries thermodynamic model. Circuit element expressions were derived based on the mathematical mechanisms of heat generation and heat transfer. And it was coupled with the equivalent circuit model to construct the thermoelectric coupling model. Considering the influence of batteries surface heat transfer conditions and environmental changes on model parameters, an adaptive estimation algorithm based on Kalman filter was proposed for temperature estimation. The above researches are based on mathematical principles to construct thermodynamic models. The parameters of the thermoelectric coupling model are easily affected by changes in the environment and operating conditions. It is difficult to fully describe the environmental changes based on the mathematical principles of thermodynamics. Compared with using Computational Fluid Dynamics (CFD) simulation analysis software (ANSYS Icepak, ANSYS Fluent) to construct the three-dimensional high-precision thermodynamic model, the simulation accuracy is lower. Therefore, it is important to construct the thermoelectric coupling model combined with the three-dimensional high-precision thermodynamic model and update model parameters online with full consideration of external conditions. Ref. [16] used ANSYS Fluent to establish a three-dimensional thermal model of the battery pack. Based on this model, the internal temperature of the battery pack under different external cooling schemes was estimated and analyzed. Ref. [17] established the three-dimensional cell thermal model based on finite elements. The first-order RC circuit model and thermal model were embedded in the volume microelement to realize thermoelectric coupling model establishment. The temperature distribution of the cell were obtained. Ref. [18] proposed the collaborative thermal simulation framework and used Modelica and ANSYS Fluent to establish equivalent circuit model and thermal model, respectively. Considering the influence of temperature on the equivalent circuit parameters, the equivalent circuit model was coupled with the thermal model using Python. The temperature field online simulation was carried out using the coupled model. The CFD simulation analysis methods used in the above researches generally have the problem of long simulation time. But multi-physics real time simulation is the basis of the lithium-ion batteries digital twin [19]. The digital twin needs to map the operating state of the lithium-ion battery in real time. CFD simulation is difficult to meet the real-time requirements of the digital twin. Therefore, it is necessary to use techniques such as model reduction to speed up the model solution and improve simulation efficiency.

For the problems of low simulation accuracy and long simulation time analyzed above in the current research, this paper proposes a construction method of the lithium-ion batteries thermoelectric coupling model based on digital twin. The main contribution of this paper is:

1. Considering the influence of thermoelectric coupling on batteries operating states, the lithium-ion batteries thermoelectric coupling model based on digital twin is established to realize accurate evaluation of the operating state.
2. Based on ANSYS TwinBuilder, the order reduction of the thermodynamic model is realized. The simulation time is reduced and the calculation efficiency is improved, while ensuring the simulation accuracy of the model. This meets the real time simulation requirements of the lithium-ion batteries digital twin.
3. Based on the variable forgetting factor recursive least squares(VFFRLS) algorithm, the parameters of the equivalent circuit model are identified online. In this way, the parameters of the lithium-ion battery thermoelectric coupling model are updated to improve the accuracy of the prediction results.

The remaining parts of this paper are as follows. Section 2 presents lithium-ion batteries digital twin structure system considering thermoelectric coupling. Section 3 presents construction of lithium-ion batteries thermoelectric coupling model based on digital twin. Section 4 presents parameters identification. Experiment results and discussions are presented in Section 5. Finally, the conclusions are drawn in Section 6.

2 | LITHIUM-ION BATTERIES DIGITAL TWIN STRUCTURE SYSTEM CONSIDERING THERMOELECTRIC COUPLING

The key to digital twin is to build a high-fidelity virtual model of physical devices. It can evaluate the operating state of the real physical world and feedback corresponding information to make decisions. Therefore, this paper proposes the lithium-ion batteries digital twin structure system considering thermoelectric coupling, which consists of five parts: physical device, virtual model, service system, twin data and connection system, as shown in Figure 1 [5, 20].

2.1 | Physical device

The physical device is the physical basis of the lithium-ion batteries thermoelectric coupling model based on digital twin, that

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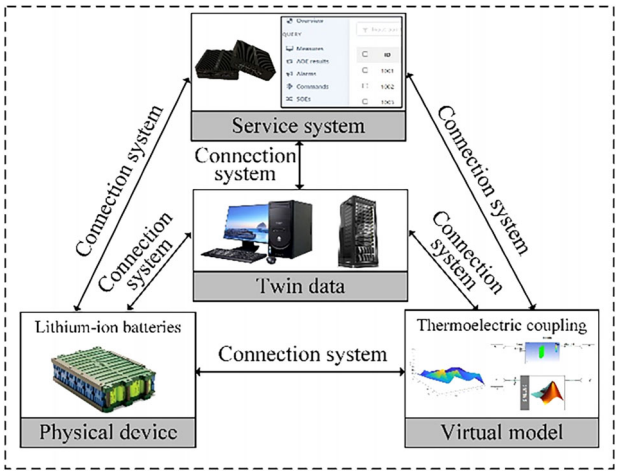

FIGURE 1 Lithium-ion batteries digital twin structure system considering thermoelectric coupling.

is, the real devices of the lithium-ion batteries. Various sensors are deployed on physical devices to monitor environmental data and operating status in real time.

2.2 | Virtual model

The virtual model is the core of the lithium-ion batteries thermoelectric coupling model based on digital twin. It integrates system models, correction algorithms, simulation calculations and other key elements. It adopts a "model-driven" + "data-driven" hybrid approach to correct and update model parameters, which not only preserves the physical characteristics of the model, but also improves the simulation accuracy [21].

2.3 | Service system

The service system integrates various information systems such as evaluation, control and optimization. It provides intelligent operation and precise control based on physical devices and virtual models. This prevents overcharging, over-discharging and high temperature operation, thereby ensuring the safe and stable operation of lithium-ion batteries.

2.4 | Twin data

It includes data related to physical devices, virtual models and service systems. And it is constantly updated and optimized with the generation of real-time data. Twin data is the core driver of digital twin operation.

2.5 | Connection system

The connection system connects the above four parts in pairs to enable effective and real-time data transmission. In this way, real-time interaction is realized to ensure the consistency and iterative optimization among various parts.

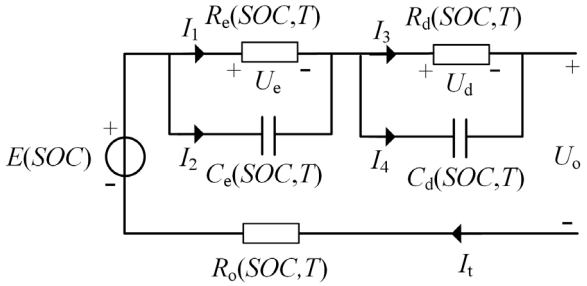

FIGURE 2 Second-order RC equivalent circuit model.

3 | CONSTRUCTION OF LITHIUM-ION BATTERIES THERMOELECTRIC COUPLING MODEL BASED ON DIGITAL TWIN

Based on the second-order RC equivalent circuit principle and thermodynamic principle of lithium-ion batteries, this section uses MATLAB Simulink and ANSYS Icepak to construct the equivalent circuit model and thermodynamic model, respectively. The lithium-ion batteries thermoelectric coupling model based on digital twin is established in ANSYS TwinBuilder. At last the model operation mechanism is explained in detail.

3.1 | Equivalent circuit model

The equivalent circuit model represents the lithium-ion battery in a specific circuit form. Common equivalent circuit models include Thevenin model, second-order RC model and GNL model. The second-order RC model has the advantages of relatively simple structure, real-time solution and high accuracy of dynamic and static characteristics description. Therefore, this paper chooses the second-order RC model for research and its equivalent circuit model is shown in Figure 2 [22].

In the figure, E represents open circuit voltage; R_e represents electrochemical polarization resistance; C_e represents electrochemical polarization capacitance; R_d represents the electrochemical concentration polarization resistance; C_d represents the electrochemical concentration polarization capacitance; R_o represents ohmic internal resistance, which is composed of electrode material, electrolyte, diaphragm resistance and contact resistance of various parts; I_t represents the current flowing through R_o; U_o represents the terminal voltage; U_e represents the voltage of the electrochemical polarization resistance; U_d represents the voltage of the electrochemical concentration polarization resistance; I_1, I_2, I_3 and I_4 represent the current flowing through R_e, C_e, R_d and C_d, respectively; T represents the temperature.

According to the equivalent circuit model shown in Figure 2, the relationship between various state parameters of batteries is

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obtained by combining Kirchhoff's law and circuit theory.

$$\begin{cases} SOC = SOC_0 - \dfrac{I_t}{C_N}\int \eta \Delta t dt \\ \dfrac{\int I_2 dt}{C_e} = I_1 R_e = U_e \\ \dfrac{\int I_4 dt}{C_d} = I_3 R_d = U_d \\ U_o = E - I_t R_o - U_e - U_d \end{cases}, \quad (1)$$

where SOC represents the state of charge; SOC_0 represents the initial SOC; C_N represents the rated capacity of the battery; η represents the Coulomb efficiency; $\triangle t$ represents the sampling period.

The state equation of the equivalent circuit model is obtained by discretization Formula (1).

$$\begin{bmatrix} SOC_{k+1} \\ U_{e,k+1} \\ U_{d,k+1} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & e^{-\frac{\Delta t}{\tau_e}} & 0 \\ 0 & 0 & e^{-\frac{\Delta t}{\tau_d}} \end{bmatrix} \begin{bmatrix} SOC_k \\ U_{e,k} \\ U_{d,k} \end{bmatrix} + \begin{bmatrix} -\dfrac{\eta \Delta t}{C_N} \\ R_e\left(1 - e^{-\frac{\Delta t}{\tau_e}}\right) \\ R_d\left(1 - e^{-\frac{\Delta t}{\tau_d}}\right) \end{bmatrix} I_{t,k}, \quad (2)$$

where k represents discrete computing ordinal; τ_d and τ_e both represent time constants, $\tau_d = R_d C_d$, $\tau_e = R_e C_e$.

Then the terminal voltage output equation can be obtained.

$$U_{o,k} = E - I_{t,k} R_o - U_{e,k} - U_{d,k}. \quad (3)$$

The terminal voltage can be substituted into Bernardi equation to obtain the thermal power of the batteries [23].

$$q = \left[I_t (U_o - E) + I_t T (\partial E / \partial T)\right] / V, \quad (4)$$

where q represents the heat generation power; $I_t(U_o\text{-}E)$ represents the irreversible thermal power caused by the difference between the terminal voltage and the open voltage; $I_t T(\partial E/\partial T)$ represents reversible reaction thermal power, depending on cell temperature, current and entropy coefficient; V represents the volume of batteries.

3.2 | Thermodynamic model

Lithium-ion batteries are their own heat sources during operation. Their heat generation power can be calculated by the above equivalent circuit model. The output current has no fixed change rule. Therefore, the heat dissipation process of lithium-ion batteries is an unsteady dynamic heat transfer process. According to the energy conservation equation, the three-dimensional heat dissipation model of lithium-ion batteries can be described as follows [24].

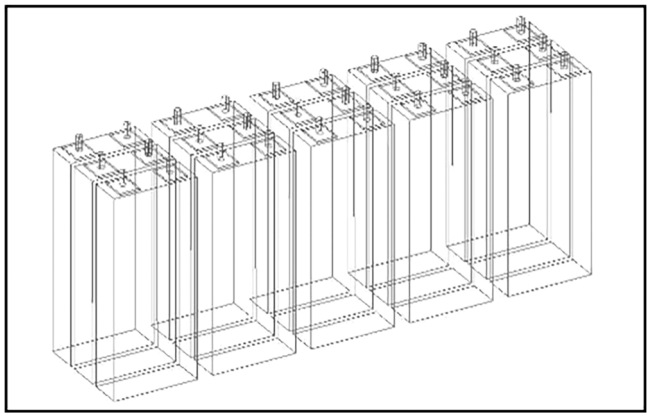

FIGURE 3 Thermodynamic model.

$$\rho C \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T) + q. \quad (5)$$

The left side of the formula represents the total heat added. The first term on the right side of the formula is the heat added by heat convection between batteries and the external environment. The second term on the right side of the formula is the heat added by the internal heat generation. ρ represents the average density; C represents the average specific heat capacity; λ represents the thermal conductivity in a direction.

The above formula is transformed into the rectangular coordinate form.

$$\rho C \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\lambda_x \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda_y \frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(\lambda_z \frac{\partial T}{\partial z}\right) + q, \quad (6)$$

where λ_x, λ_y and λ_z represent the thermal conductivity in x, y and z direction, respectively.

In this paper, the CFD simulation software ANSYS Icepak is used to build the thermodynamic model of lithium ion batteries, as shown in Figure 3.

Calculating the lithium-ion batteries temperature based on ANSYS Icepak simulation is the process of solving Formula (6). First, the heat production power of the batteries is input into the constructed thermodynamic model. Second, the boundary conditions is set and the calculation is solved. Finally, the temperature changes of the monitoring points are obtained. In this way, high-fidelity thermodynamic modeling and visualization of lithium batteries can be realized.

3.3 | Lithium-ion batteries thermoelectric coupling model construction based on digital twin

Considering the highly convoluted multi-physics nature of lithium-ion batteries, the equivalent circuit model parameters

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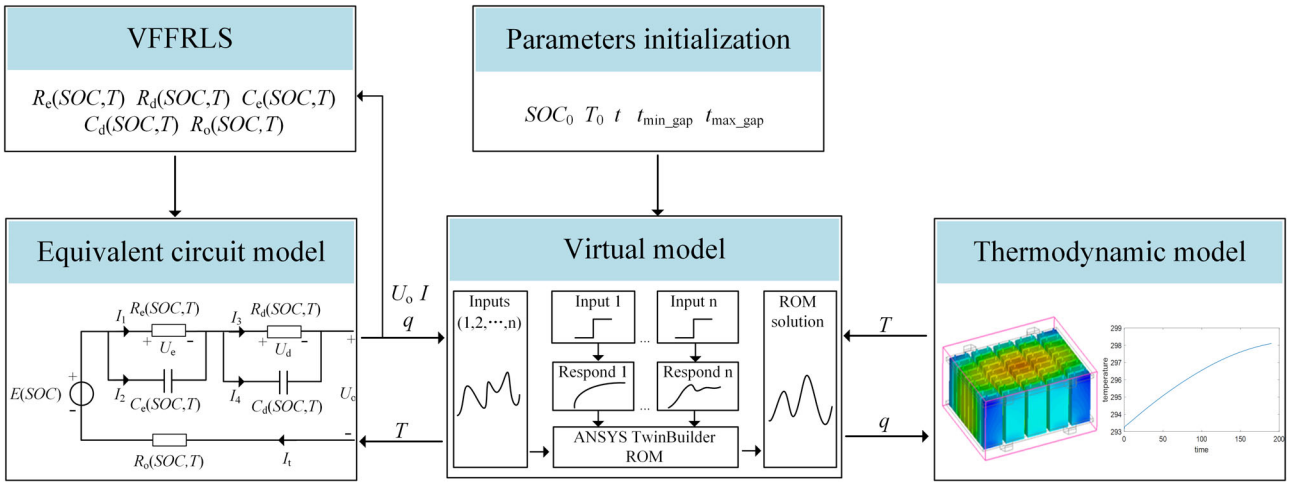

FIGURE 4 The operation mechanism of digital twin model.

are functions of temperature and SOC, and the heat generation power depends on SOC, temperature, charge and discharge mode. The equivalent circuit model and the thermal model are mutually coupled and interacting [25].

The lithium-ion batteries thermoelectric coupling model based on digital twin needs to map the batteries operating status in real time. The real-time simulation requirements are high. At present, CFD simulation using ANSYS Icepak has the advantages of high calculation accuracy and three-dimensional visualization, but the calculation takes a long time.

During the working process of the lithium-ion batteries, the heat generation power and the parameters of the equivalent circuit model change in real time. The model needs to be run repeatedly, which makes it difficult to meet the real-time requirements. Therefore, it is necessary to find a model order reduction tool that can reduce the convergence difficulty, speed up the model solving and maintain the simulation accuracy [26].

In this paper, the order reduction technology is used to reduce the order of the thermodynamic model, and then based on the ANSYS Twinbuider platform, the lithium-ion batteries thermoelectric coupling model based on digital twin is constructed. The calculation time is reduced to the second level, which greatly improves the simulation efficiency. And the result has the same accuracy as the CFD simulation, realizing accurate evaluation of the operating state of the lithium-ion batteries.

The operation mechanism of model is shown in Figure 4. Equivalent circuit model and thermodynamic model are constructed in MATLAB Simulink and ANSYS Icepak, respectively. Both the equivalent circuit model and thermodynamic model are imported into the ANSYS TwinBuilder platform. The thermodynamic model is reduced to Reduced-Order Model(ROM) . The ROM can be connected with the equivalent circuit model to form the lithium-ion batteries thermoelectric coupling model [27]. The specific process of importing the thermodynamic model into the ANSYS TwinBuilder platform for order reduction is as follows. Transient CFD simulations are performed using ANSYS Icepak to generate response curves for lithium-ion batteries. The response curve is fed to ANSYS TwinBuilder ROM application to create the ROM of the batteries. It has the accuracy of CFD analysis with the simulation speed in seconds.

At the beginning of the simulation, the initialized simulation parameters include: current, initial SOC, initial temperature, simulation time, simulation step size, circuit model parameters and thermodynamic model parameters. Equivalent circuit model calculates the batteries terminal voltage and real-time heat generation power according to Formulas (3) and (4). It sends them to thermodynamic model. Thermodynamic model outputs the temperature of the batteries and updates the equivalent circuit model parameters. Equivalent circuit model calculates the new heating power according to the modified circuit model parameters. It will be used in the next calculation to model the coupled thermoelectric process with temperature correction.

4 | PARAMETERS IDENTIFICATION

In this section, the least squares algorithm is used to identify the parameters of the equivalent circuit model to obtain the initial parameters set. Secondly, based on the recursive least squares algorithm(RLS) and VFFRLS, the parameters of the equivalent circuit model are identified and updated online. It improves the accuracy of the model and enhances interactive feedback between the thermoelectric coupling model and the lithium-ion batteries. Finally, the parameters of the thermodynamic model are identified.

4.1 | Identification of equivalent circuit model initial parameters

The initial parameters of the equivalent circuit model include the corresponding relationship between open circuit voltage

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and SOC, resistance and capacitance [28]. Hybrid pulse power characteristic experiments (HPPC) are often used for initial parameters identification. The specific experimental procedure is as follows [29]. The batteries are placed in an incubator, charged to 100% SOC with constant current and constant voltage, and discharged with constant current after fully standing. Then they are discharged 10% SOC each time and the experiment is ended when the discharge cut-off voltage is reached. The voltage and current curves are measured at different SOC points (0–100%, interval 10%), different temperatures (10°C, 25°C, 35°C), and different charge and discharge currents (−2A, 2A, 6A, 14A). The equivalent circuit model parameters including R_o, R_e, R_d, C_e and C_d are obtained by least squares fitting. Linear interpolation is performed on three dimensions of SOC, temperature and charge/discharge current. Finally, the initial parameters of the equivalent circuit model are identified.

4.2 | Online identification of equivalent circuit model parameters

The actual operation of lithium-ion batteries is a highly nonlinear time varying system. Their operating parameters are affected by factors such as temperature and aging, so they are variable. The lithium-ion batteries thermoelectric coupling model based on digital twin needs to have the function of approaching the batteries entity in the whole life cycle. However, with the continuous operation of the batteries, the least squares parameter identification method has the problem that the model parameters do not match the actual situation. In order to solve the above problems and improve the accuracy of the equivalent circuit model, the online parameter identification algorithm is introduced to update the lithium-ion batteries thermoelectric coupling model parameters.

In this paper, the RLS algorithm is used to realize the online parameters identification of the equivalent circuit model. The RLS algorithm is a commonly used parameter estimation method. It enables online parameter estimation in changing environments. It is an effective method for systems with high real-time requirements. The principle of the algorithm can be described as follows [30].

$$\begin{cases} \theta(k) = \theta(k-1) + K(k)[y(k) - \psi^{\mathrm{T}}(k)\theta(k-1)] \\ K(k) = P(k-1)\psi(k)[\psi^{\mathrm{T}}(k)P(k-1)\psi(k) + 1]^{-1} \\ P(k) = [I - K(k)\psi^{\mathrm{T}}(k)]P(k-1) \end{cases}, \quad (7)$$

where $\theta(k)$ represents the estimated value of the parameter at time k; $y(k)$ represents the actual observed value at time k; $\Psi(k)$ represents the observation vector at time k; $\Psi^{\mathrm{T}}(k)$ represents the transposition of the observation vector at time k; $\Psi^{\mathrm{T}}(k)\theta(k$-1) represents the forecast value at time k; $y(k)$-$\Psi^{\mathrm{T}}(k)\theta(k$-1) represents the forecast error at time k; $P(k)$ represents the covariance matrix, which reflects the estimation accuracy of the algorithm; I represents the identity matrix; $K(k)$ represents the gain factor at time k, multiplying the gain factor and the prediction error to obtain the correction item; finally adding the correction term and $\theta(k$-1) to obtain the estimated value of the parameter at time k.

However, the covariance matrix is a decreasing positive definite matrix in the RLS algorithm. It decreases as the number of iterations increases. The parameter correction ability gradually weakens, and filter saturation occurs. The VFFRLS algorithm with forgetting factor λ is introduced to identify the parameters of the equivalent circuit model online. The VFFRLS algorithm is an online recursive least squares algorithm, which is mainly used for parameter identification. VFF stands for "Variable Forgetting Factor", that is, the variable forgetting factor. The forgetting factor is dynamically adjusted according to the dynamic changes of the system to balance the adaptability and robustness of the model. It can weaken the influence of old data and increase the effect of new observation data. The recursive formula of VFFRLS can be described as follows.

$$\begin{cases} \theta(k) = \theta(k-1) + K(k)[y(k) - \psi^{\mathrm{T}}(k)\theta(k-1)] \\ K(k) = P(k-1)\psi(k)[\psi^{\mathrm{T}}(k)P(k-1)\psi(k) + 1]^{-1} \\ P(k) = \frac{1}{\lambda}[I - K(k)\psi^{\mathrm{T}}(k)]P(k-1) \end{cases}. \quad (8)$$

The above VFFRLS is applied to the equivalent circuit model of lithium-ion batteries. Let the input be the current I_t, and the output be $y = E\text{-}U_o$. According to Kirchhoff law and Laplace transform, the frequency domain expression of the equivalent circuit model is:

$$y(s) = I_t(s)(R_o + \frac{R_e}{1 + R_eC_es} + \frac{R_d}{1 + R_dC_ds}). \quad (9)$$

Then the model transfer function can be obtained as follows.

$$G(s) = R_o + \frac{R_e}{1 + R_eC_es} + \frac{R_d}{1 + R_dC_ds}. \quad (10)$$

The transfer function is turned into a common denominator.

$$G(s) = \frac{R_os^2 + \frac{R_o\tau_e + R_o\tau_d + R_e\tau_d + R_d\tau_e}{\tau_e\tau_d}s}{s^2 + \frac{\tau_e + \tau_d}{\tau_e\tau_d}s + \frac{1}{\tau_e\tau_d}} + \frac{\frac{R_o + R_e + R_d}{\tau_e\tau_d}}{s^2 + \frac{\tau_e + \tau_d}{\tau_e\tau_d}s + \frac{1}{\tau_e\tau_d}}. \quad (11)$$

The bilinear transformation method is used to discretize the Formula (11). Let $s = (2/T)(1\text{-}z^{-1})/(1+z^{-1})$, the discrete transfer function can be obtained as follows.

$$G(z^{-1}) = \frac{\beta_0 + \beta_1z^{-1} + \beta_2z^{-2}}{1 + \alpha_1z^{-1} + \alpha_2z^{-2}}, \quad (12)$$

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where $\alpha_1, \alpha_2, \beta_0, \beta_1$ and β_2 are undetermined coefficients. Thus, the difference equation after the frequency domain expression discretization can be obtained as:

$$y(k) = -\alpha_1 y(k-1) - \alpha_2 y(k-2) + \beta_0 I_t(k) + \beta_1 I_t(k-1) + \beta_2 I_t(k-2) \quad (13)$$

Let $\theta = [\alpha_1, \alpha_2, \beta_0, \beta_1, \beta_2]$, $\Psi(k) = [-y(k\text{-}1)\ -y(k\text{-}2)\ I_t(k)\ I_t(k\text{-}1)\ I_t(k\text{-}2)]$.

Formula (13) can be converted to the form of least square $y(k) = \Psi^T(k)\theta + e(k)$, and solved using the VFFRLS algorithm. Let $z^{-1} = (2/T\text{-}s)/(2/T+s)$. Bilinear inverse transformation is performed on the discrete transfer function.

$$G(s) = \frac{T^2(\beta_0 - \beta_1 + \beta_2)s^2 + 4T(\beta_0 - \beta_2) + 4(\beta_0 + \beta_1 + \beta_2)}{T^2(1 - \alpha_1 + \alpha_2)s^2 + 4T(1 - \alpha_2)s + 4(1 + \alpha_1 + \alpha_2)}. \quad (14)$$

Formula (14) is simplified according to Formula (11).

$$G(s) = \frac{\frac{(\beta_0 - \beta_1 + \beta_2)}{1 - \alpha_1 + \alpha_2}s^2 + \frac{4(\beta_0 - \beta_2)}{T(1 - \alpha_1 + \alpha_2)}s + \frac{4(\beta_0 + \beta_1 + \beta_2)}{T^2(1 - \alpha_1 + \alpha_2)}}{s^2 + \frac{4(1 - \alpha_2)}{T(1 - \alpha_1 + \alpha_2)}s + \frac{4(1 + \alpha_1 + \alpha_2)}{T^2(1 - \alpha_1 + \alpha_2)}}. \quad (15)$$

Authors compare Formula (15) and Formula (11), and use the coefficient correspondence method to obtain the equivalent circuit model parameters calculation formula.

$$\begin{cases} R_o = \dfrac{\beta_0 - \beta_1 + \beta_2}{1 - \alpha_1 + \alpha_2} \\ \tau_e \tau_d = \dfrac{T^2(1 - \alpha_1 + \alpha_2)}{4(1 + \alpha_1 + \alpha_2)} \\ \tau_e + \tau_d = \dfrac{T(1 - \alpha_2)}{1 + \alpha_1 + \alpha_2} \\ R_o + R_e + R_d = \dfrac{\beta_0 + \beta_1 + \beta_2}{1 + \alpha_1 + \alpha_2} \\ R_o(\tau_e + \tau_d) + R_e(\tau_e + \tau_d) = \dfrac{T(\beta_0 - \beta_2)}{1 + \alpha_1 + \alpha_2} \end{cases} \quad (16)$$

The coefficients $\alpha_1, \alpha_2, \beta_0, \beta_1$ and β_2 in the expression can be solved by VFFRLS recursive Formula (8). Then the parameters of the equivalent circuit model can be obtained by solving Formula (16). When a set of new data is obtained at time k+1, new model parameters at time k+1 can be obtained according to the above analysis. Every time a set of new data is obtained, recursion is performed to realize online identification of model parameters. The concept of twinning rate is introduced to represent the above-mentioned model update speed. It is defined as the update time of the digital twin model and the twinning rate value can be set according to the actual update requirements of the model. This method fully considers the impact of changes in lithium-ion batteries thermoelectric model operating parameters. It makes full use of interactive simulation among physical devices, sensing devices, and operational data. In this way, the digital twin model can enhance the high-fidelity virtual-real mapping between the physical devices and the digital twin models. The specific implementation process is shown in the Figure 5.

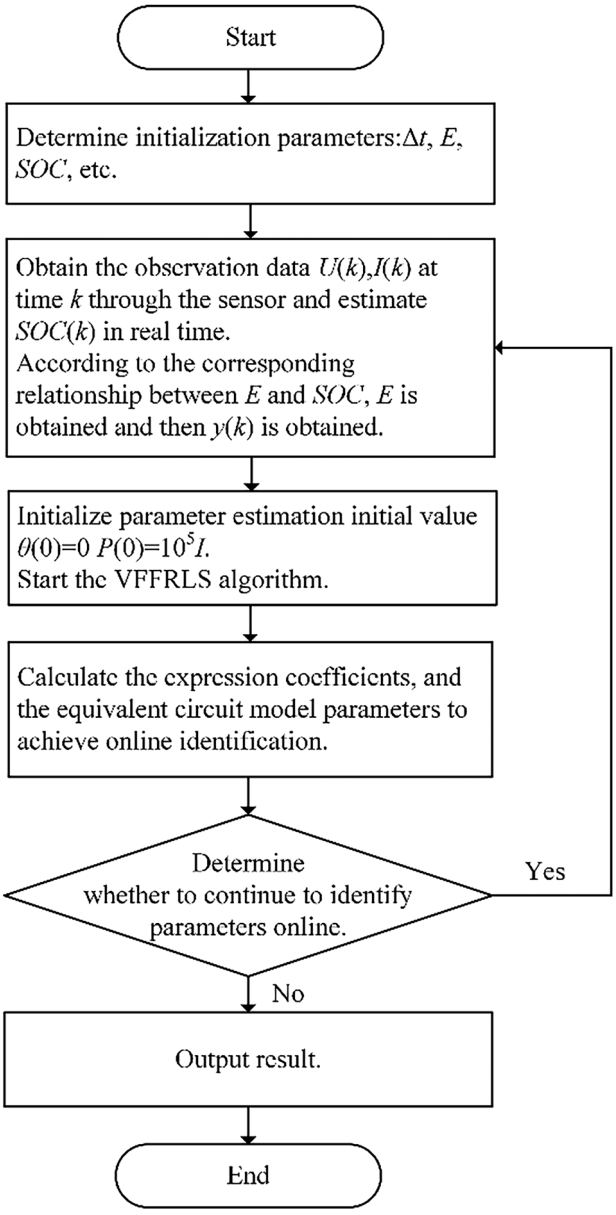

FIGURE 5 Algorithm flow chart.

4.3 | Thermodynamic model parameters identification

According to Formula (6), determining the parameters value of ρ, C, λ_x, λ_y and λ_z can obtain the temperature of monitoring points along with the running time [26].

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4.3.1 | Average density ρ

Due to complex internal structures of batteries, it is difficult to express them in detail when modeling. Therefore, the average density ρ is used to approximate the calculation.

$$\rho = \frac{\sum m_i}{\sum V_i}, \tag{17}$$

where i represents the battery cell number; $\sum m_i$ represents the mass sum of the internal materials; $\sum V_i$ represents the volume sum of the internal materials.

4.3.2 | Average specific heat capacity C

The average specific heat capacity calculation method is to measure the specific heat capacity of each material inside the battery, and then use the mass weighted method to calculate.

$$C = \frac{\sum C_i m_i}{\sum m_i}, \tag{18}$$

where C_i represents the specific heat capacity of each material inside the battery.

4.3.3 | Thermal conductivity $\lambda_x, \lambda_y, \lambda_z$

The internal composition of the battery is complex, and the difference in thermal conductivity of materials makes the thermal conductivity calculation difficult. Assuming that the battery plate is perpendicular to the x axis, heat transfer along the y and z axis is regarded as being transferred between plates in parallel, and heat transfer along the x axis is regarded as being transferred between plates in series. The thermal conductivity can be calculated by the following formula.

$$\lambda_x = \frac{l}{\sum \frac{dx_i}{\lambda_i}} = \frac{l}{\frac{dx_p}{\lambda_p} + \frac{dx_n}{\lambda_n} + \frac{dx_j}{\lambda_j}}, \tag{19}$$

$$\lambda_y = \sum \frac{\lambda_i dy_i}{b} = \frac{\lambda_p dy_p + \lambda_n dy_n + \lambda_j dy_j}{b}, \tag{20}$$

$$\lambda_z = \sum \frac{\lambda_i dz_i}{h} = \frac{\lambda_p dz_p + \lambda_n dz_n + \lambda_j dz_j}{h}, \tag{21}$$

where λ_p, λ_n and λ_j, respectively, represent the thermal conductivity of the positive electrode, negative electrode and separator inside the battery; dx_p dx_n dx_j, dy_p dy_n dy_j and dz_p dz_n dz_j represent the thicknesses of the positive electrode, negative electrode and separator along the x, y and z axis directions, respectively; l, b and h, respectively, represent the length, width and height of the battery along the x, y and z axes.

4.3.4 | Boundary conditions

Boundary condition 1: the temperature of batteries at the initial moment:

$$T(x, y, z, 0) = T_0. \tag{22}$$

Boundary Condition 2: Newton Law of Cooling:

$$-\lambda_x \frac{\partial T}{\partial x} = \alpha(T - T_\infty), x = 0, l, \tag{23}$$

$$-\lambda_y \frac{\partial T}{\partial y} = \alpha(T - T_\infty), y = 0, b, \tag{24}$$

$$-\lambda_z \frac{\partial T}{\partial z} = \alpha(T - T_\infty), z = 0, h, \tag{25}$$

where T_0 represents the initial temperature; α represents the convective heat transfer coefficient between the surrounding environment and batteries; T_∞ represents the ambient temperature.

5 | RESULTS AND DISCUSSION

This paper takes a commercial lithium-ion battery cell and battery module as the research object to carry out experimental verification. The rated capacity of the battery cell is 2Ah. The battery module is composed of 15 battery cells, which is arranged in the 3×5 structure. The rated capacity of the battery module is 30Ah. The three-dimensional structure of the battery module is shown in Figure 3 above. For the facilitate subsequent description, the battery module is numbered as shown in Figure 6.

To simplify the model, the following assumptions are made:

1. the internal materials are isotropic;
2. the density and specific heat capacity of the constituent materials remain unchanged from the influence of the external environment;
3. the thermal conductivity remains constant in all directions and positions;
4. the internal current density is equal at each position when working;
5. only heat conduction and heat transfer are considered inside batteries.

Considering the key factors affecting the temperature distribution, the lithium-ion battery cell is simplified to be composed of positive electrode material, negative electrode material, shell, positive lug and negative lug. After searching the manual and related literature, the thermodynamic parameters are shown in Table 1.

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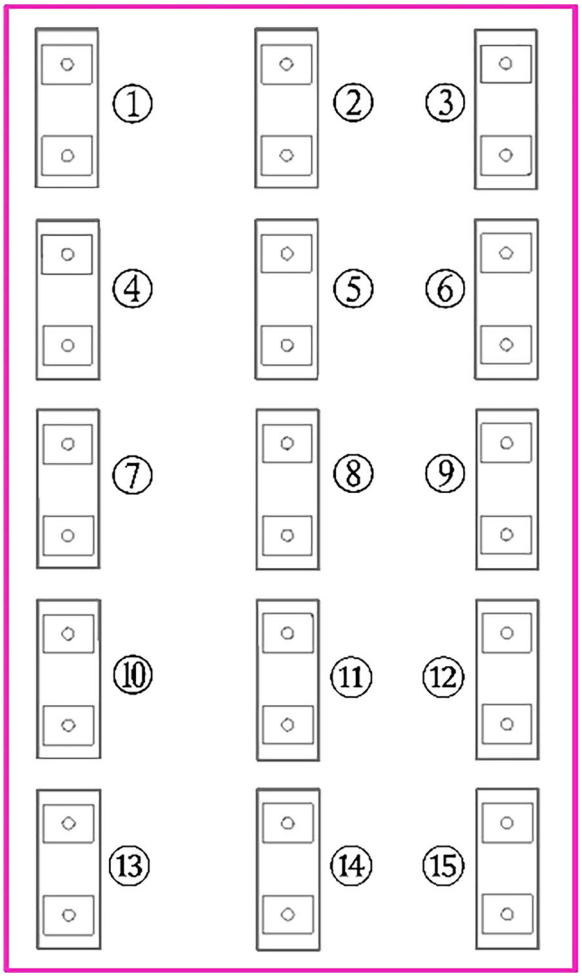

FIGURE 6 Arrangement and numbering of the battery module.

TABLE 1 Thermodynamic parameters.

Parameters	Density (kg/m^3)	Thermal conductivity (W/(m·K))
Positive electrode material	2840	3.9
Negative electrode material	1617	3.3
Shell	7817	14.4
Positive lug	2700	240
Negative lug	8933	387.6

According to Formulas (17)—(25), it can be calculated that average density $\rho = 2179$ kg/m^3, the average specific heat capacity $C = 1000$J(kg·K), and the thermal conductivities along x, y, z directions are $\lambda_x = 3$ W/(m·K), $\lambda_y = 30$ W/(m·K), $\lambda_z = 30$ W/(m·K).

In order to verify the calculation efficiency and accuracy of the digital twin model, this paper conducts simulation analysis from three aspects: whether to use reduced order model, RLS and VFFRLS algorithm voltage prediction accuracy, and verification of current discharge at different rates.

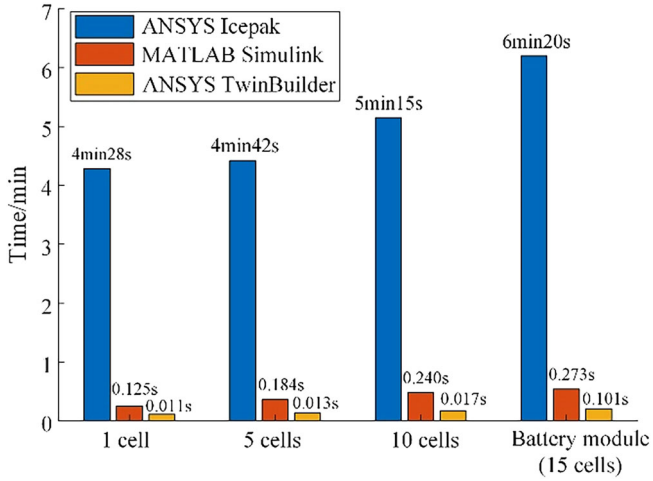

FIGURE 7 Simulation time comparison of different battery types in ANSYS Icepak and ANSYS TwinBuilder.

5.1 | Whether to use reduced order model

At the ambient temperature of 20°C, firstly, four battery types including 1 cell, 5 cells, 10 cells and battery module (15 cells) are selected for modeling and temperature field simulation in ANSYS Icepak. A step response file is also generated. Then, ANSYS TwinBuilder generates an LTI ROM reduced order model based on the above step response file. Finally, the reduced order model is used to simulate the temperature field. Considering that the simulation time of the three-dimensional high-precision thermodynamic model of lithium-ion battery is longer than that of the reduced-order model established in ANSYS TwinBuilder, the mathematical mechanism model of lithium-ion battery mentioned in the Section 1 introduction can also be regarded as a reduced-order model. Based on the mathematical principles of thermal transfer and thermal generation, authors use MATLAB Simulink to construct a mathematical mechanism thermodynamic model of lithium-ion batteries. In order to verify the computational efficiency of the reduced-order model established in ANSYS TwinBuilder, the author compared the simulation time of the three models. The simulation time of different battery types in ANSYS Icepak, MATLAB Simulink and ANSYS TwinBuilder is shown in Figure 7.

It can be seen from Figure 7 that after reducing the order of the thermodynamic model based on ANSYS TwinBuilder, the battery simulation time is reduced from minutes to seconds. Compared with the three-dimensional high-precision model, the simulation time reduction reaches 99%, and the calculation efficiency is significantly improved. As the simulation scale expanded from 1 cell to the battery module (15 cells), the simulation time of ANSYS Icepak increases by nearly 2 min, but the simulation time of ANSYS TwinBuilder and MATLAB Simulink remains at the second level. The simulation time of the mechanism model built in MATLAB Simulink is longer than that of the reduced-order model built in ANSYS TwinBuilder.

The three-dimensional high-precision model can simply and fully consider the impact of environment and operating state

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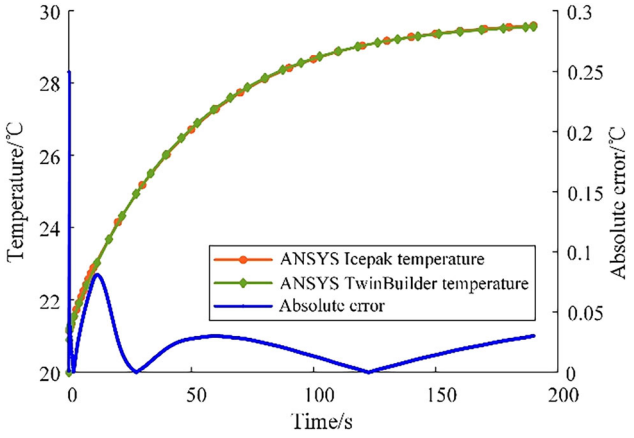

FIGURE 8 Simulation temperature and error of 1 cell in ANSYS Icepak and ANSYS TwinBuilder.

changes on model parameters. It is obvious that the simulation accuracy of the model established in ANSYS Icepak is the highest. At the same time, according to Figure 7, the simulation efficiency of the reduced-order model established in ANSYS TwinBuilder is the highest. Therefore, 1 cell is selected for comparative analysis in the simulation temperature changes of ANSYS Icepak and ANSYS TwinBuilder to prove the simulation accuracy of the reduced-order model. The comparison results are shown in Figure 8.

It can be seen from Figure 8 that the temperature simulation results based on ANSYS TwinBuilder are almost the same as those of ANSYS Icepak. There is a certain error at the beginning of the simulation, and as the simulation time prolongs, the error gradually decreases and remains within 0.1°C. Therefore, the reduced order model not only has the CFD simulation accuracy but also greatly improves the simulation efficiency. It realizes multi-physics real time simulation and provides an effective method for the construction of thermoelectric coupling model of lithium-ion batteries based on digital twin.

5.2 | RLS and VFFRLS algorithm voltage prediction accuracy

At the ambient temperature of 20°C, the discharge experiment is carried out for the battery module. The voltage data of each battery cell is obtained. Considering that the center temperature of the battery module is high and the risk probability is high, this paper selects the center battery cell ⑧ of the battery module for algorithm verification. The obtained battery cell ⑧ voltage and current data is analyzed. The RLS algorithm and VFFRLS algorithm are used to identify the parameters of the equivalent circuit model online. The twinning rate value is set to 1 s. The simulation voltage is calculated by using the identification results, and compared with the experimental voltage to verify the identification accuracy. The comparison results are shown in Figure 9.

It can be seen from the figure that the simulated voltage obtained from the identification results of the RLS and VFFRLS

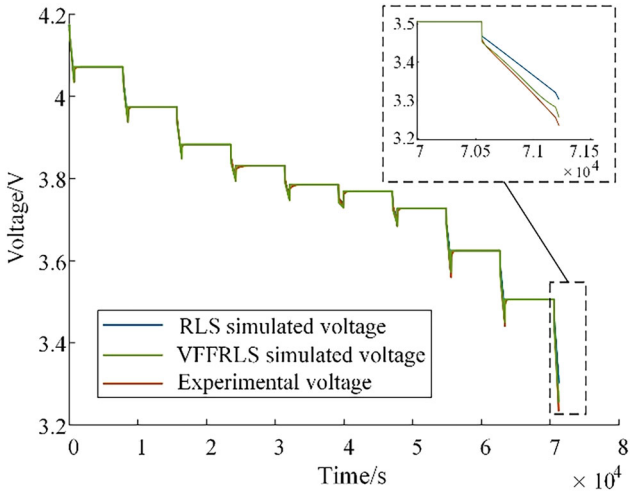

FIGURE 9 The actual voltage and simulated voltage calculated based on the RLS and VFFRLS algorithm.

TABLE 2 Comparison of error evaluation indicators.

	RLS	VFFRLS
M_{AE}	0.0015	0.0009
R_{MSE}	0.0057	0.0029

algorithms almost completely coincides with the actual voltage results. But the VFFRLS algorithm is more accurate at the end of the simulation. In order to compare the parameter identification accuracy of the two algorithms more directly, the data in Figure 9 Is extracted. The error evaluation index in Formula (26) is used for analysis [30].

$$\begin{cases} M_{AE} = \frac{1}{N}\sum_{k=1}^{N}\left(\left|U_k - \hat{U}_k\right|\right) \\ R_{MSE} = \sqrt{\frac{1}{N}\sum_{k=1}^{N}\left(U_k - \hat{U}_k\right)^2} \end{cases}. \tag{26}$$

In the formula: M_{AE} is the average absolute error; R_{MSE} is the root mean square error; U_k is the actual value of the terminal voltage at time k; $\hat{U}_k$ is the voltage simulation value at time k; N is the number of experimental data.

The calculated evaluation results are shown in Table 2.

It can be seen from the table that the average absolute error and root mean square error of the VFFRLS algorithm are smaller than RLS. Therefore, the accuracy of VFFRLS algorithm is higher. It realizes the parameters update of the model and improves the accuracy of prediction results.

5.3 | Verification of current discharge at different rates

At the ambient temperature of 20°C, 1C, 2C, and 3C discharge experiments were carried out for the battery module. The

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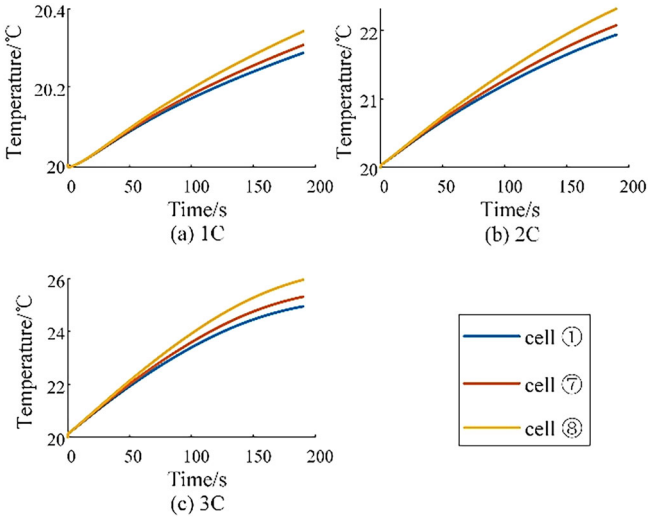

FIGURE 10 Simulation temperature of battery module in 1C to 3C discharge experiment at 20°C.

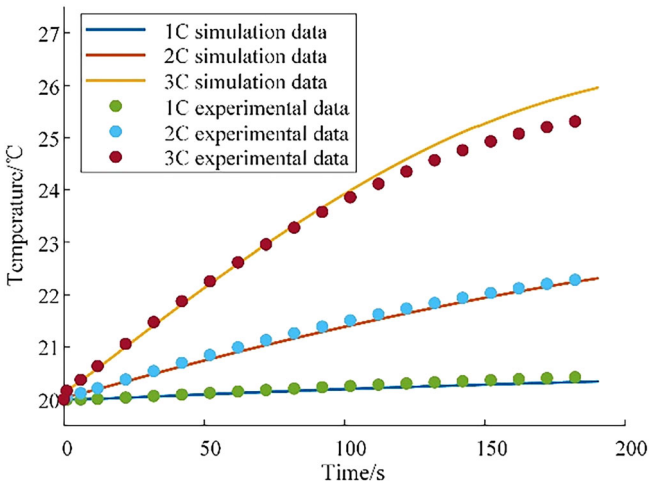

FIGURE 11 1C to 3C discharge experimental temperature and simulation temperature of cell ⑧.

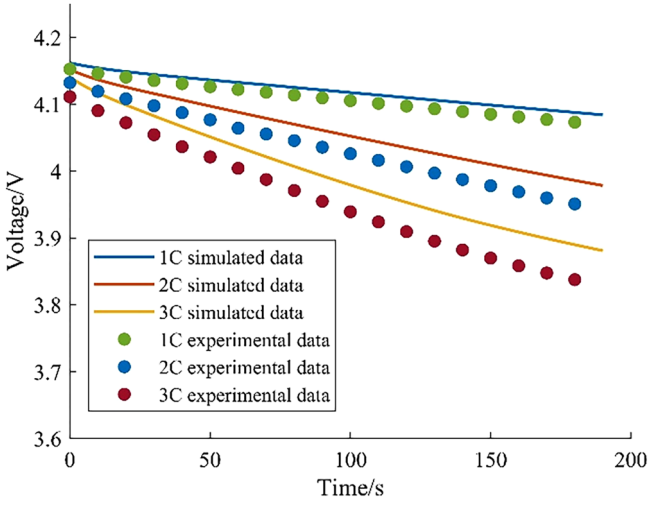

FIGURE 12 1C to 3C discharge experimental voltage and simulation voltage of cell ⑧.

temperature and voltage changes of the battery cells were recorded. At the same time, the constructed lithium-ion batteries thermoelectric coupling model based on digital twin is used to carry out simulation analysis under the same experimental conditions to verify the accuracy of the model.

The temperature of cells in the battery module is analyzed. Considering that the center temperature of the battery module is high and the risk probability is high, the center cell ⑧, edge cell ⑦ and corner cell ① of the module are selected as samples. The selection principles of cells can be summarized as follows. It can be seen from Figures 3 and 6 that the battery module has a centrally symmetrical structure. This paper focuses on the simulation analysis of a single battery module, ignoring the mutual influence between modules. It is assumed that the internal material is isotropic, and the current density at each position inside is equal during operation in the paper. It can be considered that the temperature changes of corner cells ① ③ ⑬ ⑮ are almost the same during the charging and discharging process. Therefore, the author selected corner cell ① for verification. The selection principles of edge cells are the same as that of corner cells. The temperature changes obtained are shown in Figure 10. It can be seen from the figure that the center temperature of the battery module is high and the corner temperature is low, and as the battery discharge rate increases, the battery temperature increases. Therefore, it is particularly important to monitor the temperature change of lithium-ion batteries. Reasonable and effective decisions can be made according to the temperature to prevent over-temperature operation.

Considering the high temperature at the center of the battery module, the probability of accidents is high. The central battery cell ⑧ of the battery module is selected for further temperature and voltage verification. Under the 1C to 3C discharge experiment, the experimental temperature and simulation temperature of the center cell ⑧ is shown in Figure 11.

From the temperature comparison results in the Figure 11, It can be seen that the temperature of the cell is rising during the discharge process. Under 1C, 2C, and 3C discharge rates, the temperature rises rapidly at the initial stage of discharge, and relatively flat in the later stage. As the discharge rate increases, the steady-state temperature of the cell also increases. Compared with the experimental results, it can be seen that the simulation temperature error of the discharge process is within 1°C, which verifies the accuracy of the model.

Under the 1C to 3C discharge experiment, the experimental voltage and simulation voltage of the center battery ⑧ is shown in Figure 12.

From the voltage comparison results in the Figure 12, It can be seen that the voltage of the cell is droping during the discharge process. Compared with the experimental results, it can be seen that as the rate increases, the relative error at the end of the discharge gradually increases. The error at the end of 3C discharge reaches 1.2%, but the error is controlled within 0.35% at the low rate 1C discharge stage, which verifies the

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accuracy of the method proposed in this paper in engineering applications.

6 | CONCLUSION

This paper proposes a construction method of lithium-ion batteries thermoelectric coupling model based on digital twin. Through simulation analysis, the calculation efficiency and accuracy of the model are verified. The main conclusions are:

1. The digital twin structure system is proposed. Considering the coupling between the equivalent circuit model and the thermodynamic model of the lithium-ion batteries, the thermoelectric coupling model based on digital twin is established on ANSYS TwinBuilder. It can evaluate operating status more efficiently and accurately so as to reduce the probability of fire, explosion and other safety accidents. It has reference significance for the development of batteries digital twin technology.
2. Based on ANSYS TwinBuilder, the order of thermodynamic model is reduced. The simulation accuracy is high and the simulation time is reduced to the second level, which improves the simulation efficiency. It can guarantee the real-time simulation of the model, and provides an effective method for the simulation, design and optimization management of lithium-ion batteries.
3. The VFFRLS algorithm is used to realize the online identification of the equivalent circuit model parameters in the lithium-ion battery thermoelectric coupling model. The problem of updating the model parameters is solved. It enhances the interactive feedback between the physical devices and virtual models and improves the real time mapping ability of the model.

AUTHOR CONTRIBUTIONS

Lingchong Liu: Writing—review & editing. Shufeng Dong: Writing—review & editing. Bin Nan: Writing—review & editing. Kaicheng Lu: Writing—review & editing.

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CONFLICT OF INTEREST STATEMENT

The authors declare no conflict of interest.

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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