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Multi-Physics Lithium-Ion Battery Modeling for Deep Learning Applications: Data Development and Thermal Risk Analysis

Tobias Weber^{1*}, Hanna Müller¹

Abstract

The swift expansion of electric vehicle adoption demands significant improvements in durability, safety, and dependability for advanced high-capacity battery systems. Consequently, there is a strong need for data-oriented battery management strategies capable of decoding intricate battery signals and guiding appropriate control of the coupled multi-physical processes inside batteries. At present, battery informatics is gaining traction as an effective strategy, harnessing sophisticated machine learning methods to generate reliable forecasts of battery capability, degradation state, and hazard levels—yet its advancement is severely constrained by insufficient data availability. In response, this work offers one of the pioneering contributions to synthetic and experimental data creation, integrating lab-based measurements with comprehensive three-dimensional (3-D) multi-physics simulations to establish a robust deep learning pipeline accompanied by detailed evaluation of performance metrics and thermal hazard anticipation. In particular, Part I addresses the construction and rigorous verification of the battery simulation framework, conducted in two main phases to confirm its predictive fidelity: initially, validation of the multi-physics approach was performed using measurements from two widely used commercial Li-ion cells—Panasonic NCR18650B and 18650BD; subsequently, an in-depth investigation of the thermal–electrochemical coupling was carried out, yielding valuable model-derived understanding such as temporal voltage profiles and identification of peak local temperature regions (hot spots). This carefully validated model produces high-quality, interpretable datasets suitable for training the hybrid convolutional neural network and long short-term memory architecture (CNN-LSTM), which will be detailed in Part II.

Keywords Machine learning, Li-ion batteries, Data development, Multi-physics modeling, Hot spot

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Introduction

Progress toward a net-zero emissions future requires a 25% reduction in transportation-related greenhouse gas emissions, bringing them down to roughly 6 Gt by 2030 [1]. Transitioning to electrified vehicles is a cornerstone strategy for eliminating carbon emissions from road transport. Automotive service conditions impose exceptionally rigorous specifications on forthcoming Lithium-ion (Li-ion) battery technologies, including a minimum calendar life of 10 years, at least 1000 full charge–discharge cycles, an operational temperature range of -30 to 52 °C, and a target pack-level cost of \$100/kWh [2]. Sophisticated, adaptive management of battery internal states has emerged as one of the most powerful means to realize high-efficiency, extended-lifetime, and high-safety Li-ion systems [3, 4].

Reliable forecasting of battery operational characteristics and aging behavior is a foundational requirement for next-generation smart battery management systems (BMS); however, this task remains challenging due to the highly nonlinear, interdependent physicochemical phenomena within the cell [5–8]. Over many years, substantial effort has been invested in developing multi-physics and multi-scale computational models that describe battery response by numerically solving coupled partial differential equations governing species/charge transport, thermal energy balance, and their dependence on external inputs [9–12]. Such physics-based simulations offer considerable advantages for virtual prototyping and the refinement of electrode materials, single cells, and entire battery modules or packs—greatly reducing reliance on resource-intensive hardware testing and facilitating customized control algorithms—yet their utility for real-time decision-making is constrained by significant computational overhead. Furthermore, conventional multi-physics models exhibit limited ability to assimilate continuous measurement data, thereby hindering full exploitation of tightly integrated sensor–model frameworks [13]. Additionally, resolving spatially heterogeneous phenomena—such as localized overheating (hot spots), extreme local reaction kinetics, or reactant starvation—necessitates multi-dimensional representations (2D or 3D), which dramatically increase the computational burden due to the elaborate description of coupled transport and reaction processes required for comprehensive analysis.

Recent advancements in battery informatics demonstrate strong potential for accurately forecasting diverse battery characteristics, thereby promoting enhanced safety and operational efficiency through data-driven machine learning (ML) techniques that uncover hidden patterns and relationships in sensor and diagnostic information [14–17]. To date, progress in battery informatics has relied on numerous data-centric investigations focused on battery performance, aging processes, and risk assessment. For example, Li *et al.* [18] achieved a precise state of charge (SOC) estimation for Li-ion batteries using a convolutional neural network integrated with long short-term memory (CNN-LSTM), attaining a root mean square error (RMSE) below 0.31 %. Similarly, Severson *et al.* [19] forecasted battery endurance using a data-driven ML approach, achieving top-tier cycle-life prediction accuracy of 9.1% based on a training set of 124 commercial lithium iron phosphate/graphite cells. In another case, Zhao *et al.* [20] assessed battery failure risks in practical scenarios via an ensemble of ML algorithms—including support vector machine, gradient boosting decision tree, and others—resulting in a classification error of just 7.7 % after training on 94 matched pairs of failure-positive and safety-negative instances. Such developed models hold promise as foundational structures for creating digital twins of battery ecosystems. In general, these ML approaches depend on authentic battery measurements, making their broader applicability contingent on the volume and quality of available data [21, 22]. Regrettably, acquiring substantial quantities of high-quality experimental battery data proves challenging and costly, particularly for training large-scale ML systems [23].

As an alternative, recent initiatives have utilized multi-physics battery simulations to expand the pool of training examples for battery informatics applications [24–28]. In this approach, physics-based battery models are applied across a wide range of scenarios to generate extensive synthetic datasets, which are subsequently used for ML model training. Data of superior fidelity obtained from 3D simulations play an essential role in enabling instantaneous state estimation and propelling the evolution of AI-supported battery management systems (BMS) in electric vehicles. Relying solely on physical testing falls short of meeting these goals due to constraints such as higher costs. For instance, Li *et al.* [24] constructed a Pseudo-2-Dimensional (P2D) model to supply data for multiple ML techniques—such as random forests, artificial neural networks, and extreme gradient boosting—ultimately yielding SOC estimates with an error of 0.358%; Park *et al.* [25] applied a P2D framework to a Li-Fe battery, generating coupled thermal and electrochemical profiles to train a deep neural network that accelerated performance forecasting by three orders of magnitude. While P2D models offer excellent accuracy, they suffer from poor computational speed. More recently, Yu *et al.* [26] introduced a physics-informed deep learning strategy that merges a reduced electrochemical battery representation with deep neural networks, thereby speeding up dataset creation and markedly improving the precision, resilience, and transferability of purely data-driven ML predictions for battery SOC. Nonetheless, the final performance of any ML model is inevitably tied to the fidelity of the underlying multi-physics simulations. Therefore, comprehensive validation of these multi-physics battery models is indispensable to guarantee the trustworthiness of ML solutions trained on simulated data.

In the present study, we tackle the two primary challenges outlined earlier for battery informatics—namely, limited data availability and concerns over data trustworthiness—through three key pillars: 1) Rigorous validation of a three-dimensional (3-D) multi-physics Li-ion battery model using diverse experimental benchmarks, encompassing current-voltage profiles and thermal progression; 2) Generation of a comprehensive dataset spanning multiple operational regimes, incorporating variables such as surface cooling heat transfer coefficient, discharge C-rate, coolant temperature, and anisotropic thermal conductivity of the battery; 3) Assessment of the efficacy of this data-generation strategy by constructing and evaluating a data-driven CNN-LSTM predictive model. The current contribution primarily emphasizes pillar 1, with pillars 2 and 3 elaborated in Part II. Overall, these findings illustrate the effectiveness of combining 3-D multi-physics-informed data augmentation with ML techniques to produce reliable, high-precision surrogate models suited for next-generation sophisticated battery architectures.

Battery Data Development

Operating principles of batteries

Lithium-ion batteries operate as rechargeable electrochemical power sources that accumulate and deliver energy via the reversible movement of lithium ions between opposing electrodes. A conventional Li-ion cell includes a cathode, an anode, and an intervening separator, as conceptually shown in **Figure 1(a)** and captured photographically in **Figure 1(b)**. The positive electrode is ordinarily built from a lithium-containing metal oxide, and the negative electrode is most often graphite or a lithium-alloy material. An organic-solvent-based electrolyte containing a dissolved lithium salt enables ionic transport between the two electrodes. The separator, a microporous film that blocks electron conduction, physically isolates the cathode from the anode, eliminating the risk of direct contact and short-circuiting.

In discharge mode, lithium ions are extracted from the anode material, diffuse through the electrolyte and across the separator, and insert themselves into the cathode structure. At the same time, electrons are released from the anode and travel through the external circuit to reach the cathode, thereby creating an electric current that powers external devices.

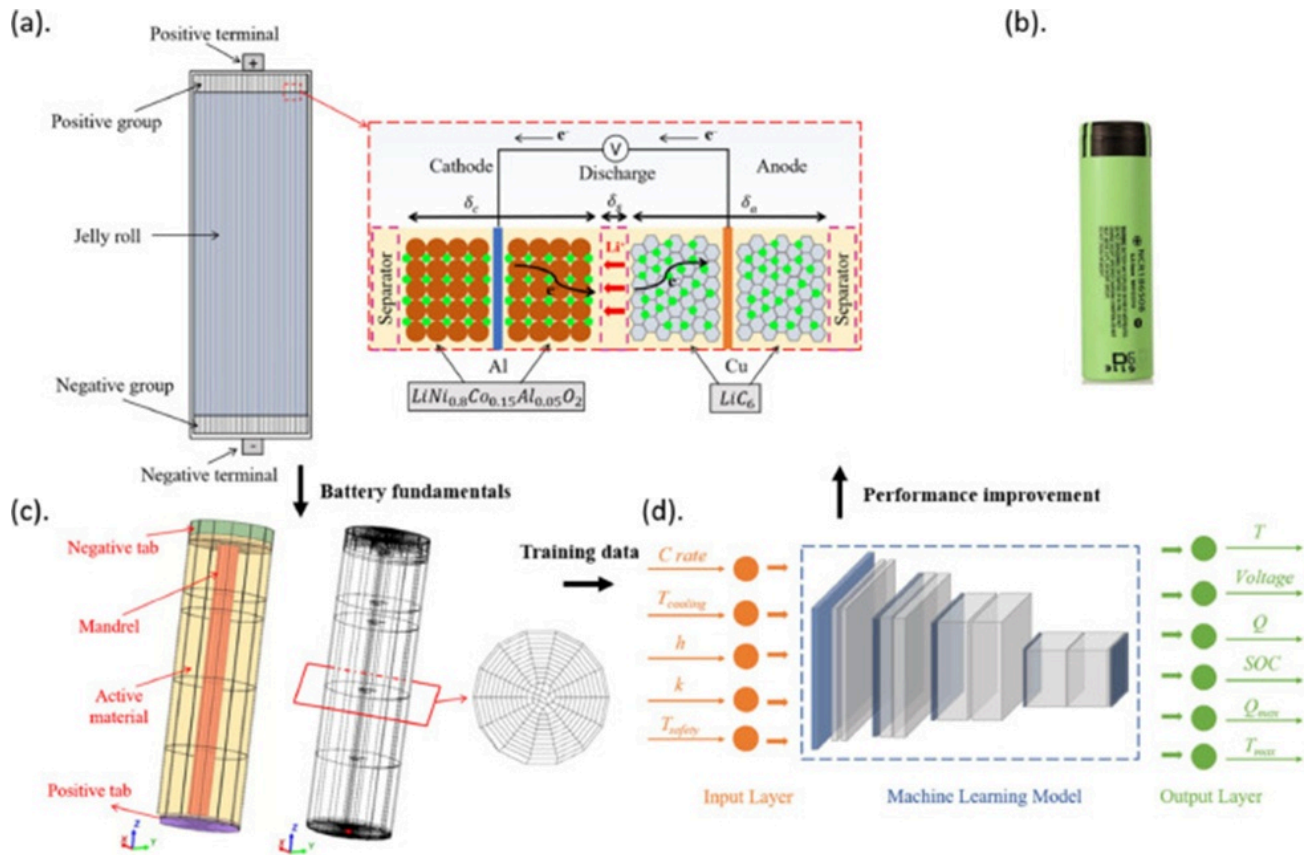
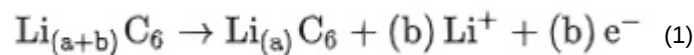


Figure 1. The modeling framework for battery informatics. (a) Schematic of Li-ion battery, structures, and operating principles, (b) The Panasonic NCR18650B battery, (c) Li-ion battery geometry and computational domain, and (d) Schematics of an ML model for battery performance prediction.

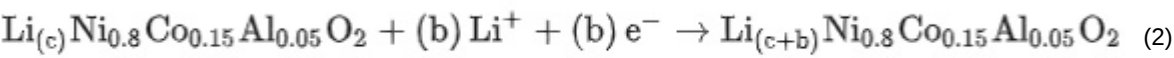
The present research examines two widely available commercial Li-ion cylindrical cells: Panasonic NCR18650B and 18650BD [29]. Each cell contains a spirally wound jelly-roll assembly together with protective safety elements. The jelly-roll stack comprises a positive electrode layer (NCA: Nickel Cobalt Aluminum Oxide (LiNi_{0.8}Co_{0.15}Al_{0.05}O₂)), a polyolefin separator, and a graphite-based negative electrode, as depicted in **Figure 1(a)**. Panasonic cells typically employ an electrolyte composed of lithium hexafluorophosphate (LiPF₆) dissolved in a 1:1 mixture of ethyl carbonate and ethyl methyl carbonate; this mixture is volatile and can evaporate readily into the atmosphere following any leakage [30]. The polyolefin separator interrupts electronic pathways and prevents internal shorts, while aluminum and copper foils serve as current collectors for the positive and negative electrodes, respectively.

The core electrochemical processes occurring at discharge are [31]:

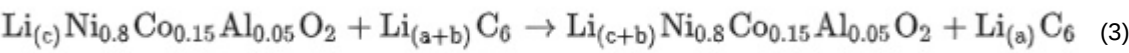
At the negative electrode:



At the positive electrode:



Overall cell reaction:



Electrochemical and thermal responses of the NCR18650BD variant were characterized at multiple C-rates on a battery cycler (NEWARE BTS-4000) [29]. Surface temperatures were monitored with five NTC thermistors placed on the cell exterior, providing readings accurate to ± 0.2 °C. Experiments were conducted at an ambient temperature of 24 °C with a charge cut-off voltage of 4.2 V. After complete charging, constant-current discharge was performed at 0.5C, 1C, or 2C. In a separate campaign, an NCR18650B cell was evaluated using the electronic load module of a fuel-cell test platform (Scribner 850e) at discharge rates of 0.3C and 0.9C while maintained at 25 °C ambient temperature. The principal geometric features and test conditions for the studied Li-ion cells are presented in Table 1.

Table 1. Geometrical and operating parameters of Li-ion batteries in this study [29].

Parameter	Panasonic NCR18650B	Panasonic NCR18650BD
Empty Cell	Panasonic NCR18650B	Panasonic NCR18650BD
Height (mm)	65	65
Diameter (mm)	18	18
Mass (g)	45.8	49.0
Rated capacity (mAh)	3200	2980
Nominal voltage (V)	3.6	3.6
Maximum charge voltage (V)	4.2	4.2
Minimum discharge voltage (V)	2.5	2.5
Energy density (Wh kg ⁻¹)	243	217
Positive electrode	NCA	NCA
Negative electrode	Graphite	Graphite
Electrolyte	EC + EMC + LiPF ₆	EC + EMC + LiPF ₆
Separator	Polyolefin	Polyolefin
Jelly roll length (mm)	60.0	60.0
Jelly roll inner/outer diameter (mm)	4 / 17.2	4 / 17.5
Positive electrode thickness (Lc, mm)	140 × 10 ⁻³	138 × 10 ⁻³
Negative electrode thickness (La, mm)	160 × 10 ⁻³	149 × 10 ⁻³
Separator thickness (Ls, mm)	32 × 10 ⁻³	32 × 10 ⁻³
Cathode tab thickness (mm)	1	1

Anode tab thickness (mm)	4	4
Initial temperature (°C)	25	24
C-rate (C)	0.3 / 0.9	0.5 / 1 / 2

Multi-physics modeling of the battery

To capture the strong nonlinear interplay between electrochemical and thermal phenomena, a comprehensive multi-physics battery model was formulated using the finite element method. The model geometry includes the negative current collector tab, mandrel, outer casing, active electrode material, and positive current collector tab. The full-cell computational domain employed in the simulation software AutoLion™ is presented in **Figure 1(c)**. This modeling framework relies on porous-electrode theory combined with concentrated-solution theory [32]. The main simplifying assumptions are listed below:

- 1) The electrolyte behaves as a concentrated binary electrolyte solution.
- 2) Side reactions and gas evolution are not taken into account.
- 3) Reaction kinetics are represented via the Butler–Volmer equation.
- 4) Solid-phase lithium-ion transport occurs solely by diffusion.
- 5) The active materials in both electrodes consist of uniform-sized spherical particles.
- 6) Any volume variation during cycling is ignored.
- 7) Electrolyte-phase ion movement results from the combined effects of diffusion and migration.
- 8) Local thermodynamic equilibrium exists at every electrode/electrolyte boundary.

Governing equations

Electrochemical reaction rates for the anode and cathode processes **Eqs. 1 and 2** are described with the Butler–Volmer kinetic expression:

$$\vec{i}_{nj} = i_{oj} \left[\exp \left(\frac{a_{aj} F}{RT} \eta_j \right) - \exp \left(-\frac{a_{cj} F}{RT} \eta_j \right) \right] \quad (4)$$

Where a_{aj} and a_{cj} are the anodic and cathodic transfer coefficients for reaction j , i_{nj} (A m⁻³) is the local electrode reaction current density, i_{oj} (A m⁻³) is the exchange current density, F (C mol⁻¹) stands for Faraday's constant, T (K) is absolute temperature, and R (J K⁻¹ mol⁻¹) denotes the gas constant.

Charge balance in the electrolyte phase reads:

$$\nabla \cdot (k^{eff} \nabla \phi_e) + \nabla \cdot (k_D^{eff} \nabla \ln c_e) = -j^{Li} \quad (5)$$

Where ϕ (V) represents the electrolyte potential, subscript e refers to the electrolyte, c is the lithium-ion concentration (mol m⁻³), k^{eff} (S m⁻¹) is the effective conductivity of the electrolyte, and k_D^{eff} (m² s⁻¹) is the diffusion-related conductivity term, expressed as:

$$k_D^{eff} = \frac{2RTk^{eff}}{F} (t_+^0 - 1) \left(1 + \frac{d \ln f_{\pm}}{d \ln c_e} \right) \quad (6)$$

In which t_+^0 is the Li⁺ transference number with respect to the solvent velocity and $f_{\pm}$ is the mean molar activity coefficient. Charge conservation within the solid phase is written:

$$\nabla \cdot (\sigma^{eff} \nabla \phi_s) = j^{Li} \quad (7)$$

Where σ^{eff} (S m⁻¹) denotes the effective electronic conductivity of the solid matrix, which depends on the intrinsic material conductivity σ (S m⁻¹) and the solid volume fraction ε_s according to:

$$\sigma^{eff} = \varepsilon_s \sigma \quad (8)$$

Lithium-ion mass conservation in the electrolyte is governed by:

$$\frac{\partial(\varepsilon_e c_e)}{\partial t} = \nabla \cdot (D_e^{eff} \nabla c_e) + \frac{1-t_+^0}{F} j^{Li} \quad (9)$$

Where D_e^{eff} (m² s⁻¹) is the effective diffusivity in the electrolyte, computed via the Bruggeman correction [33]:

$$D_e^{eff} = D_e \varepsilon_e^{1.5} \quad (10)$$

Lithium diffusion inside the solid active material particles is described by:

$$\frac{\partial c_s}{\partial t} = \frac{D_s}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial c_s}{\partial r} \right) \quad (11)$$

Where r represents the radial position within a spherical particle, and c_s is the solid-phase lithium concentration.

The overall energy balance takes the form:

$$\frac{\partial(\rho c_p T)}{\partial t} = \nabla \cdot (k \nabla T) + q_r + q_j \quad (12)$$

Where ρ (kg m⁻³) is the effective density, c_p (J kg⁻¹ K⁻¹) is the specific heat capacity, k (W m⁻¹ K⁻¹) is the effective thermal conductivity, q_r (W m⁻³) is the volumetric heat release from electrochemical reactions, and q_j (W m⁻³) is the ohmic heat generation from ionic and electronic resistances, calculated as:

$$q_r = j^{Li} (\phi_s - \phi_e - U_j) + T \frac{\partial U_j}{\partial T} \quad (13)$$

$$q_j = \sigma^{eff} \nabla \phi_s \nabla \phi_s + k^{eff} \nabla \phi_e \nabla \phi_e + k^{eff} \nabla \ln c_e \nabla \phi_e \quad (14)$$

With U_j being the equilibrium open-circuit voltage of reaction j .

Overall, the battery modeling approach outlined above closely resembles frameworks commonly applied to Li-air batteries [34–36] and redox flow batteries [37–39], particularly in the formulation of transport phenomena and the depiction of electrochemical reaction kinetics.

Initial and boundary conditions

Uniform initial values are assumed for the primary variables throughout the domain.

$$c_e = c_e^0, c_s = c_s^0 \text{ and } T = T^0 \quad (15)$$

Zero-flux (Neumann) boundary conditions are imposed for lithium-ion concentration and electrical potentials at all domain boundaries, as indicated below.

$$\frac{\partial c_e^{Li}}{\partial n} = 0, \frac{\partial \phi_s}{\partial n} = 0 \text{ and } \frac{\partial \phi_e}{\partial n} = 0 \quad (16)$$

Surface heat transfer via convection is incorporated through the boundary condition:

$$-k \frac{\partial T}{\partial n} = h (T - T_a) \quad (17)$$

Where h ($\text{W m}^{-2} \text{K}^{-1}$) denotes the convective heat transfer coefficient at the battery exterior, and T_a (K) represents the temperature of the coolant or the surrounding air in the case of natural convection.

Numerical procedures

The complete set of governing equations, boundary conditions, model parameters, and material properties utilized in this study is summarized in **Table 2**. These values were obtained either through direct experimental measurements or extracted from established literature sources. Simulations were conducted using finite element discretization in the AutoLion™ platform, with a fixed time step of 5 s. A maximum of 100 iterations was allowed per time step, and convergence was enforced when residuals fell below 1×10^{-8} . The electrical mesh featured 4 elements along the length and 2 along the height, while the thermal mesh employed 15 elements circumferentially, as depicted in **Figure 1(c)**. All computations were run on a conventional desktop PC equipped with an Intel(R) Core(TM) i7-6700K processor operating at 4.00 GHz and 16 GB of RAM.

Table 2. Model parameters.

Parameter	Value

Density of negative/positive electrode (kg cm ⁻³)	2200 × 10 ⁶ / 3600 × 10 ⁻⁶
Specific heat of jelly roll (J kg ⁻¹ K ⁻¹)	1150 / 1150
Bruggeman tortuosity exponent	1.5
Thermal conductivity of separator (W cm ⁻¹ K ⁻¹)	0.005
Electrical conductivity of negative/positive electrode (S m ⁻¹)	100 / 3.8
Charge transfer coefficient	0.5
Diffusion coefficient of negative/positive electrode – solid phase (cm ² s ⁻¹)	4.9 × 10 ⁹ / 1.0 × 10 ⁻¹¹
Mass fraction of active material in the negative/positive electrode	0.94 / 0.94
Porosity of the negative/positive electrode	0.24 / 0.34

Data generation

The established multi-physics model served as the basis for producing a large volume of simulation data across diverse operational scenarios. A comprehensive dataset encompassing battery capacity, terminal voltage, state of charge (SOC), and temperature profiles was generated by running physics-based simulations across a broad range of conditions. These included variations in C-rate, coolant/ambient temperature, surface convective heat transfer coefficient, and anisotropic thermal conductivities in the axial and in-plane orientations, as detailed in [Table 3](#). The resulting data supported training a hybrid LSTM-CNN network to forecast voltage-capacity curves and temperature-capacity relationships. Comparable strategies leveraging data-driven surrogate models have appeared in recent literature [\[40-42\]](#). It should be emphasized that, despite validation of the 3D physics-based model against limited experimental measurements, numerical inaccuracies or instances of solver divergence may compromise the reliability of certain generated data points. Such flawed data can significantly impair the performance of machine learning models. Consequently, rigorous data quality assessment and filtering were performed before their use in ML training, as implemented in the present work.

Table 3. Data generation using the 3-D physics-based model for machine learning applications.

Parameter	Values/Range	Number of data points
Discharge C-rate (C)	0.5, 1.0, 1.5, 2.0, 2.5, 3.0	–
Ambient temperature (°C)	0 – 50	306
Heat transfer coefficient (W m ⁻² K ⁻¹)	1 – 80	480
Axial thermal conductivity (W m ⁻¹ K ⁻¹)	0.1 – 9.0	540
In-plane thermal conductivity (W m ⁻¹ K ⁻¹)	1 – 90	540

[Figure 1\(d\)](#) provides a schematic overview of the data-driven machine learning workflow, underscoring the complementary integration of the multi-physics battery model with the LSTM-CNN approach for precise battery performance forecasting. Input sequences are first processed by a 1-D convolutional layer with 6 filters and a kernel size of 4, enabling the extraction of spatial patterns from the voltage-capacity and temperature-capacity profiles across varying conditions. These extracted features are subsequently fed into an LSTM module with a hidden layer dimension of 256, which captures temporal dependencies to predict battery voltage and temperature responses under diverse discharge rates, heat transfer coefficients, ambient temperatures, and thermal conductivity values. Comprehensive details regarding the LSTM-CNN network structure and training methodology are provided in Part II [\[43\]](#).

In total, 1686 simulation cases were generated, with 80% allocated for model training and the remaining 20% reserved for testing. To ensure uniform sequence lengths during LSTM-CNN training, zero-padding was applied: short sequences were padded with zeros at the start or end until they reached the target length, corresponding, for example, to the voltage window from 4.2 V (maximum charge) to 2.5 V (cut-off discharge). Additionally, an alignment procedure was employed to guarantee that all input sequences began at the identical reference point, thereby preserving temporal coherence across the dataset.

Results and Discussion

The numerical investigations presented in this section aimed to rigorously validate the developed battery model through direct comparisons of predicted performance with experimental data, as well as parametric analyses examining how various material properties and operating parameters influence the battery's electrochemical and thermal responses.

Model validation

Figure 2 illustrates the agreement between predictions from the multi-physics battery model and experimental discharge curves [29] at three different C-rates: 0.5 C, 1 C, and 2 C. In general, the model demonstrates acceptable accuracy, with average deviations of 3.5% for battery voltage and 7% for surface temperature. The simulated voltage profiles closely match the experimental trends, including the pronounced voltage drop near 3 V. As anticipated, the battery temperature rises during discharge at varying rates primarily due to Joule heating. At the higher 2 C rate, the surface temperature reaches approximately 42 °C, reflecting insufficient heat removal by surface cooling compared to the 0.5 C case. Notably, the predicted temperature serves as a critical metric for assessing battery safety, particularly when evaluated against established safety limits (such as 50 °C).

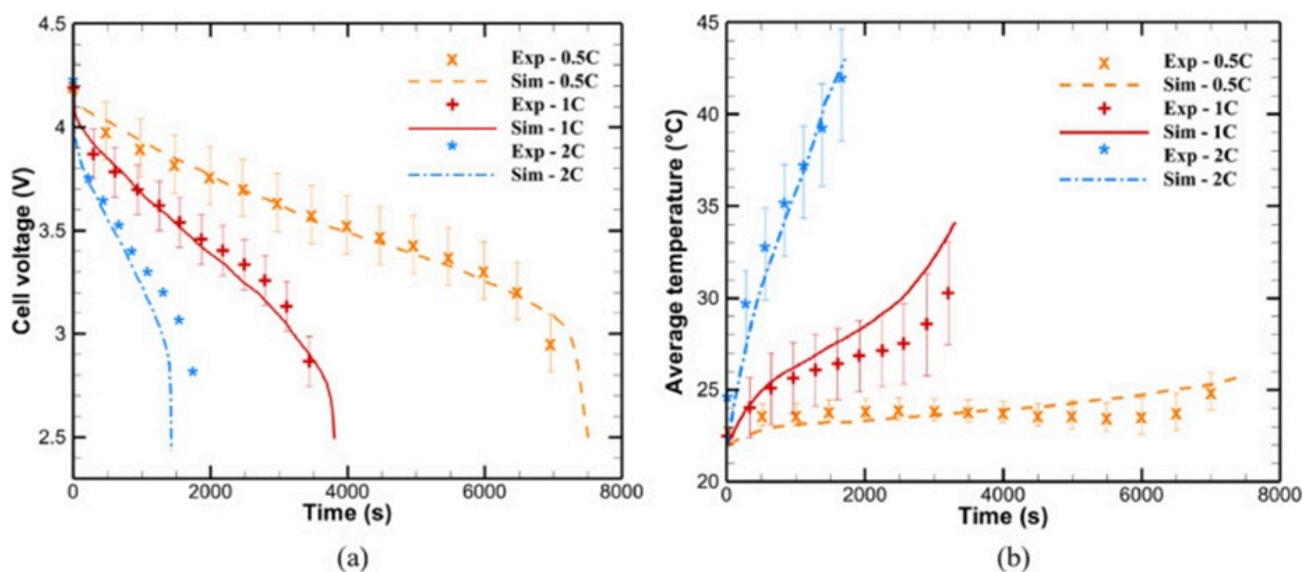


Figure 2. Experimental validation of the multi-physics battery model compared to measured curves [29] for the Panasonic NCR18650BD cell.

Figure 3 provides additional validation using a separate experimental dataset for the Panasonic NCR18650B cell at two discharge rates. Excellent correspondence is again achieved, with an average error of 4.9% at the 0.3 C rate. The simulated voltage-capacity profiles align well with the experimental measurements, confirming the model's predictive fidelity. Further validation was conducted at 0.9 C, starting from a partial charge state of 80% SOC, demonstrating the model's robust forecasting performance across arbitrary initial SOC levels.

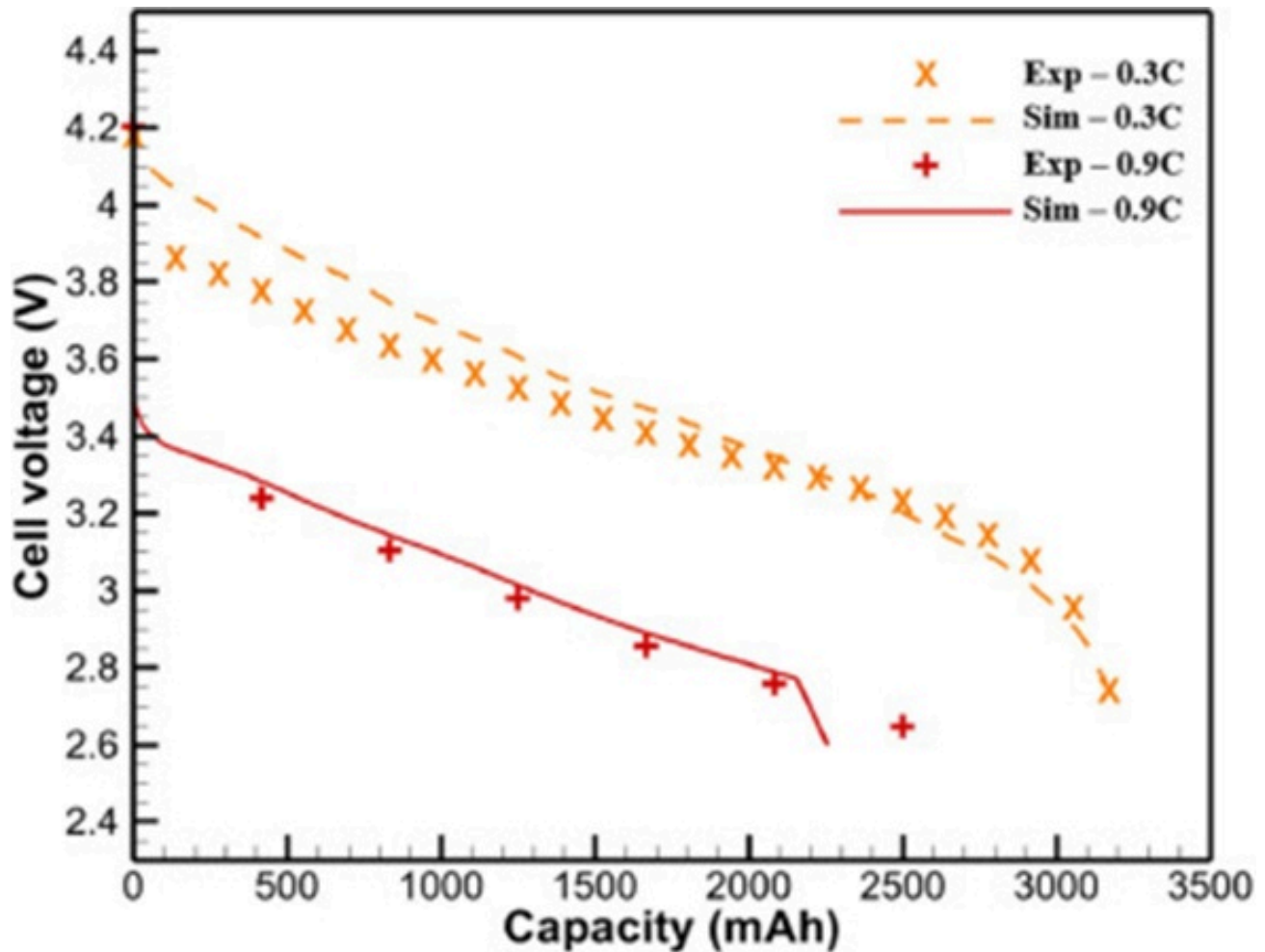


Figure 3. Experimental validation of the physics-based model against data for the Panasonic NCR18650B cell.

Analysis of battery thermal distribution

Spatial temperature variations within the battery are essential for effective safety monitoring, yet they are difficult to capture experimentally in isolation. The multi-physics model, however, readily provides detailed local temperature fields. For example, [Figure 4](#) displays the temperature distribution in a battery during 2 C discharge, with anisotropic thermal conductivities of 1 and 10 W m⁻¹ K⁻¹, a convective heat transfer coefficient $h = 20$ W m⁻² K⁻¹, and ambient temperature $T_{amb} = 22$ °C. The temperature field exhibits the expected pattern: elevated temperatures in the core region and cooler conditions near the surface, consistent with principles of conduction and convection. Analysis of the maximum temperature—a primary concern for thermal runaway risks—reveals that the central region experiences hotspots approximately 2 °C warmer than the surface and 5 °C higher than the top of the battery.

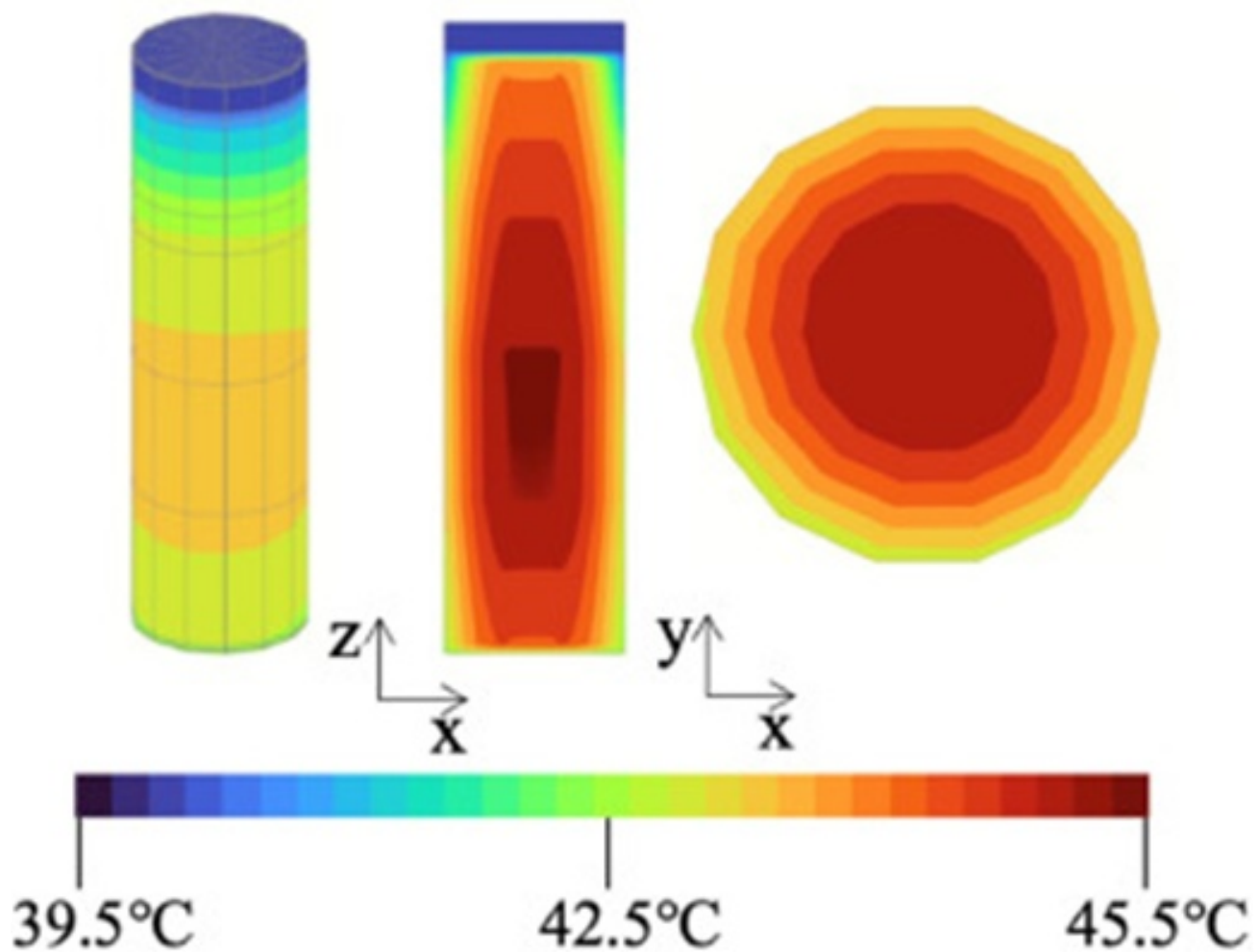


Figure 4. Spatial temperature distribution in the Panasonic NCR18650BD battery during 2C discharge, with anisotropic thermal conductivities of 1 & 10 $\text{W m}^{-1} \text{K}^{-1}$, $h = 20 \text{ W m}^{-2} \text{K}^{-1}$, and $T_{\text{amb}} = 22^\circ \text{C}$.

Influence of thermal conductivity in batteries

Lithium-ion batteries consist of layered composite materials, which give rise to strongly anisotropic heat transfer characteristics. This work explored the consequences of this directional dependence by applying separate thermal-conductivity values along the axial and radial directions within the jelly-roll structure.

Figure 5 demonstrates how contrasting pairs of thermal conductivities ($0.1 \& 1 \text{ W m}^{-1} \text{K}^{-1}$ versus $9 \& 90 \text{ W m}^{-1} \text{K}^{-1}$) affect the spatial temperature field inside the cell. Results reveal that poor thermal conductivity produces a dramatically steeper internal temperature gradient, with a peak temperature of 70°C , even while the outer surface remains close to the acceptable safety limit of 50°C . According to Fourier's law, materials possessing low thermal conductivity exhibit high thermal resistance, which directly accounts for this steep gradient.

Comparing the two conductivity sets further highlights that insufficient local heat conduction can drive dangerously elevated temperatures at specific locations and increase the risk of initiating thermal runaway. Thus, raising the local thermal conductivity represents an effective strategy for suppressing hot spots within the cell. As illustrated in **Figure 5b**, incorporation of highly conductive materials markedly lowers the peak temperature down to 44°C .

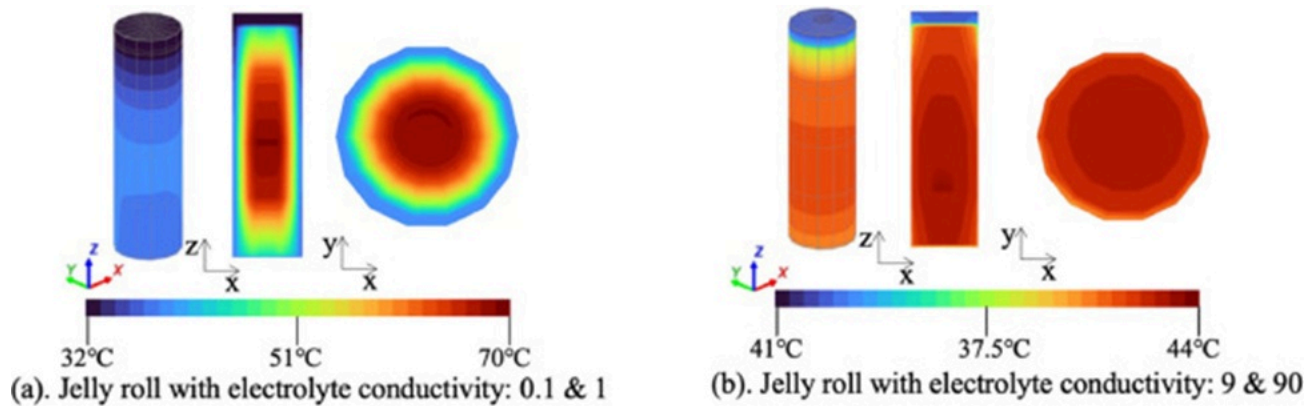


Figure 5. Three-dimensional temperature profiles in the Panasonic NCR18650BD cell using thermal conductivities of: (a) 0.1&1 $\text{W m}^{-1}\text{K}^{-1}$; (b) 9&90 $\text{W m}^{-1}\text{K}^{-1}$, at 2 C discharge rate, $h = 20 \text{ W m}^{-2}\text{K}^{-1}$, and ambient temperature $T_{\text{amb}} = 22^\circ\text{C}$.

Additional insight into the role of thermal conductivity on overall cell behavior appears in [Figure 6](#), which compares three conductivity scenarios ($k = 0.1 \text{ \& } 1$, $1 \text{ \& } 10$, and $9 \text{ \& } 90 \text{ W m}^{-1}\text{K}^{-1}$) during 2C discharge with $h = 20 \text{ W m}^{-2}\text{K}^{-1}$ and $T_{\text{amb}} = 22^\circ\text{C}$. Throughout most of the discharge process, differences in voltage and capacity remain small. Noticeable divergence only emerges near the end of discharge. This pattern arises because heat generation is relatively modest from 100 % to ≈ 30 % SOC. Still, both reversible entropic heat and irreversible Joule heating rise sharply in the final stage (≈ 30 % to 0 % SOC) [44], magnifying the temperature spread among the different conductivity cases and thereby accentuating voltage deviations. The variation is also linked to core temperature differences: higher core temperatures accelerate electrochemical kinetics and ionic/electronic transport, which, in turn, reduce polarization losses and enhance overall energy efficiency [45].

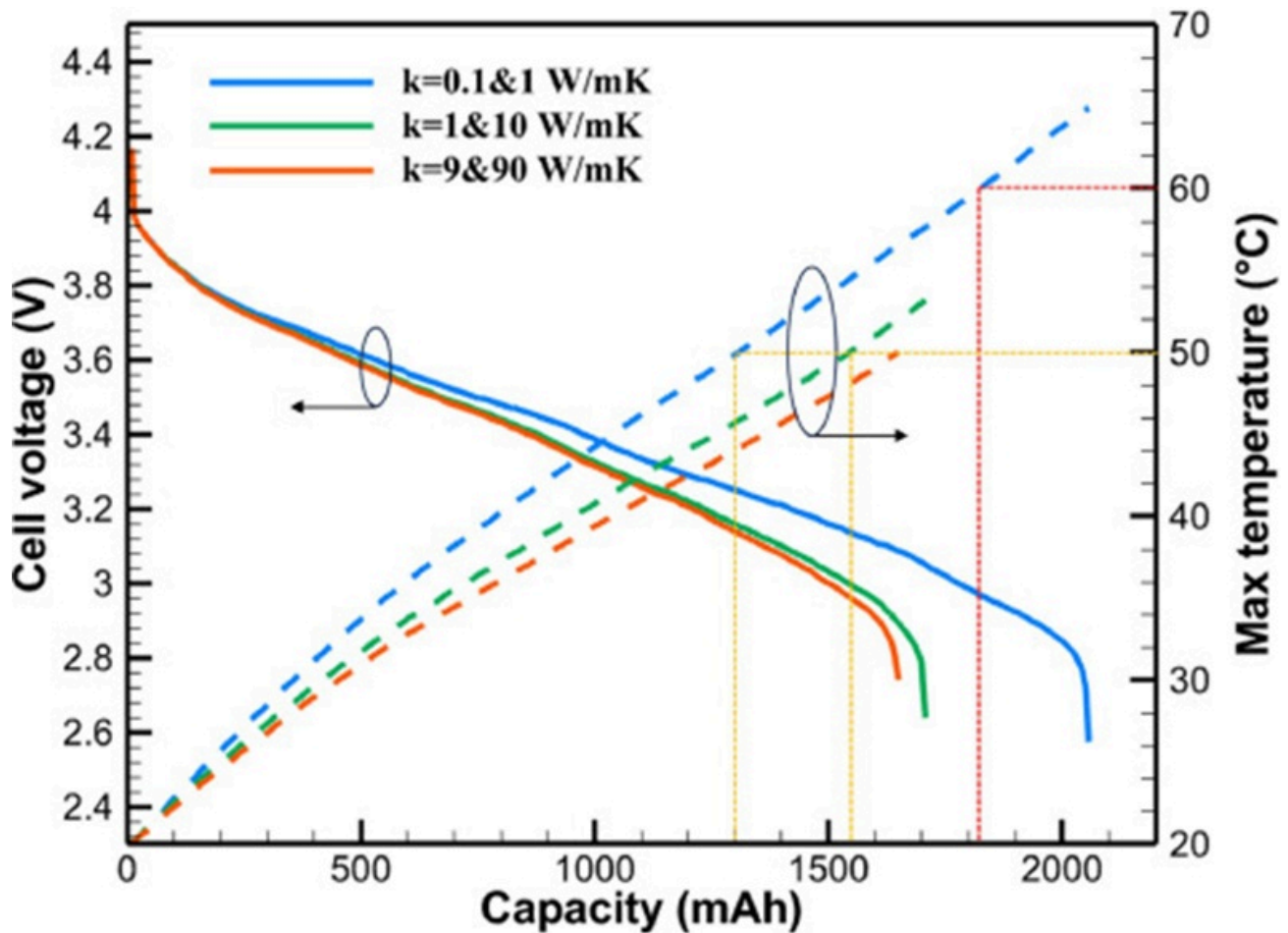


Figure 6. Discharge performance curves together with maximum (hotspot) temperature of the Panasonic NCR18650BD cell for different thermal conductivity pairs at 2 C rate, $h = 20 \text{ W m}^{-2}\text{K}^{-1}$ and $T_{\text{amb}} = 22^\circ\text{C}$.

Given the critical safety temperature limits of batteries, the peak temperature directly governs the usable discharge capacity. **Figure 6** shows that cells with low thermal conductivity experience a much quicker temperature climb. In the low-conductivity case, discharge terminates at only 1300 mAh when the 50°C threshold is met and at 1800 mAh when the 60°C threshold is met, underscoring how severely reduced thermal conductivity constrains the extractable capacity.

Impact of convective heat transfer coefficient

To evaluate how external cooling intensity influences cell behavior, four values of the convective heat transfer coefficient h (ranging from 1 to $80 \text{ W m}^{-2}\text{K}^{-1}$) were simulated for the Panasonic NCR18650BD under continuous 2°C discharge, corresponding to different cooling regimes from very weak to strong forced convection.

Figure 7 indicates that temperature naturally increases over time due to the combined effects of ohmic and entropic heating throughout the discharge. Nonetheless, the cell response diverges significantly depending on whether natural or forced convection dominates. In the natural convection regime ($h < 30 \text{ W m}^{-2}\text{K}^{-1}$), the maximum temperature surpasses the critical safety thresholds of 50°C or 60°C , forcing early discharge termination at roughly 1200 mAh or 1800 mAh, respectively. Raising h to $10 \text{ W m}^{-2}\text{K}^{-1}$ provides only a modest extension of capacity (≈ 1700 mAh before hitting 50°C). By contrast, applying strong forced convection (higher h values) enables the cell to deliver nearly its full theoretical capacity without violating thermal limits.

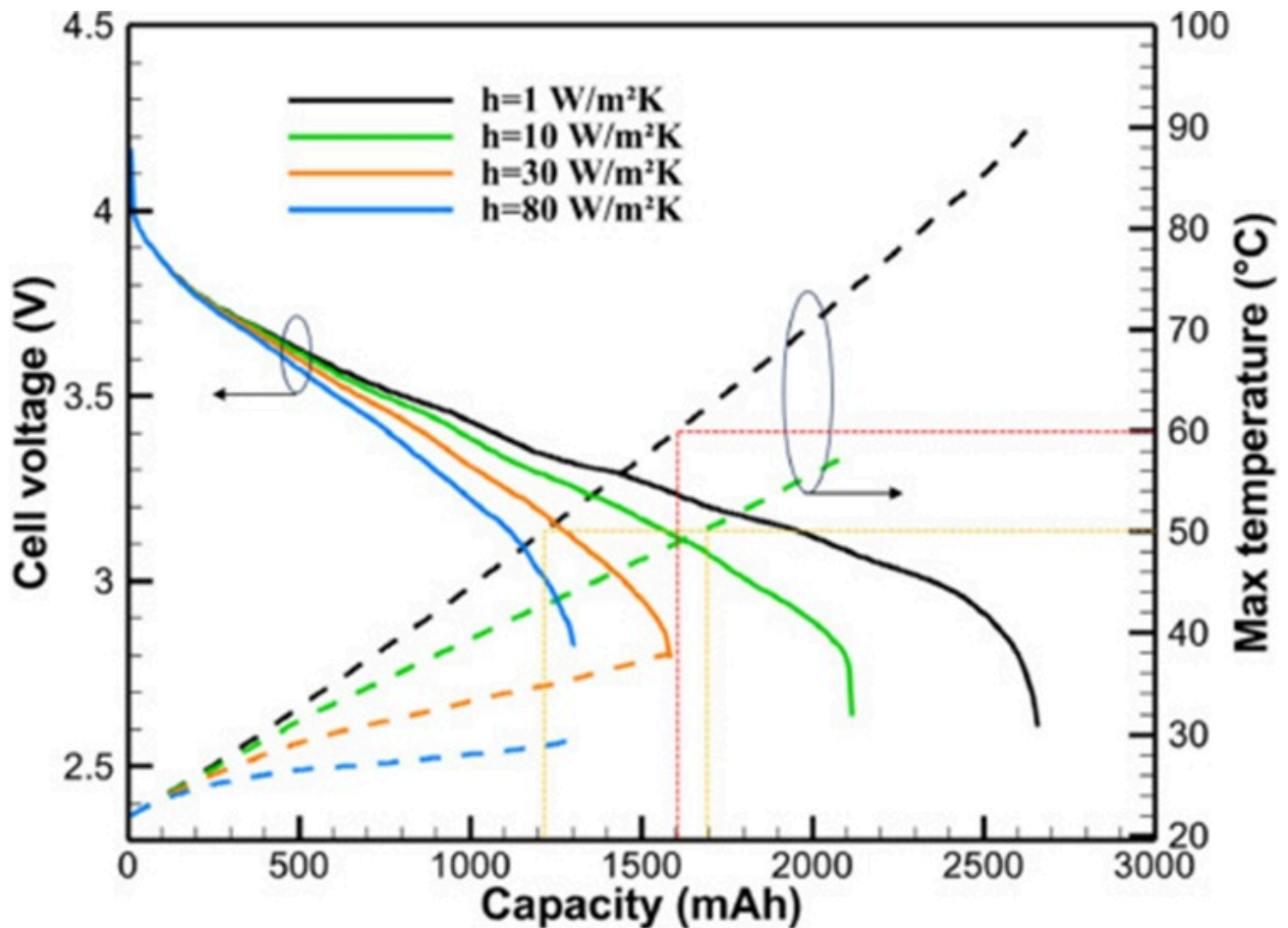


Figure 7. Voltage profiles and maximum (hotspot) temperature of the Panasonic NCR18650BD cell during discharge at ambient temperature under various convective heat transfer coefficients. Remaining conditions: $k = 1\&10\text{ W m}^{-1}\text{K}^{-1}$, $T_{\text{amb}} = 22\text{ }^{\circ}\text{C}$, 2 C discharge rate.

Effects of ambient temperature

Here is the paraphrased version, maintaining the original structure, all numbers, and placing figure references in brackets:

Ambient temperature constitutes another vital factor in convective cooling processes. Standard indoor room temperature typically hovers around $20\text{ }^{\circ}\text{C}$, whereas the highest temperature ever recorded worldwide is $60\text{ }^{\circ}\text{C}$. **Figure 8** presents the maximum battery temperature and corresponding capacity at a 2 C discharge rate under three different ambient temperatures: $20\text{ }^{\circ}\text{C}$, $40\text{ }^{\circ}\text{C}$, and $60\text{ }^{\circ}\text{C}$. The data reveal that the battery's peak temperature rises more quickly during the initial phase in the $40\text{ }^{\circ}\text{C}$ and $60\text{ }^{\circ}\text{C}$ cases than in the $20\text{ }^{\circ}\text{C}$ baseline, as both internally generated waste heat and the elevated ambient conditions (transferred via the cooling airflow) contribute to cell heating. The rate of temperature increase noticeably decelerates once the temperature exceeds $20\text{ }^{\circ}\text{C}$, at which point the cooling mechanism becomes active. Elevated ambient temperatures result in higher battery voltage, owing to warmer cell temperatures that enhance ionic transport and electrochemical kinetics. In the $60\text{ }^{\circ}\text{C}$ scenario, the battery temperature stays below $50\text{ }^{\circ}\text{C}$ and $60\text{ }^{\circ}\text{C}$ until the discharged capacity reaches 600 mAh and 1000 mAh, respectively—corresponding to less than one quarter and one half of the nominal capacity without thermal restrictions (approximately 2700 mAh). This $60\text{ }^{\circ}\text{C}$ case clearly illustrates the substantial capacity sacrifice required to maintain battery safety in extremely hot environments. By comparison, the usable capacity at $40\text{ }^{\circ}\text{C}$ was markedly greater than in the extreme heat case, achieving 1200 mAh and 2200 mAh while respecting the $50\text{ }^{\circ}\text{C}$ and $60\text{ }^{\circ}\text{C}$ temperature thresholds, respectively. At an ambient temperature of $20\text{ }^{\circ}\text{C}$, the battery

delivered its full capacity (1700 mAh) while maintaining a very safe maximum temperature of 40 °C, comfortably below the critical safety limit.

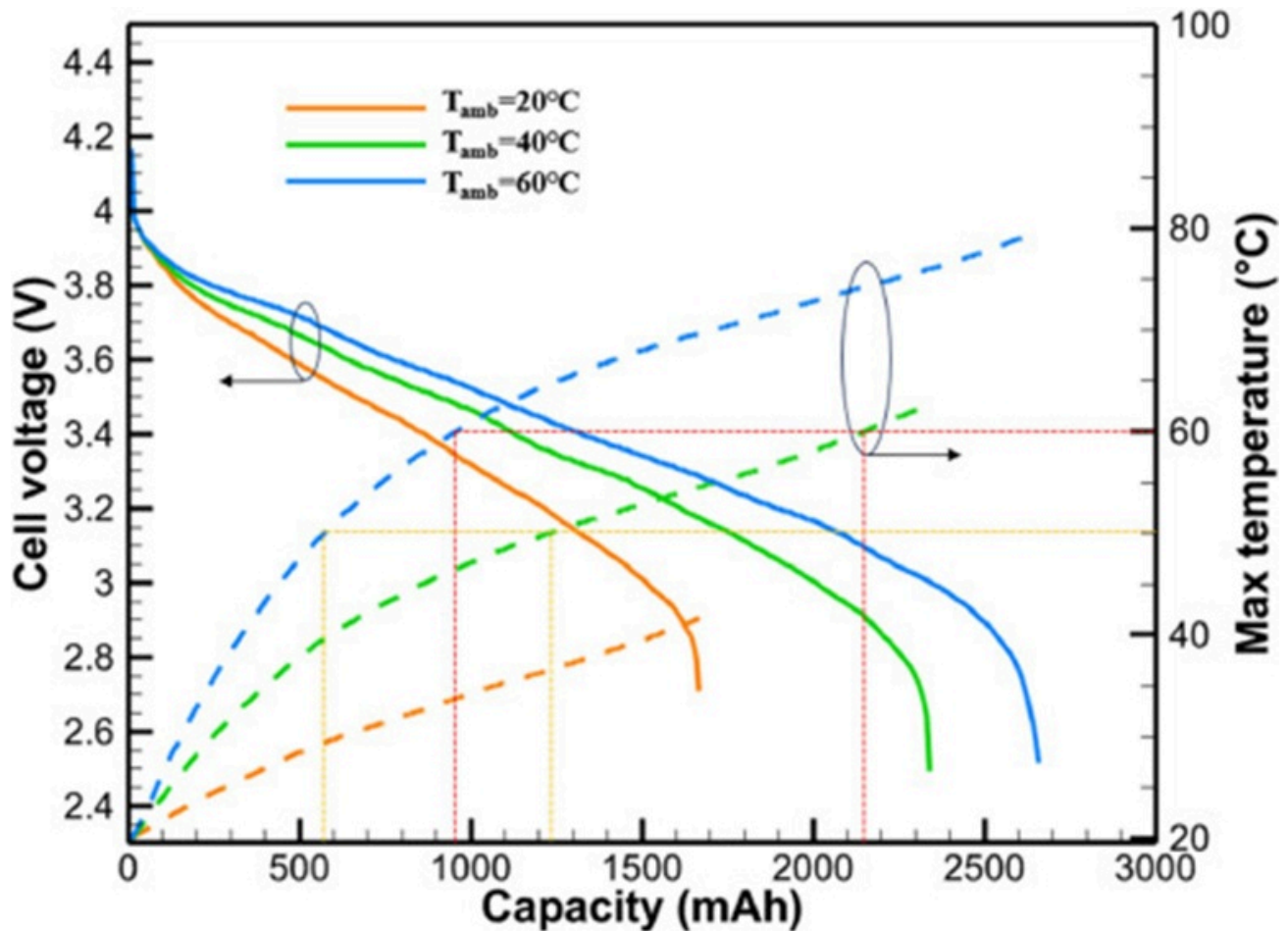


Figure 8. Battery voltage and maximum temperature (hot spot) of the Panasonic NCR18650BD cell operating at $h = 20 \text{ W m}^{-2} \text{ K}^{-1}$ and a 2 C discharge rate across various ambient temperatures.

Conclusion

This work represents one of the essential steps toward cost-effective, data-driven battery informatics. A multi-physics battery model was constructed to numerically simulate battery behavior by solving the relevant physical and electrochemical governing equations. A detailed analysis of the generated data showed excellent agreement with two independent sets of experimental curves, with the maximum error below 7% for the cell voltage-capacity profiles. An extensive parametric investigation was performed to confirm the influence of varying thermal conductivities, heat transfer coefficients, and ambient temperatures on battery performance. The findings revealed that battery behavior is highly sensitive to low thermal conductivity, which promotes localized high temperatures (hot spots) that may initiate thermal runaway and compromise battery safety.

Furthermore, elevated cooling parameters—specifically higher heat transfer coefficients—proved effective in increasing the usable battery capacity by delaying the rise of the maximum battery temperature (hot spot) toward the critical safety threshold. Finally, the results demonstrated that batteries become particularly vulnerable under extremely high ambient temperatures (60 °C) due to excessively rapid local temperature increases, resulting in the loss of nearly half the

theoretical capacity during safe operation. The comprehensive validation and evaluation of this multi-physics battery model confirm its feasibility and reliability for generating numerical data to advance battery informatics.

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Conflict of interest

None

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None

Ethics statement

None

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