

## Article

# Control Volume Free Element Method for Simulating Thermal Runaway of Lithium-Ion Battery

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## Abstract

The safety of lithium-ion batteries is a critical concern, and this paper introduces a novel simulation approach for thermal runaway using the control volume free element method (CVFrEM). This method uniquely integrates the geometric adaptability of mesh-free techniques with the local conservation properties inherent to the finite volume method. The governing equations for heat generation and heat transfer within the battery are discretized through the CVFrEM framework, thereby ensuring strict energy conservation at the local control volume level. To accurately capture the nonlinear Arrhenius kinetics governing the internal reactions, a coupled solution algorithm is implemented within the CVFrEM formulation. The proposed method is rigorously validated against both experimental data and reference results, confirming its predictive accuracy and exceptional numerical stability, particularly in scenarios involving steep thermal gradients. Overall, this work offers a promising numerical tool for predicting thermal runaway events and provides valuable insights for advancing battery safety simulations.

**Keywords:** control volume free element method; mesh-free method; lithium-ion battery; thermal runaway; 3D simulation

## 1. Introduction

Lithium-ion batteries (LIBs) have become the dominant energy storage technology for electric vertical takeoff and landing aircraft (eVTOL) due to their high energy density, long cycle life, and low self-discharge rates [1]. However, as the demand for higher energy density increases, charge/discharge rates increase and operating environments become harsher, safety concerns regarding thermal runaway have become a critical bottleneck restricting the further development of LIBs [2,3]. Thermal runaway is a catastrophic chain reaction characterized by a rapid, uncontrollable rise in temperature, often leading to fire, explosion, and the release of toxic gases [4,5]. To mitigate these risks, accurate prediction and simulation of the thermal runaway process are essential for the design of effective battery thermal management systems and safety protection strategies.

The simulation of thermal runaway necessitates a comprehensive understanding of the intricate electrochemical and thermodynamic phenomena occurring inside a battery cell [6]. This process is typically initiated by abusive conditions—mechanical, electrical, or thermal—that set off a cascade of exothermic reactions. Common abuse scenarios include nail penetration, overcharging, and external heating. The chain of events generally begins



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with the breakdown of the solid electrolyte interphase (SEI) layer, which subsequently triggers reactions between the anode and the electrolyte and between the cathode and the electrolyte, as well as electrolyte decomposition [7,8].

Mathematically, these processes are described by coupled partial/ordinary differential equations governing heat transfer and species conservation. The heat generation rate is typically modeled using Arrhenius kinetics, making the system highly nonlinear and stiff. While 1D and 2D models have been widely used to study cell-level behaviors [9,10], 3D simulations are increasingly necessary to capture the spatial heterogeneity of temperature fields and the propagation of thermal runaway in battery modules [11].

The numerical solution of the governing equations for thermal runaway is challenging due to the steep temperature gradients, the coupling of heat transfer, electric fields, and chemical reactions. The dominant numerical methods employed in commercial software (such as ANSYS Fluent or COMSOL Multiphysics) are the finite volume method (FVM) and the finite element method (FEM) [11].

FVM discretizes the computational domain into control volumes and applies the integral form of the governing equations, ensuring that fluxes across control volume boundaries are balanced [12]. This approach is robust for problems involving convection-dominated heat transfer and complex boundary conditions. FVM is widely favored in computational fluid dynamics (CFD) and heat transfer for its strict conservation of mass and energy and is particularly effective in simulating thermal-abuse scenarios in lithium-ion batteries [13]. However, FVM can struggle with accurately capturing sharp thermal fronts and steep gradients, which are characteristic of thermal runaway events.

FEM is also widely used in simulating the thermal behavior of lithium-ion batteries. It offers high accuracy for complex geometries and boundary conditions, making it suitable for detailed cell-level thermal analysis [14]. FEM uses variational principles to minimize the residuals of the governing equations, leading to a system of algebraic equations that can be solved numerically. However, FEM is much more expensive than FVM because it requires domain integration and uses coefficient matrices with larger bandwidths.

Furthermore, both FVM and FEM are mesh-dependent methods. Therefore, the quality of the mesh will directly affect the accuracy. Moreover, for highly nonlinear problems, distorted elements can cause divergence during iteration. To overcome mesh distortion issues, researchers have explored mesh-free methods [15–17], such as smoothed particle hydrodynamics (SPH) [18] and the element-free Galerkin (EFG) method [19]. Lin and Wang proposed a space–time mesh-free method to simulate the heat transfer in porous media such as batteries [20]. Susuki et al. used an interface-modified reproducing kernel particle method to simulate the thermal runaway of lithium-ion batteries [21]. Their work shows the great potential of mesh-free methods in simulating thermal runaway. However, these methods have difficulties in enforcing boundary conditions [22] and local conservation laws, which are critical for accurately capturing the energy balance during thermal runaway events.

The control volume free element method (CVFrEM) has emerged as a promising numerical technique. CVFrEM combines the geometric flexibility of mesh-free methods with the local conservation properties of FVM [23]. Additionally, the isoparametric elements used in FEM and their shape functions are used to calculate field variables and their gradients [24]. Unlike traditional FEM/FVM, CVFrEM does not require a predefined mesh topology; instead, it uses scattered nodes to construct local elements, with a control volume defined around each node to ensure the conservation of mass, momentum, and energy. Because of the delta property of the shape functions, the boundary conditions can be easily enforced [25], which is particularly advantageous for simulating the complex boundary conditions and multi-physical problems.

In this paper, we propose a novel numerical framework based on CVFrEM to simulate the thermal runaway process of lithium-ion batteries. The primary contributions of this work are as follows:

- **Formulation:** We derive the discrete governing equations for battery heat generation and heat transfer using the CVFrEM scheme, ensuring energy conservation at the local control volume level.
- **Coupling:** We implement a coupled algorithm to handle the nonlinear Arrhenius kinetics of the chemical reactions within the CVFrEM framework.
- **Validation:** The proposed method is validated against experimental data and reference results, demonstrating its accuracy and superior stability in handling steep thermal gradients.

This study aims to provide a robust and meshfree numerical tool for predicting battery thermal runaway, offering new insights into battery safety simulation.

## 2. Materials and Methods

### 2.1. Heat Transfer in Battery

The general heat transfer equation in solids can be expressed as:

$$\rho C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x_i} \left( k_{ij} \frac{\partial T}{\partial x_j} \right) + Q \quad (1)$$

where  $\rho$  is the density,  $C_p$  is the specific heat capacity,  $T$  is the temperature,  $t$  is time,  $k_{ij}$  is the thermal conductivity tensor, and  $Q$  represents the volumetric heat generation rate due to chemical reactions. The repeated indices  $i$  and  $j$  imply summation over the spatial dimensions, following Einstein notation. For isotropic materials, such as battery shells, the thermal conductivity tensor simplifies to a scalar  $k_{ij} = k\delta_{ij}$ , where  $\delta_{ij}$  is the Kronecker delta. However, the battery jelly is a composite material composed of the anode, cathode, separator, and electrolyte. As a result, the thermal conductivity of the jelly is anisotropic, and the thermal conductivity tensor can be expressed as:

$$k'_{ij} = \begin{pmatrix} k'_{x'x'} & 0 & 0 \\ 0 & k'_{y'y'} & 0 \\ 0 & 0 & k'_{z'z'} \end{pmatrix} \quad (2)$$

where  $k'_{x'x'}$ ,  $k'_{y'y'}$ , and  $k'_{z'z'}$  are the thermal conductivities along the principal axes of the jelly, which can be determined experimentally or through homogenization techniques. The conductivity tensor can be transformed to the global coordinate system using the rotation matrix  $\mathbf{R}$ :

$$k_{ij}^{\text{global}} = R_{ik} k'_{kl} R_{jl} \quad (3)$$

where  $R_{ik}$  is the rotation matrix that aligns the local principal axes of the jelly with the global coordinate system, and  $k'_{kl}$  is the thermal conductivity tensor in the local coordinate system. Since the local and global coordinate systems are related by a rigid-body rotation, the rotation matrix is orthogonal and satisfies  $R^T R = I$ . The rotation matrix can be constructed based on the orientation of the jelly layers and the geometry of the battery cell. Using the tensor transformation, the rotation matrix can be defined as:

$$R_{ij} = \begin{pmatrix} \partial x' / \partial x & \partial x' / \partial y & \partial x' / \partial z \\ \partial y' / \partial x & \partial y' / \partial y & \partial y' / \partial z \\ \partial z' / \partial x & \partial z' / \partial y & \partial z' / \partial z \end{pmatrix} \quad (4)$$

where  $x'$ ,  $y'$ , and  $z'$  denote the local coordinates of the jelly roll, and  $x$ ,  $y$ , and  $z$  denote the global coordinates of the battery cell. For the blade-type jelly roll, the local coordinate system is typically aligned with the blade geometry, with the  $x'$ -axis along the length, the  $y'$ -axis along the width, and the  $z'$ -axis along the thickness. For the rolled-type jelly roll, the local coordinate system is typically aligned with the winding structure, with the  $x'$ -axis along the radial direction, the  $y'$ -axis along the circumferential direction, and the  $z'$ -axis along the axial direction.

The jelly is a layered structure, and the thermal conductivity along the thickness direction is much smaller than that along the in-plane direction. The conductivity along the thickness direction can be calculated using the series model [8]:

$$k_{\text{thickness}} = \sum_{\alpha} d_{\alpha} \left( \sum_{\alpha} \frac{d_{\alpha}}{k_{\alpha}} \right)^{-1} \quad (5)$$

where  $d_{\alpha}$  and  $k_{\alpha}$  are the thickness and thermal conductivity of the  $\alpha$ -th layer, respectively. The conductivity along the in-plane direction, by contrast, can be calculated using the parallel model:

$$k_{\text{in-plane}} = \frac{\sum_{\alpha} d_{\alpha} k_{\alpha}}{\sum_{\alpha} d_{\alpha}} \quad (6)$$

At the battery boundary, heat transfer can be modeled using convective and radiative boundary conditions. The convective heat flux can be expressed as:

$$q_{\text{conv}} = -k_{ij} \frac{\partial T}{\partial x_j} n_i = h(T_{\text{surface}} - T_{\infty}) \quad (7)$$

where  $h$  is the convective heat transfer coefficient,  $T_{\text{surface}}$  is the temperature at the battery surface, and  $T_{\infty}$  is the ambient temperature. The radiative heat flux can be expressed as:

$$q_{\text{rad}} = -k_{ij} \frac{\partial T}{\partial x_j} n_i = \epsilon \sigma (T_{\text{surface}}^4 - T_{\infty}^4) \quad (8)$$

where  $\epsilon$  is the emissivity of the battery surface, and  $\sigma$  is the Stefan–Boltzmann constant.

For the battery surface, there is usually a thin shell or casing, which can be simplified as a thermal resistance layer. The heat flux through the shell can be expressed as:

$$q_{\text{shell}} = \frac{T_{\text{jelly}} - T_{\text{surface}}}{R_{\text{shell}}} \quad (9)$$

where  $T_{\text{jelly}}$  is the temperature of the jelly, and  $R_{\text{shell}}$  is the thermal resistance of the shell, which can be calculated as:

$$R_{\text{shell}} = \frac{d_{\text{shell}}}{k_{\text{shell}}} \quad (10)$$

For metal shells, the thermal conductivity is usually high, and the thermal resistance can be neglected. However, because the shell and the jelly are usually not in perfect contact, there is usually a thermal contact resistance between them, which can be expressed as:

$$q_{\text{contact}} = \frac{T_{\text{jelly}} - T_{\text{surface}}}{R_{\text{contact}}} \quad (11)$$

where  $R_{\text{contact}}$  is the thermal contact resistance, which can be determined experimentally or through empirical correlations.

## 2.2. Reactions and Heat Source

The total heat generation rate  $Q$  in the battery can be expressed as the sum of the transformation of electric energy ( $Q_{\text{ele}}$ ) and the heat generated by the reactions ( $Q_{\text{R}}$ ):

$$Q = Q_{\text{ele}} + Q_{\text{R}} \quad (12)$$

Five main reactions contribute to heat generation during thermal runaway: SEI decomposition; reaction of intercalated Li with the solvent at the anode; separator melting; and decomposition of the cathode and electrolyte. The rate of each reaction can be calculated using Arrhenius kinetics, which can be expressed as:

$$R_x = A_x c_x^{n_{x,1}} (1 - c_x)^{n_{x,2}} \exp\left(-\frac{E_x}{RT}\right) g_x, T > T_{\text{onset},x} \quad (13)$$

where  $A_x$  is the frequency factor for the reaction,  $c_x$  is the concentration of the reactant,  $n_{x,1}$  and  $n_{x,2}$  are the reaction orders,  $E_x$  is the activation energy,  $R = 8.314 \text{ J}/(\text{mol K})$  is the universal gas constant, and  $g_x$  is a correction term that represents the effects of other factors. The subscript  $x$  denotes the specific reaction (SEI, anode, separator, cathode, or electrolyte), and  $T_{\text{onset},x}$  is the onset temperature for each reaction. The concentration of the reactant  $c_x$  can be calculated using the following equation:

$$\frac{\partial c_x}{\partial t} = -R_x \quad (14)$$

while the heat generation rate of each reaction can be expressed as:

$$Q_x = R_x W_x \Delta H_x V_r \quad (15)$$

where  $W_x$  is the specific content of the reactant,  $\Delta H_x$  is the enthalpy change of the reaction, and  $V_r$  is the volume ratio of active material.

Previous work has shown that SEI can be regenerated through the Li-solvent reaction at the anode [7,26]. The rate of SEI regeneration can be expressed as:

$$R_{\text{SEI,regen}} = -K_r R_{\text{anode}} \quad (16)$$

where  $K_r$  is the regeneration coefficient, which can be determined experimentally. For the Li-solvent reaction at the anode, the correction term  $g_{\text{anode}}$  can be expressed as:

$$g_{\text{anode}} = \exp\left(-\frac{C_{\text{SEI}}}{C_{\text{SEI},0}^{\text{ref}}}\right) \quad (17)$$

According to Equation (14), the reaction rate is an exponential function of temperature. When the temperature increases, the reaction rate also increases exponentially, leading to a higher heat-generation rate and potentially triggering thermal runaway. Unlike the reaction onset temperature, the runaway trigger temperature  $T_{\text{tr}}$  is the temperature at which thermal runaway actually occurs. It is typically higher than the onset temperature and depends on the specific conditions of the battery system.

When thermal runaway occurs, the separator melts and the anode and cathode come into contact, leading to a short circuit. The heat generation rate of the short circuit can be expressed as [9,27]:

$$Q_{\text{ele}} = \frac{1}{\Delta\tau} \left( \Delta H_{\text{ele}} - \int_0^t Q_{\text{ele}}(t) dt \right) \quad (18)$$

where  $\Delta H_{ele}$  is the enthalpy change associated with the electric energy, and  $\Delta \tau$  is the time interval over which the short circuit occurs.

### 2.3. Numerical Methods

The control volume free element method is a numerical technique that combines the advantages of FVM and FEM. In CVFrEM, the computational domain is discretized into a set of scattered nodes, and local collocated elements are constructed around each node, as shown in Figure 1. Inside the local elements, control volumes are defined using half of the distance between neighboring nodes. Using the Green–Gauss formula [12], the governing equation (Equation (1)) is transformed into conservation form and then integrated over these control volumes:

$$\int_{V_c} \rho C_p \frac{\partial T}{\partial t} dV = \int_{\Gamma_c} \left( k_{ij} \frac{\partial T}{\partial x_j} \right) n_i d\Gamma + \int_{V_c} Q dV \quad (19)$$

where  $V_c$  is the control volume,  $\Gamma_c$  is the boundary of the control volume, and  $n_i$  is the outward normal vector on the control volume boundary.

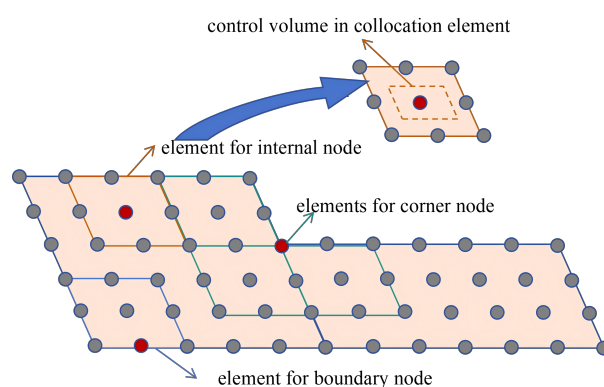


**Figure 1.** Collocation elements and the control volume.

The field variables and their gradients are approximated using shape functions associated with the local elements, similar to FEM. This approach allows for greater flexibility in handling complex geometries and boundary conditions, while also maintaining the conservation properties of FVM. Using the shape functions, the temperature field can be expressed as [25,28]:

$$T(\mathbf{x}) = N_\alpha(\xi) T^\alpha \quad (20)$$

where  $N_\alpha(\xi)$  are the shape functions,  $T^\alpha$  are the nodal temperatures, and the repeated  $\alpha$  indicates summation over all nodes in the local element. Therefore, the temperature gradient can be expressed as:

$$\frac{\partial T}{\partial x_j} = \frac{\partial N_\alpha(\xi)}{\partial x_j} T^\alpha \quad (21)$$

The gradients of the shape functions can be calculated using the isoparametric mapping technique, which maps the local element to a standard reference element:

$$\frac{\partial N_\alpha(\xi)}{\partial x_j} = \frac{\partial N_\alpha(\xi)}{\partial \xi_k} \frac{\partial \xi_k}{\partial x_j} \quad (22)$$

where  $\xi_k$  are the coordinates in the reference element, and  $\frac{\partial \xi_k}{\partial x_j}$  is the Jacobian of the transformation. At a corner node, multiple local elements can be constructed, and the shape functions from each element are combined to form a complete approximation of the field

variables and their gradients [29]. Like the field variables, the global coordinates can also be approximated using the shape functions:

$$\mathbf{x} = N_\alpha(\boldsymbol{\xi})\mathbf{x}^\alpha \quad (23)$$

Thus, one can obtain the gradients of the shape functions in the global coordinate system by substituting the above equations into the Jacobian matrix:

$$\frac{\partial \xi_k}{\partial x_j} = \left( \frac{\partial x_j}{\partial \xi_k} \right)^{-1} = \left( \frac{\partial N_\alpha(\boldsymbol{\xi})}{\partial \xi_k} x_j^\alpha \right)^{-1} \quad (24)$$

Substituting these approximations into Equation (19) and applying numerical integration techniques, such as Gaussian quadrature, the discretized equations can be obtained for each node:

$$\rho C_p V_c \frac{\partial T}{\partial t} = \sum_{k=1}^{N_f} \sum_{\beta=1}^{N_{\Gamma_k}} \left( k_{ij} \frac{\partial N_\alpha(\boldsymbol{\xi}_{k\beta})}{\partial x_j} n_i A_{k\beta} \right) T^\alpha + \int_{V_c} Q dV \quad (25)$$

In the above equation, the lumped mass matrix is used to simplify the time integration.  $N_f$  is the number of faces of the control volume,  $N_{\Gamma_k}$  is the number of quadrature points on the  $k$ -th face, and  $A_{k\beta}$  is the area associated with the  $\beta$ -th quadrature point on the  $k$ -th face. In CVFrEM, each node has its own control volume, and the control volumes of adjacent nodes may overlap. In Equation (25), only temperature  $T$  is the independent unknown variable, while the thermal conductivity and heat capacity are assumed to be known or a function of temperature.

On the physical boundary of the domain, because of the interpolation property of the shape functions, the unknown variable in CVFrEM is the nodal temperature. Hence, the essential boundary conditions can be enforced directly by enforcing temperature at the boundary nodes:

$$T(\mathbf{x}_{\text{boundary}}) = T_{\text{boundary}} \quad (26)$$

Then, heat fluxes can be calculated using the values at those boundary nodes by Equations (7) and (21). This is an advantage over some other mesh-free methods, such as the element-free Galerkin method, where the unknowns consist only of interpolation-function parameters and special treatment is required to enforce the essential boundary conditions.

The natural boundary conditions can be imposed by replacing the fluxes by boundary values. For example, for the convective boundary condition, the heat flux can be expressed as Equation (7). The first term on the right-hand side of Equation (25) represents the summation of heat flow over the surfaces of a control volume. For a given control surface  $k$ , the heat flow is

$$\int_{\Gamma_k} -k_{ij} \frac{\partial T}{\partial x_j} n_i d\Gamma = \sum_{\beta=1}^{N_{\Gamma_k}} \left( -k_{ij} \frac{\partial N_\alpha(\boldsymbol{\xi}_{k\beta})}{\partial x_j} n_i A_{k\beta} \right) T^\alpha = \sum_{\beta=1}^{N_{\Gamma_k}} q_{k\beta} A_{k\beta} \quad (27)$$

At the boundary where the heat flux is specified, the corresponding boundary values  $q_{k\beta} = \bar{q}$  are used to replace the fluxes in the integral over the control surface. Therefore, by substituting Equation (7) into Equation (19), the integral over the control surface can be expressed as:

$$\int_{\Gamma_k} -k_{ij} \frac{\partial T}{\partial x_j} n_i d\Gamma = \int_{\Gamma_k} h(T_{\text{surface}} - T_\infty) d\Gamma = \sum_{\beta=1}^{N_{\Gamma_k}} \left( N_\alpha(\boldsymbol{\xi}_{k\beta}) T^\alpha - T_\infty \right) h_{k\beta} A_{k\beta} \quad (28)$$

Similarly, for the radiative boundary condition, the heat flux can be expressed as Equation (8), and the integral over the control volume boundary can be expressed as:

$$\int_{\Gamma_k} -k_{ij} \frac{\partial T}{\partial x_j} n_i d\Gamma = \int_{\Gamma_k} h_r(T)(T_{\text{surface}} - T_{\infty}) d\Gamma = \sum_{\beta=1}^{N_{\Gamma}} \left( N_{\alpha}(\xi_{\beta}) T^{\alpha} - T_{\infty} \right) h_{r\beta}(T_{\text{surface}}, T_{\infty}) A_{\beta} \quad (29)$$

where  $h_r = \epsilon\sigma(T_{\text{surface}}^2 + T_{\infty}^2)(T_{\text{surface}} + T_{\infty})$  is the radiative heat transfer coefficient at the  $\beta$ -th boundary node, and  $A_{\beta}$  is the area associated with the  $\beta$ -th boundary node.

For the time derivative, the implicit backward difference formula is used:

$$\frac{\partial T^{n+1}}{\partial t} \approx \frac{(1+2\beta)T^{n+1} - (1+3\beta)T^n + \beta T^{n-1}}{(1+\beta)\Delta t} \quad (30)$$

When  $\beta = 0$ , the scheme reduces to the first-order backward Euler method, which is unconditionally stable and suitable for stiff problems. When  $\beta = 1$ , the scheme reduces to the second-order backward differentiation formula (BDF2), which is also unconditionally stable and provides higher accuracy.

The final discretized equation for each node can be expressed as:

$$R^{n+1,\gamma} = \left( \frac{(1+2\beta)\rho C_p V_c}{(1+\beta)\Delta t} T^{n+1,\gamma} + \sum_{k=1}^{N_f} \sum_{\beta=1}^{N_{\Gamma_k}} \left( q_i(\xi_{k\beta}) n_i A_{k\beta} \right) \right) - \frac{(1+3\beta)\rho C_p V_c}{(1+\beta)\Delta t} T^{n,\gamma} + \frac{\beta\rho C_p V_c}{(1+\beta)\Delta t} T^{n-1,\gamma} - \int_{V_c} Q dV \quad (31)$$

where  $R^{n+1,\gamma}$  is the residual of the discretized equation at node  $\gamma$  and time step  $n+1$ , and  $q_i$  is the heat flux vector. If the boundary is inside the domain,  $q_i$  can be calculated using the gradient of the temperature calculated by collocation elements. For the physical boundary,  $q_i$  can be calculated using the boundary conditions. Apparently, the residual  $R^{n+1,\gamma}$  is a function of the temperature at time step  $n+1$ , and the temperature at time step  $n+1$  can be solved by  $\mathbf{R}^{n+1} = 0$  using iterative methods such as Newton–Raphson. In the Newton–Raphson method, the temperature at time step  $n+1$  is updated iteratively using the following equation:

$$\frac{\partial \mathbf{R}^{n+1}(\mathbf{T}_{(m)}^{n+1})}{\partial \mathbf{T}_{(m)}^{n+1}} \Delta \mathbf{T}_{(m+1)}^{n+1} = \mathbf{R}^{n+1}(\mathbf{T}_{(m)}^{n+1}) \quad (32)$$

where  $\mathbf{T}_{(m)}^{n+1}$  is the temperature vector at iteration  $m$ , and  $\Delta \mathbf{T}_{(m+1)}^{n+1}$  is the temperature increment for the next iteration. At the first iteration,  $m = 0$ ,  $\mathbf{T}_{(0)}^{n+1}$  is typically taken as the temperature field from the previous time step, i.e.,  $\mathbf{T}_{(0)}^{n+1} = \mathbf{T}^n$ . Then, we solve the increment  $\Delta \mathbf{T}_{(m+1)}^{n+1}$  from Equation (32) and update the temperature for the next iteration using:

$$\mathbf{T}_{(m+1)}^{n+1} = \mathbf{T}_{(m)}^{n+1} + \Delta \mathbf{T}_{(m+1)}^{n+1} \quad (33)$$

Subsequently, the residual,  $\mathbf{R}^{n+1}$ , and the Jacobian matrix,  $\frac{\partial \mathbf{R}^{n+1}}{\partial \mathbf{T}^{n+1}}$ , are recalculated using the updated temperature, and the process is repeated until convergence is achieved. When the residual is sufficiently small,  $\|\mathbf{R}^{n+1}\|_2 < \epsilon$ ,  $\mathbf{R}^{n+1} \approx 0$  holds. Hence, the solution is considered converged, and the temperature field at time step  $n+1$  is obtained.

For multiphysics coupling problems, the choice of the time step is crucial. When the temperature is low, the reaction rates are slow, and a large time step can be used to accelerate the simulation. However, as the temperature rises, the reaction rates increase rapidly, necessitating a smaller time step to capture the rapid changes in temperature

and heat generation. More critically, the temperature rise is primarily driven by the heat generated from the reactions, which is significantly larger than the heat dissipation during thermal runaway. Furthermore, because the activation energies of the reactions vary considerably, the reaction rates may differ substantially even at the same temperature. If the time step is too large, the temperature rise will be overestimated, even potentially leading to divergence of the simulation. Conversely, if the time step is too small, the heat-transfer simulation becomes prohibitively slow and computationally expensive. This is known as a stiff problem, which is a common challenge in multi-physics simulations. It can also be observed that the contribution of the reactions serves as a source term in the heat transfer equation. Therefore, there is no need to fully couple the heat transfer and reaction models, which would significantly increase the computational cost.

In this paper, we employ a separated iteration algorithm with a two-way coupling strategy to solve the heat transfer and reaction models. As shown in Figure 2, the temperature is guessed at the beginning of each time step, and the reaction rates are calculated using Equation (13) based on the guessed temperature. Then, the heat generation rate is calculated based on the reaction rates using Equation (15), and the heat transfer equation (using Equation (32)) is solved to update the temperature. Using the updated temperature, the reaction rates are recalculated, and the process is repeated until convergence is achieved.

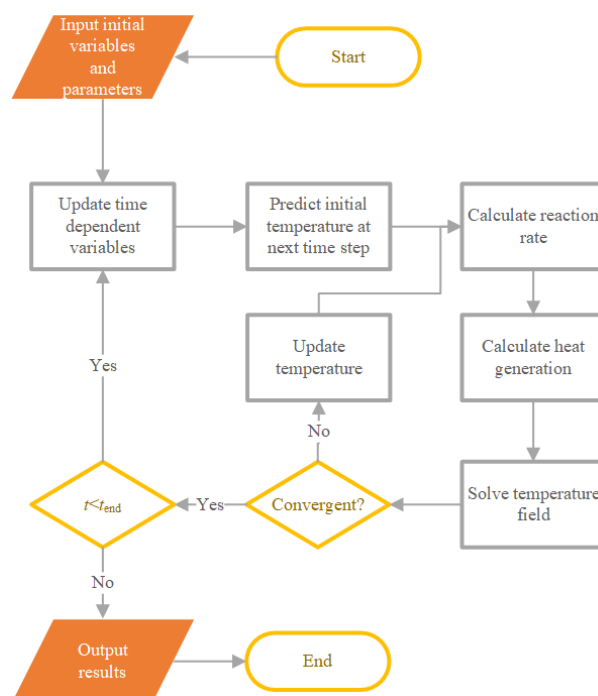


**Figure 2.** Separated iteration algorithm for thermal runaway of lithium-ion batteries.

Because the temperature changes slowly during the initial stage but rises rapidly during thermal runaway, an adaptive time-stepping scheme is employed to ensure numerical stability and accuracy. Initially, a relatively large time step  $t_0$  is used to accelerate the computation. During the simulation, the time step is halved to improve stability if the convergence criterion is not satisfied within four iterations for three consecutive time steps. Conversely, if convergence is achieved in fewer than three iterations for three consecutive time steps, the time step is increased by a factor of 1.5 to accelerate the computation. To maintain sufficient accuracy, the time step is bounded above by  $t_{\max}$  and below by  $t_{\min}$ . The procedure is summarized in the following pseudocode:

#### Adaptive time step

- 1: Initialize  $t = 0$ ,  $\Delta t = t_0$ , and the counters  $n_{\text{slow}} = 0$  and  $n_{\text{fast}} = 0$ .

- 2: While  $t < t_{\text{end}}$ , set  $\mathbf{T}^{n+1,0} = \mathbf{T}^n$ .
- 3: For iteration  $m = 0, 1, \dots$ , calculate the reaction rates and temperature.
- 4: If  $\|\mathbf{T}^{n+1,m+1} - \mathbf{T}^{n+1,m}\|_2 < \epsilon$ , accept  $\mathbf{T}^{n+1} = \mathbf{T}^{n+1,m+1}$  and record the number of iterations; otherwise, reduce time step size by half and return to step 3.
- 5: If convergence requires more than four iterations, increment  $n_{\text{slow}}$  and reset  $n_{\text{fast}}$ ; otherwise, reset  $n_{\text{slow}}$ . If convergence requires fewer than three iterations, increment  $n_{\text{fast}}$ ; otherwise, reset  $n_{\text{fast}}$ .
- 6: If  $n_{\text{slow}} = 3$ , set  $\Delta t = \max(\Delta t/2, t_{\text{min}})$  and reset  $n_{\text{slow}}$ . If  $n_{\text{fast}} = 3$ , set  $\Delta t = \min(1.5\Delta t, t_{\text{max}})$  and reset  $n_{\text{fast}}$ .
- 7: Advance the time:  $t \leftarrow t + \Delta t$ , and return to step 2.

In the test cases presented below, the time step is equal to the maximum time step size for most of the time steps. However, when thermal runaway occurs, a smaller time step is needed for better convergence and accuracy.

### 3. Numerical Results and Discussion

#### 3.1. The Blade-Type Battery

Taking the experiments conducted by Feng et al. [27,30] as an example, the proposed method is used to simulate the thermal runaway process of a 25 Ah large-format lithium-ion battery. According to Wang et al. [31], cathode decomposition follows a two-stage reaction process. The kinetic parameters of the reactions are listed in Table 1, and the material properties of the battery are listed in Table 2. The battery consists of two pouch cells, a shell, a cover, and two terminals, as shown in Figure 3. Because the shell is very thin ( $d = 1 \text{ mm}$ ) and the thermal conductivity is very high ( $k = 237 \text{ W/(m K)}$ ), the thermal resistance of the shell is only  $4.2 \times 10^{-6} \text{ m}^2 \text{ K/W}$ . Hence, the shell can be simplified as a boundary condition with a convective heat transfer coefficient of  $h_{\text{conv}} = 10 \text{ W/(m}^2 \text{ K)}$ . However, the contact resistance between the shell and the jelly is significant, with  $R_c = 0.156 \text{ m}^2 \cdot \text{K/W}$  according to the data reported by Feng et al. [9]. Thus, the effective heat transfer coefficient between the shell and the jelly can be calculated as:

$$h_{\text{eff}} = \frac{1}{1/h_{\text{conv}} + R_c} \quad (34)$$

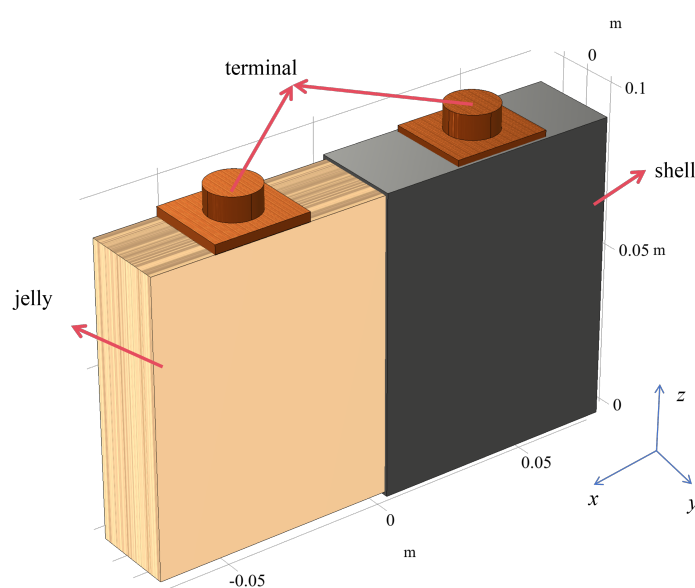


**Figure 3.** A large-format blade-type lithium-ion battery [27].

In this case, the battery is blade-type, and each layer lies in the x-z plane. Therefore, the effective thermal conductivity in the x-z plane can be calculated using the parallel model, as shown in Equation (6). In the y-direction, the effective thermal conductivity can be calculated using the series model, as shown in Equation (5). As listed in Table 2, the first value is the effective thermal conductivity of the jelly in the stacking direction (y-direction). The other two values are the effective thermal conductivities in the x and z directions, respectively.

**Table 1.** The reaction parameters for different battery components.

| Parameter                               | SEI                        | Anode                                                                 | Separator                | Cathode,1               | Cathode,2                   | Electrolyte              |
|-----------------------------------------|----------------------------|-----------------------------------------------------------------------|--------------------------|-------------------------|-----------------------------|--------------------------|
| $\Delta H_x$ (J/kg)                     | $2.57 \times 10^5$ [8]     | $1.714 \times 10^6$ [8]                                               | $-2.332 \times 10^5$ [8] | $7.7 \times 10^4$ [31]  | $8.4 \times 10^4$ [31]      | $8.0 \times 10^5$ [9]    |
| $W_x$ (kg/m <sup>3</sup> ) <sup>a</sup> | 318                        | 318                                                                   | 56                       | 566                     | 566                         | 341                      |
| $c_{x0}$                                | 0.150 [8]                  | 1.000 [9]                                                             | 1.000 [9]                | 0.999 [9]               | 0.999 [9]                   | 1.000 [8]                |
| $n_{x,1}$ [8]                           | 1.0                        | 1.0                                                                   | 1.0                      | 1.0                     | 1.0                         | 1.0                      |
| $n_{x,2}$ [8]                           | 0.0                        | 0.0                                                                   | 0.0                      | 1.0                     | 1.0                         | 0.0                      |
| $T_{\text{onset},x}$ (K)                | 323 [9]                    | 323 [9]                                                               | 393 [27]                 | 453 [31]                | 493 [31]                    | 413 [9]                  |
| $E_{a,x}$ (eV)                          | 1.401 [7]                  | 0.342 [9]                                                             | 4.355 [9]                | 1.192 [31]              | 1.647 [31]                  | 1.763 [9]                |
| $A_x$ (1/s)                             | $1.667 \times 10^{15}$ [8] | $0.035(T \leq 260^\circ\text{C})$<br>$5.0(T > 260^\circ\text{C})$ [9] | $1.5 \times 10^{50}$ [9] | $1.75 \times 10^9$ [31] | $1.077 \times 10^{12}$ [31] | $3.0 \times 10^{15}$ [9] |
| $g_x$                                   | 1                          | $\exp\left(-\frac{C_{\text{SEI}}}{C_{\text{SEI},0}}\right)$ [8]       | 1                        | 1                       | 1                           | 1                        |

<sup>a</sup> Calculated based on the mass of the reactants [9].

**Table 2.** The material properties of the battery components.

| Materials | Density (g/cm <sup>3</sup> ) | Specific Heat (J/g·K) | Conductivity (W/m·K) |
|-----------|------------------------------|-----------------------|----------------------|
| Jelly [9] | 2.309                        | 1.10                  | 1.5, 30, 30          |
| Terminal  | 8.9                          | 0.39                  | 380                  |

Following the experimental setup, the battery is placed in a chamber and subjected to the heat–wait–seek protocol to induce thermal runaway. At  $t = 0$  s, the chamber temperature is set to  $T_{\text{chamber}} = 50^\circ\text{C}$  and then increased gradually to  $T_{\text{chamber}} = 94^\circ\text{C}$  at an average rate of  $0.05^\circ\text{C}/\text{min}$ , thereby initiating the exothermic reactions. The battery temperature is subsequently measured using thermocouples, while the chamber temperature is maintained at the battery temperature to minimize heat loss. Once thermal runaway is triggered at  $T = 260^\circ\text{C}$ , the battery is cooled using a fan. During this stage, the forced-convection heat transfer coefficient is set to  $h_{\text{conv}} = 25 \text{ W}/(\text{m}^2 \text{ K})$ , and the chamber temperature is set to room temperature,  $T_{\text{chamber}} = 25^\circ\text{C}$ . Because Feng et al. did not report when the fan was switched off, it is assumed to remain in operation throughout this stage. Following the onset of thermal runaway, the battery voltage drops sharply owing to the internal short circuit. According to Feng et al. [30], the internal short circuit is triggered at  $T_{\text{isc}} = 260^\circ\text{C}$ , which is identical to the thermal-runaway trigger temperature. Unlike the reaction onset temperatures,  $T_{\text{isc}}$  is not an inherent material property; it varies with the internal state and local conditions of the cell. As measured in the experiment, the internal short circuit releases a total energy of  $Q_{\text{ele}} = 3.17 \times 10^5 \text{ J}$  over a duration of  $\tau = 10$  s. For the initial stage, the regeneration of SEI is also important, as it affects the slow increase in temperature before the onset of thermal runaway. In this case, the SEI regeneration-rate coefficient,  $K_r$ , is set to 6.0.

Because of the symmetry of the battery, only half of the battery is simulated, and the other half is mirrored. The mesh for the battery is shown in Figure 4, which is divided into two zones because of the different material properties of the jelly and the terminal. Mesh a and Mesh b consist of the same number of nodes, but the coordinates of the latter are randomly adjusted to verify robustness. The maximum time step is set to  $\Delta t = 10$  s, and the time step is adaptively adjusted based on the temperature rise rate. To verify time-step sensitivity, simulations are also conducted with a maximum time step of  $\Delta t = 5$  s. In this case, the convergence criterion is set to  $10^{-6}$  for the  $L_2$  norm of the temperature increment.

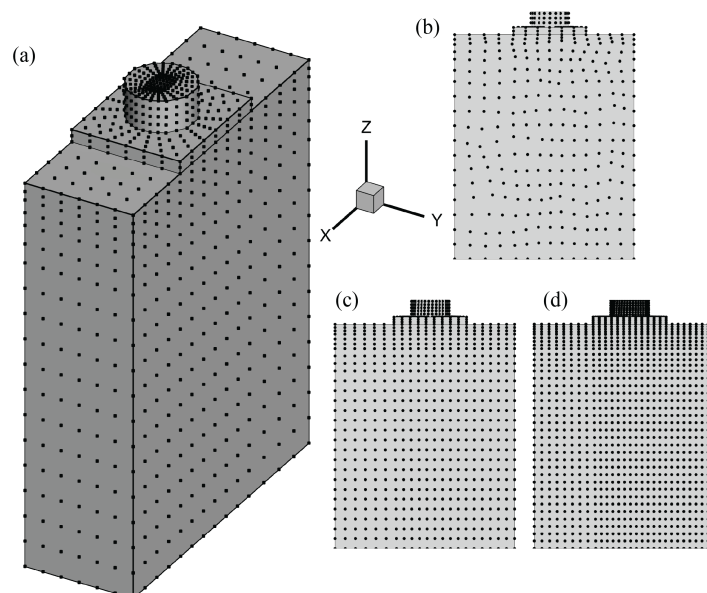


**Figure 4.** Meshes for the blade-type lithium-ion battery: (a) 6705 nodes, (b) 6705 randomly adjusted nodes, (c) 21,748 nodes, and (d) 50,537 nodes.

The temperature evolution at the center of the battery is presented in Figure 5, showing good agreement with the experimental data [27]. The results with  $\Delta t = 10$  s and  $\Delta t = 5$  s are compared, showing negligible differences, which indicates that the chosen time step is appropriate. The maximum temperature is  $T = 905$  °C, which is higher than the experimental results. The relative error of the maximum temperature is 6.1%. The primary reason for the discrepancy is that the exact cooling parameters are not given in Feng et al.'s report, and venting occurred in the experiment but was not considered in this paper. Venting is complex and difficult to model in this stage, which can significantly affect the temperature evolution during thermal runaway. To simulate the effects of venting, coupling with CFD should be considered [5]. In this study, we focus on the thermal behavior inside the battery. Therefore, the venting effects are not included in the simulation results presented in this study.

Figure 6 compares the temperature contours computed using different meshes. The irregular mesh leads to almost the same temperature distribution as Mesh a. However, both Mesh a and b slightly overestimate the temperature. As shown in Figure 7, the results for Mesh c and Mesh d are closely matched, indicating that Mesh c is sufficiently refined for accurate temperature prediction. In fact, the maximum temperature difference between Mesh a and Mesh d is less than 0.015 °C, which means that even the coarser meshes provide reasonably accurate results. In Figures 6 and 7, the temperature range is small because both the heating and reactions are slow. Feng et al.'s measurements also show that, until thermal runaway is triggered, the temperature difference between locations in the battery remains below 1 °C, consistent with the simulation results.

During the initial stage, the temperature rises gradually under the heat–wait–seek protocol, with a rate comparable to that of the chamber temperature. This initial temperature rise subsequently accelerates the exothermic reactions, as illustrated in Figure 8. As a result, even though external heating was terminated upon reaching  $T = 94\text{ }^{\circ}\text{C}$ , the battery temperature continued to rise owing to the heat released by the ongoing reactions. When the temperature reached  $T = 260\text{ }^{\circ}\text{C}$ , the separator melted, causing direct contact between the anode and cathode and triggering an internal short circuit. Consequently, the rate of temperature rise increased sharply, as shown in Figure 9. The predicted rate of temperature rise is in good agreement with the results reported by Feng et al. [30], demonstrating that the proposed method can accurately capture the thermal runaway process of lithium-ion batteries.

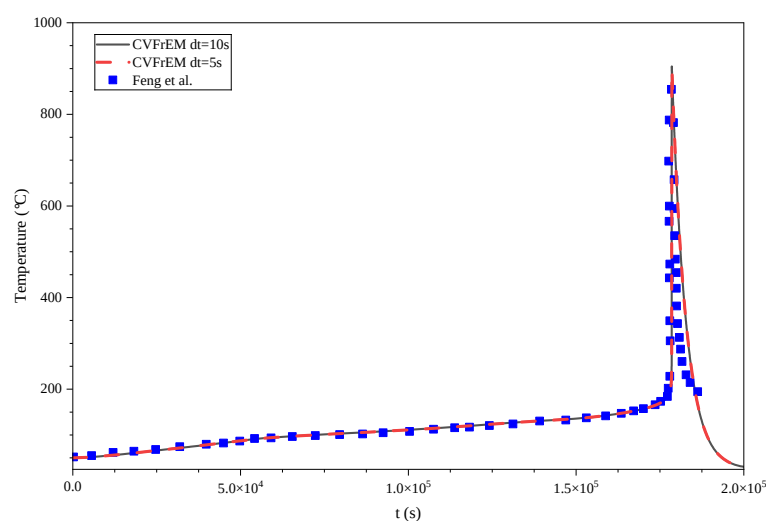


**Figure 5.** The temperature curve at the center of the blade-type battery (Mesh b) [9].

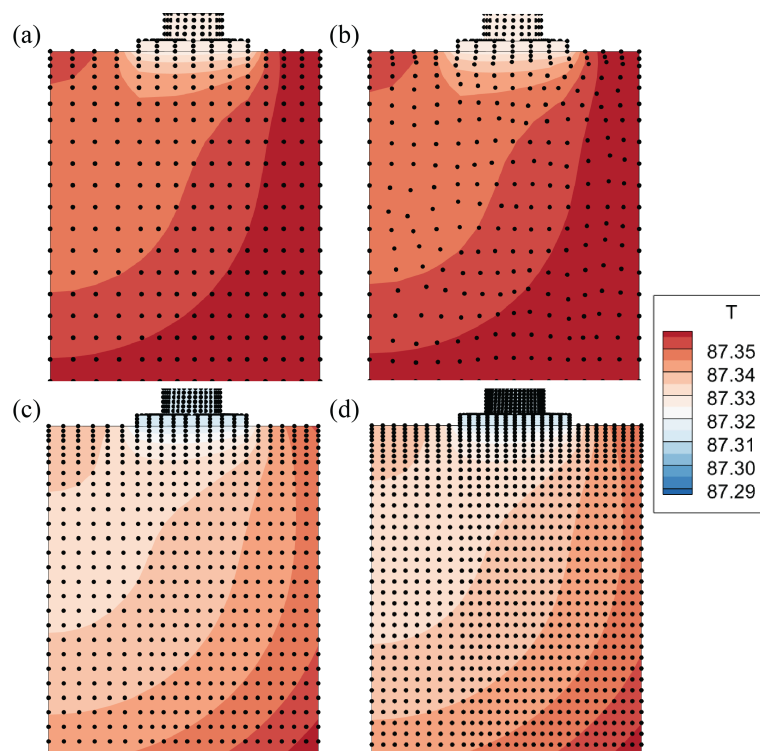


**Figure 6.** Comparison of temperature contours computed using different meshes: (a) 6705 nodes, (b) 6705 randomly adjusted nodes, (c) 21,748 nodes, and (d) 50,537 nodes.

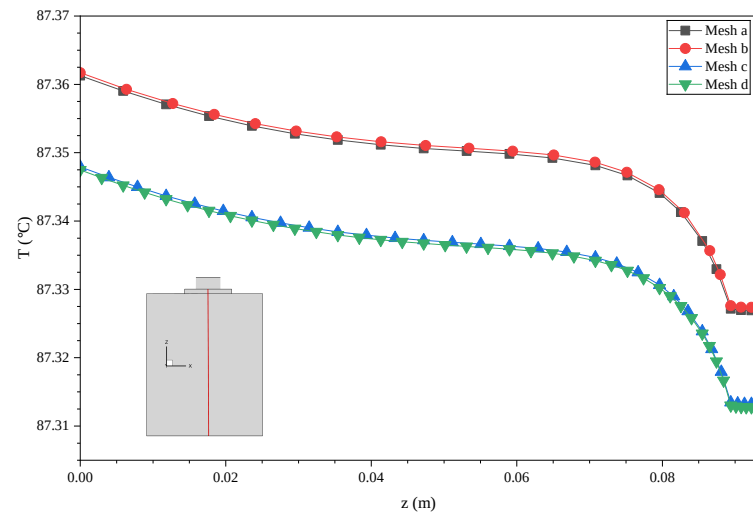


**Figure 7.** Comparison of temperatures computed using different meshes along the pathline.

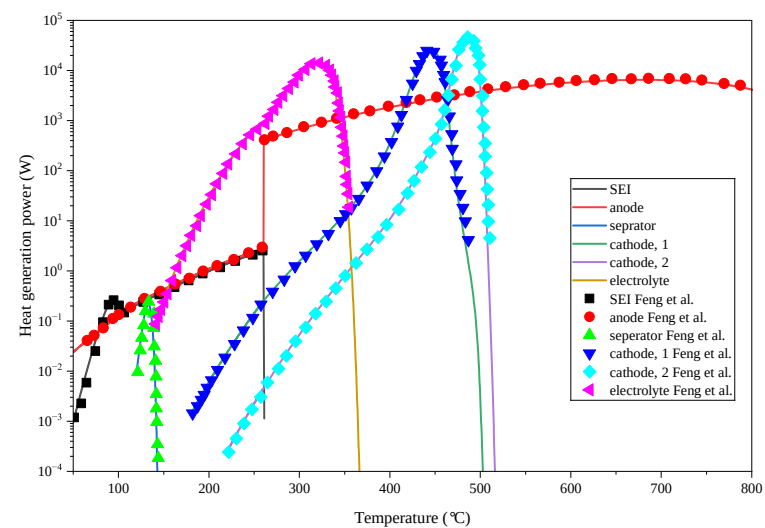


**Figure 8.** The heat generation power vs. temperature [9].

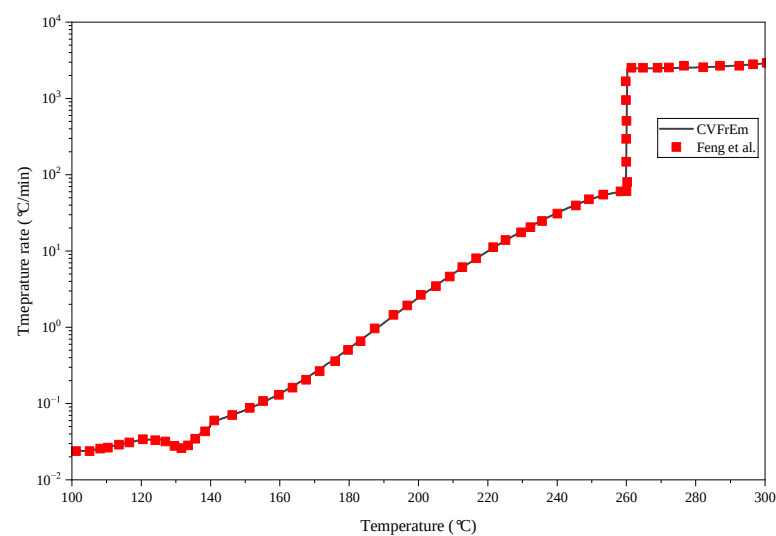


**Figure 9.** The temperature rise vs. temperature [9].

Figure 10 shows the temperature distribution at different times. During the heating stage (Figure 10a), the temperature distribution is relatively uniform because the chamber temperature rises slowly. Because the terminals act as heat sinks, the temperature near them is lower than elsewhere in the battery, as shown in Figure 10b. Thus, the thermal runaway starts at the bottom of the battery. When the thermal runaway is triggered, the temperature suddenly rises. Therefore, the temperature near the lower surface of the battery is much higher than that near the upper surface, as shown in Figure 10c,d. As shown in Figure 11, the temperature at different locations evolves over time, highlighting the non-uniform heating and the progression of thermal runaway within the battery. At the top of the battery, the onset time of thermal runaway is delayed at about 9 s compared to the bottom, due to the relatively slower temperature rise in this region. Because the thermal conductivity of terminal is relatively high, the temperature at top of the terminal rise almost the same as the top surface of the battery.

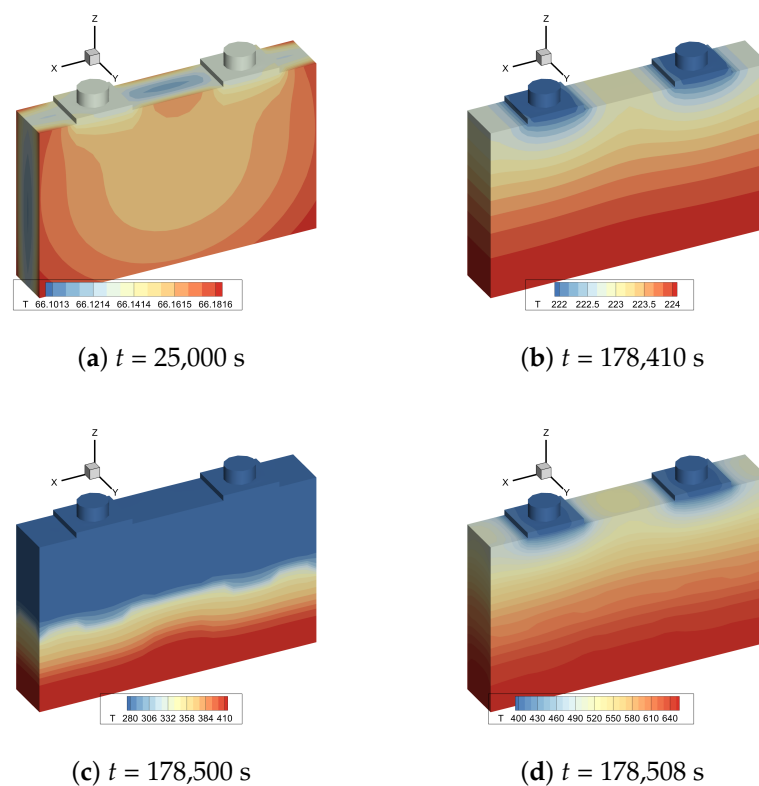


**Figure 10.** The temperature evolution over time at different locations.

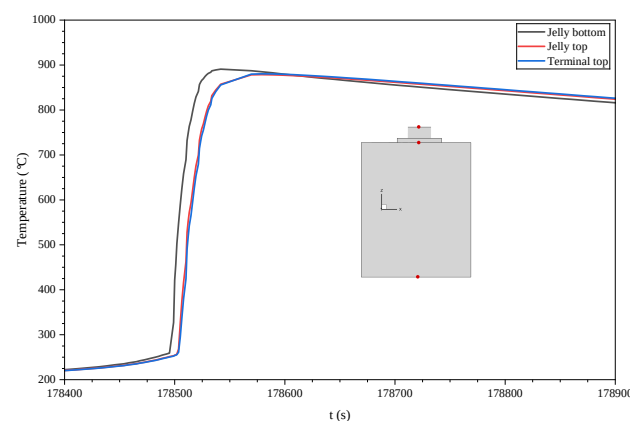


**Figure 11.** The temperature evolution over time at different locations.

### 3.2. Oven Test of Roll-Type Battery

Here, we simulate a more complex battery geometry: that of a roll-type 18650 cell, shown in Figure 12. The initial experimental setup is similar to that used by Kim et al. [8], in which the battery is placed in an oven and heated to trigger thermal runaway. The kinetic parameters of the reactions are listed in Table 3, and the material properties of the battery are listed in Table 4. In this case, each layer is wound to form the cylindrical structure. Therefore, the radial effective thermal conductivity (the first value)  $k_r$  is different from the axial and tangential effective thermal conductivities  $k_a$  and  $k_t$ . Therefore, we have

$$x' = r; y' = \theta; z' = y; \quad (35)$$

However, our model uses the Cartesian coordinate system. Thus, we have to transform the thermal conductivities from the cylindrical coordinate system to the Cartesian coordinate system using Equation (3). The transformation matrix is given by

$$\mathbf{R} = \begin{bmatrix} \cos \theta & -\sin \theta & 0 \\ 0 & 0 & 1 \\ \sin \theta & \cos \theta & 0 \end{bmatrix} \quad (36)$$

The thickness of the shell is  $d = 0.5$  mm. The initial temperature of the battery is set to  $T_0 = 35$  °C, and the oven temperature is set to  $T_{\text{oven}} = 155$  °C. The convective heat transfer coefficient between the battery and the oven is set to  $h_{\text{conv}} = 7.17$  W/(m<sup>2</sup> K), and the emissivity of the battery surface is set to  $\epsilon = 0.8$ . According to Kim et al.'s report [8], the volume ratio of the active material is 0.767, and the SEI regeneration-rate coefficient is 1.0. The air in the mandrel and the shell are isotropic and inactive.

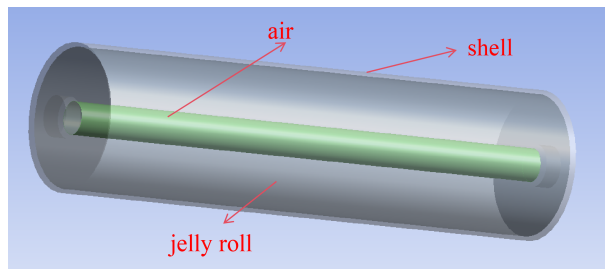


**Figure 12.** The geometry of the roll-type 18650 battery.

**Table 3.** The reaction parameters for the components of an 18650 battery.

| Parameter                      | SEI                        | Anode                                                       | Cathode                    | Electrolyte                |
|--------------------------------|----------------------------|-------------------------------------------------------------|----------------------------|----------------------------|
| $\Delta H_x$ (J/kg)            | $2.57 \times 10^5$ [7]     | $1.714 \times 10^6$ [7]                                     | $3.14 \times 10^5$ [7]     | $1.55 \times 10^5$ [32]    |
| $W_x$ (kg/m <sup>3</sup> ) [8] | 610                        | 610                                                         | 1220                       | 406.9                      |
| $c_{x0}$ [7]                   | 0.15                       | 0.75                                                        | 0.96                       | 1                          |
| $n_{x,1}$ [7]                  | 1.0                        | 1.0                                                         | 1.0                        | 1.0                        |
| $n_{x,2}$ [7]                  | 0.0                        | 0.0                                                         | 1.0                        | 0.0                        |
| $T_{\text{onset},x}$ (K)       | 293                        | 293                                                         | 293                        | 293                        |
| $E_{a,x}$ (eV)                 | 1.401 [7]                  | 1.401 [7]                                                   | 1.271 [7]                  | 2.841 [32]                 |
| $A_x$ (1/s)                    | $1.667 \times 10^{15}$ [7] | $2.5 \times 10^{13}$ [7]                                    | $6.667 \times 10^{11}$ [7] | $5.14 \times 10^{25}$ [32] |
| $g_x$ [8]                      | 1                          | $\exp\left(-\frac{C_{\text{SEI}}}{C_{\text{SEI},0}}\right)$ | 1                          | 1                          |

Because of the symmetry of the battery, only one quarter of the battery is simulated, and the other three quarters are mirrored. The meshes shown in Figure 13 consist of 7221, 55,796, and 430,417 nodes, respectively. The geometry is partitioned into three zones to account for the different material properties. Maximum time step sizes of  $\Delta t = 1$  s and

5 s are employed in this case. The convergence criterion is set to  $10^{-5}$  for the  $L_2$  norm of the temperature increment. In addition to the results reported in the literature, the simulation results are compared with those obtained using the FEM software COMSOL Multiphysics, version 6.3 [33]. The FEM model comprises 59,556 elements, and simulations are performed using both linear and quadratic Lagrange elements. The reaction rates are calculated using the partial differential equation module in COMSOL. The maximum time step size of COMSOL is restricted to  $\Delta t = 1$  s, and the strict adaptive time-stepping option of COMSOL is employed to ensure numerical stability.

**Table 4.** The material properties of the battery components.

| Materials       | Density (g/cm <sup>3</sup> ) | Specific Heat (J/g·K) | Conductivity (W/m·K) |
|-----------------|------------------------------|-----------------------|----------------------|
| Jelly roll      | 1.99 [8]                     | 1.40 [8]              | 0.897, 29.5, 29.5    |
| Aluminium shell | 2.70                         | 0.89                  | 237                  |
| Air in mandrel  | 0.0012                       | 1.01                  | 0.03                 |

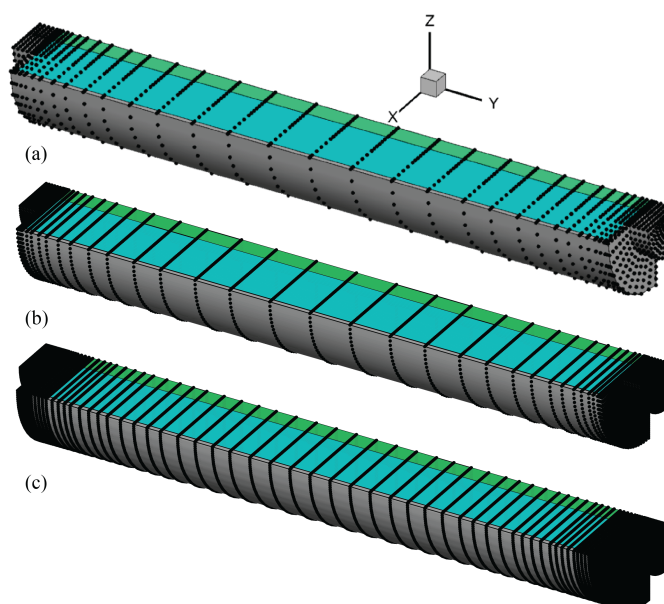


**Figure 13.** The mesh for the roll-type 18650 battery: (a) a coarse mesh consisting of 7221 nodes, (b) a refined mesh with 55,796 nodes, and (c) a further refined mesh with 430,417 nodes.

Figure 14 shows the temperature evolution at the center of the battery, which is in good agreement with the data reported by Kim et al. The maximum temperature predicted by CVFrEM is lower than that reported in the literature, and FEM predicts an even lower temperature. Compared with the results in the literature, the error of the maximum temperature predicted by CVFrEM is 4.4%. Meanwhile, the results using different time steps are almost identical, indicating that the time step is sufficiently small. At the initial stage, the temperature rises gradually under the oven heating. Even though all the reactions are triggered, the rates are very slow because the temperature is low, as shown in Figure 15. After about 13 min, a significant portion of the SEI has decomposed, as shown in Figure 16. Then, the anode and electrolyte reactions are triggered, and the heat generation rate increases significantly. At this stage, the temperature rise is driven by SEI decomposition, the anode reaction, and heating from the oven. At about 20 min, the SEI decomposition is almost complete, and the temperature is close to the oven temperature. Meanwhile, the anode reaction rate decreases as the anode-reactant concentration declines. Therefore, the heat generation rate decreases, and the temperature rises slowly. After about 40 min, when the temperature reaches 165 °C

( $t = 41$  min), the anode and cathode reaction rates accelerate, and the heat-generation rate increases significantly. A few minutes later, the runaway occurs at  $t \approx 47$  min, and the center temperature reaches  $169^\circ\text{C}$  and rises sharply. Because the battery is small, its specific surface area is large, and heat dissipation is significant. Thus, the maximum temperature ( $216.6^\circ\text{C}$  at  $t \approx 55$  min) is much lower than the former case.

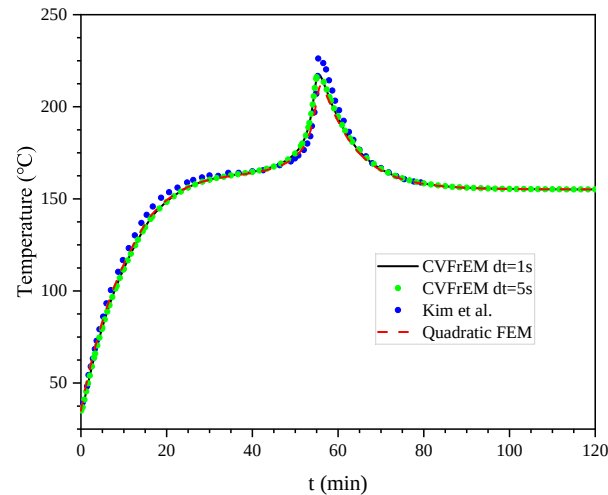


**Figure 14.** The temperature evolution at the center of the 18650 battery [8].

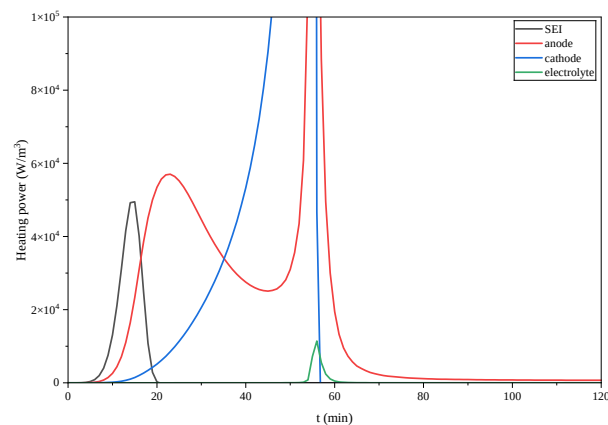


**Figure 15.** The variations of the average heating powers in the 18650 battery.

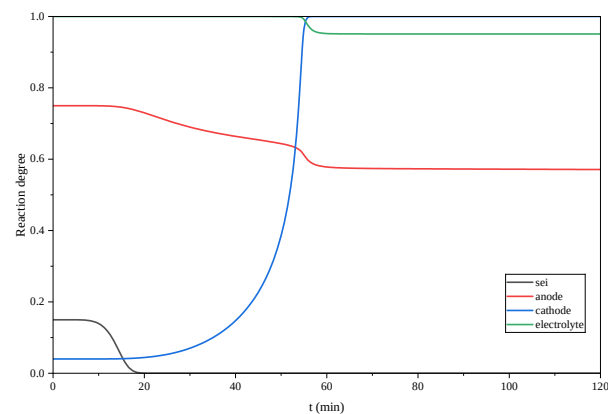


**Figure 16.** The variations of the average concentrations of the reactants in the 18650 battery.

The temperature contours at different times are shown in Figure 17. The contours show that, in the initial stage, the outer layer of the battery is at a higher temperature than the inner layer;

however, when the reactions are triggered, the inner layer is at a higher temperature than the outer layer. Figure 18 compares the temperature distribution along the line ( $x = 5, z = 0.0$ ) mm using different meshes. Even the coarsest mesh provides results that are in good agreement with the finer meshes, with maximum errors of only 0.35% at  $t = 10$  min and 0.52% at  $t = 54$  min. However, compared with FEM results, the deviations are larger, and the relative error exceeds 2% at  $t = 54$  min. In addition, FEM yields lower temperature gradients, especially near the interface between the shell and the jelly. This is because FEM tends to smear the heat transfer across interfaces, leading to artificial diffusion. As a result, heat spreads more rapidly than it should. According to Figure 14, the temperature computed by FEM rises faster in the early stage but lags behind the CVFrEM prediction at later times. Because heat flows into the battery during the initial stage and out of it during the later stage, the artificial diffusion of FEM causes the model to absorb more heat initially and release it more rapidly subsequently. The heat fluxes between the jelly and the shell are listed in Table 5, where the relative flux error is defined as  $2|q_+ - q_-|/(|q_+| + |q_-|)$ . Although CVFrEM is only locally conservative, the heat fluxes across the interfaces are still well balanced.

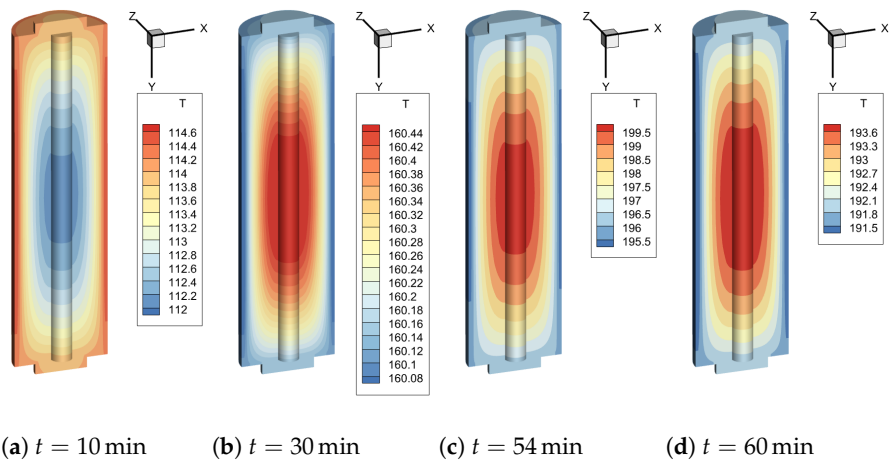


Figure 17. The temperature distribution at different times in the 18650 battery.

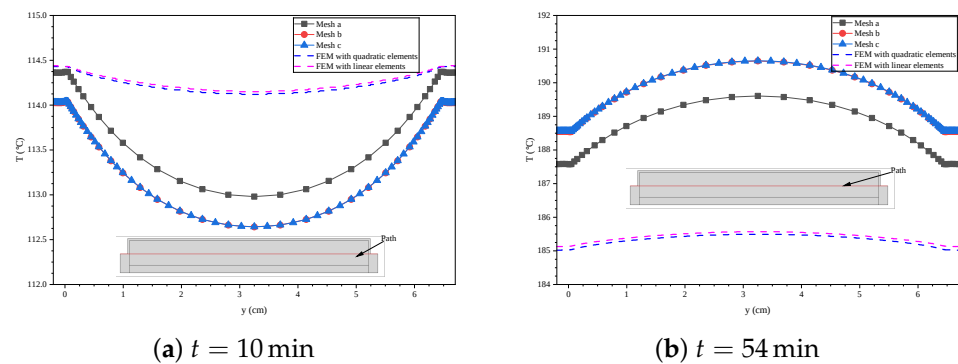


Figure 18. The temperature distribution along the path line  $x = 5.0, z = 0.0$  mm.

Table 5. The heat flux between the shell and the jelly roll at ( $x = 5.0, y = 64.5, z = 0.0$ ) mm at  $t = 10$  min.

| Meshes/Methods     | Shell Side (W/m <sup>2</sup> ) | Jelly Roll Side (W/m <sup>2</sup> ) | Relative Error |
|--------------------|--------------------------------|-------------------------------------|----------------|
| CVFrEM with Mesh a | 3457                           | 3165                                | 0.088          |
| CVFrEM with Mesh b | 3300                           | 3234                                | 0.020          |
| CVFrEM with Mesh b | 3300                           | 3234                                | 0.020          |

Table 5. Cont.

| Meshes/Methods              | Shell Side (W/m <sup>2</sup> ) | Jelly Roll Side (W/m <sup>2</sup> ) | Relative Error |
|-----------------------------|--------------------------------|-------------------------------------|----------------|
| CVFrEM with Mesh c          | 3181                           | 3245                                | 0.020          |
| FEM with linear elements    | 1784                           | 672.4                               | 0.610          |
| FEM with quadratic elements | 1558                           | 834.1                               | 0.905          |

4. Conclusions

In this paper, we developed a novel simulation method for the thermal and chemical behavior of lithium-ion batteries using the control volume free element method. The non-isotropic heat transfer equation is solved using CVFrEM, where collocation elements are generated for each node, and the shape functions are used to approximate the field variables and their gradients. Then, the governing equation is transformed into the integral form, and the discretized equations are obtained using numerical integration techniques. In addition, to address the stiffness of the thermal-runaway problem, we propose a separated-iteration algorithm with a two-way coupling strategy to couple the heat-transfer and reaction models. The proposed method is then used to simulate the thermal runaway process of a large-format, blade-type lithium-ion battery and a roll-type 18650 lithium-ion battery. The results show that the proposed method can accurately capture the thermal runaway process of lithium-ion batteries, and the predicted temperature evolution is in good agreement with the experimental data. The proposed method can be used to simulate the thermal and chemical behavior of lithium-ion batteries, and to optimize the design of lithium-ion batteries to improve their safety and performance.

**Author Contributions:** Conceptualization, B.R. and S.-D.W.; methodology and software, H.-Y.L. and X.-W.G.; validation, T.P.; investigation, M.C.; writing—original draft preparation, H.-Y.L.; writing—review and editing, B.R. and X.-W.G. All authors have read and agreed to the published version of the manuscript.

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**Data Availability Statement:** All data generated or analyzed during this study are included in this published article.

**Conflicts of Interest:** The authors declare no conflicts of interest.

Abbreviations

The following abbreviations are used in this manuscript:

|        |                                    |
|--------|------------------------------------|
| LIB    | Lithium-ion battery                |
| SEI    | Solid electrolyte interphase       |
| CVFrEM | Control volume free element method |
| FEM    | Finite element method              |
| FVM    | Finite volume method               |

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