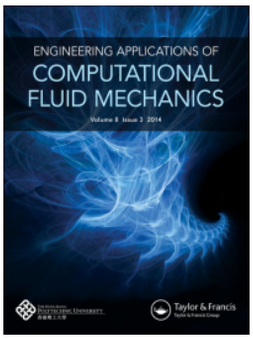

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Thermal runaway and flame propagation in battery packs: numerical simulation and deep learning prediction

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ABSTRACT

The widespread application of lithium-ion battery technology faces a significant challenge from the inherent risk of thermal runaway and consequent fire spread. This paper proposes an intelligent framework for predicting the temperature distribution and thermal runaway propagation in a battery pack across diverse conditions, including various battery types, ambient temperatures, and fire heat release rates. First, we generate an extensive numerical database, comprising 36 simulations of battery jet flame and thermal runaway processes that are validated by experimental data. Subsequently, a dual-agent artificial intelligence (AI) model is employed to forecast the cell-to-cell thermal runaway propagation and evolution of temperature field in the battery pack. The results demonstrate the accuracy and reliability of the deep-learning approach in capturing battery thermal runaway dynamics. Quantitatively, the AI-based methodology achieves a relative error below 10% for thermal runaway time predictions in database-contained scenarios and below 30% for extrapolated cases. The model also shows excellent performance in predicting temperature field distributions, with an R⊃2 value exceeding 0.99 and a maximal MSE of 1.52 s⊃2. This study underscores the potential of AI method in improving the battery safety management, thereby facilitating timely interventions, preventive maintenance and fire safety of battery energy storage system.

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KEYWORDS
Lithium-ion battery; smart energy; CFD simulation; fire modelling; jet flame; artificial intelligence

Nomenclature

Symbols

A	Pre-exponential factor [s^{-1}]
E	Activation energy [J/mol]
T	Temperature [°C]
t	Time [s]
y_i	Predicted value
$\hat{y}_i$	Simulated value

Subscripts

sim	Simulation

Abbreviation

AI	Artificial intelligence
ANN	Artificial neural network
CFD	Computational fluid dynamics
CNN	Convolutional neural network
DMC	Dimethyl carbonate
EMC	Ethyl methyl carbonate
FDS	Fire dynamics simulator
GNN	Graph neural network
HRR	Heat release rate
HWS	Heat-wait-seek
LCO	Lithium cobalt oxide
LES	Large eddy simulation
LFP	Lithium iron phosphate
LIB	Lithium-ion batteries
MAE	Mean absolute error
MPINN	multiphysics-informed neural network
MSE	Mean squared error
NMC	Lithium nickel manganese cobalt oxide
R^2	Coefficient of determination
ReLU	Rectified linear units
SEI	Solid electrolyte interface
SoC	State of charge
SoH	State of health
SP	Speed of propagation
TR	Thermal runaway

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1. Introduction

The escalating demand for high-performance Lithium-ion batteries (LIBs), driven by the ever-expanding applications in portable electronic devices, electric vehicles, and battery energy storage systems, has accentuated the imperative for ensuring their safety and reliability (Bravo Diaz et al., 2020). However, the widespread adoption of battery technology faces a significant challenge in the form of the inherent risk of thermal runaway (Feng et al., 2020). Thermal runaway refers to the uncontrollable increase in temperature within a battery (Feng et al., 2014; Feng et al., 2018), leading to potential overheating, fire or even explosion (Wang et al., 2012; Wang et al., 2019). The ability to predict and mitigate thermal runaway is crucial for bolstering safety measures, optimizing battery performance, and fostering the sustainable integration of energy storage technologies.

To address these challenges, advancements in battery management technologies have introduced innovative approaches for monitoring and improving battery performance. For instance, state of charge (SoC) and state of health (SoH) estimation methods have significantly enhanced battery reliability and safety. Chen et al. (2024) proposed a performance simulation method that couples aging effects with battery models to better understand degradation mechanisms and their influence on overall battery performance. Meanwhile, an adaptive optimization-backpropagation neural network (AO-BPNN) method has been developed for SoC estimation under high-rate pulse conditions, enabling real-time and precise monitoring of battery conditions (Fu et al., 2023). These approaches provide a robust foundation for predicting battery behaviour and preventing failures, thereby complementing efforts to manage thermal runaway.

In addition to advancements in battery management systems, many studies have focused on thermal runaway prediction via experimental methods (Chen et al., 2019; Ditch & Zeng, 2023; Liu et al., 2022; Liu et al., 2024; Mallick & Gayen, 2023; Wang et al., 2020) and modelled the thermal runaway of a single battery (Kim et al., 2024; Kong et al., 2021; Shelkea et al., 2022; Zhang et al., 2021). For example, Kong et al. (2021) used OpenFoam to simulate thermal runaway behaviours of lithium-ion batteries with different battery materials and heating conditions. Zhang et al. (2021) conducted 3-D simulations of $LiFePO_4$/graphite cell thermal runaway triggered by local overheating based on the energy conservation equation. Shelkea et al. (2022) combined numerical and experimental methods to examine thermal runaway in large-format 21700-type cylindrical lithium-ion batteries using both the heat-wait-seek (HWS) protocol and under isothermal conditions. Kim et al. (2024) developed a battery thermal runaway model considering combustion for efficiently simulating thermal runaway of a single pouch cell.

Comparatively, the numerical simulations of the thermal runaway propagation in battery packs are still limited and challenging in terms of thermal runaway mechanisms and flame behaviours. Some researchers (Hoelle et al., 2023; Hu et al., 2021; Jia et al., 2020; Kong et al., 2022; Larsson et al., 2016; Takagishi et al., 2022; Zhang et al., 2023; Zhang et al., 2024) have investigated the thermal runaway behaviour of battery packs through simulations. Larsson et al. (2016) addressed this gap by presenting a model predicting thermal runaway propagation in lithium-ion battery packs, emphasizing cell-to-cell effects. Hu et al. (2021) explored the impact of insulation on self-heating ignition in LIB ensembles using a numerically affordable 3-D anisotropic homogeneous model. Takagishi et al. (2022) introduced a 3-D heating test simulation model for Li-ion cylindrical cells and modules, demonstrating efficacy in evaluating thermal runaway behaviour. Zhang et al. (2023) developed a 3D simulation model of thermal runaway in 18650 lithium-ion batteries, incorporating thermal decomposition, gas generation and combustion, as well as solid particle ejection and heat transfer. Kong et al. (2022) presented a coupled conjugate heat transfer and CFD model to predict the thermal runaway evolution and jet fire behaviour in 18650 lithium-ion batteries under thermal abuse. Zhang et al. (2024) developed a preliminary 3D thermal runaway propagation model for battery packs, achieving high simulation accuracy and effectively capturing propagation trends. However, the computational intensity and time-consuming nature of simulating battery thermal runaway make them impractical for real-time prediction of such events. These limitations highlight the necessity of developing a more efficient approach capable of addressing the complexities of thermal runaway propagation and flame behaviours in battery packs.

To address the challenges in predicting the propagation of thermal runaway and flame in a large battery pack with many cells, the use of artificial intelligence (AI) method is emerging. Recent applications of AI techniques have improved the accuracy of fire detection, the efficiency of fire engineering design and the capacity of fire forecast (Huang & Tam, 2024). For examples, Tam et al. (2022) utilized graph neural networks (GNN) to predict temperature field and fire propagation in complex building. Similarly, Li and Zhao (2020) employed convolutional neural networks (CNN) for fire detection, showcasing its superiority compared with other algorithms using manually extraction features. Wang, Zhang, and Huang (2022, 2023) harnessed AI for training in smoke

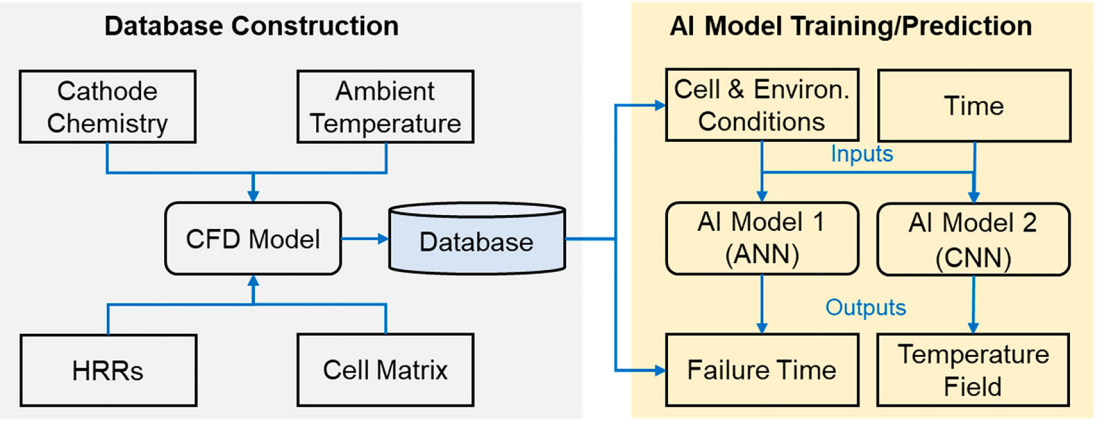

Figure 1. Framework of training AI model for predicting thermal runaway propagation in battery packs.

and fire image recognition, enabling real-time fire information assistance in firefighting scenarios. Ouyang et al. (2023) employed a fuzzy system and a multi-task CNN-LSTM model to predict thermal runaway propagation in lithium-ion battery packs, addressing the challenges posed by data uncertainty and limited availability.

This utilization of AI holds promises in accelerating the computation speed of battery thermal runaway, which has helped mitigate safety concerns associated with lithium-ion batteries (Zhao et al., 2024). For example, Meng et al. (2023) present an integrated methodology utilizing fault tree analysis, dynamic Bayesian network, and support vector regression to dynamically predict risks, providing a systematic approach to enhance safety in lithium-ion batteries. Kim et al. (2023) introduce a multiphysics-informed neural network (MPINN) for accurate estimation and prediction of thermal runaway, incorporating governing physics laws to surpass traditional artificial neural networks. Yan et al. (2022) employ an artificial neural network (ANN) for effective prediction of temperature variations in lithium-ion battery packs, thereby improving safety assessments. Daniels et al. (2024) propose a machine learning model for precise faulty cell position prediction, enhancing safety and cost efficiency. While these models have improved the state-of-the art significantly, they are limited with respect to providing real-time information during actual battery failure processes. The development of AI-based methods tailored for thermal runaway and flame propagation is essential to address these gaps and ensure the safe application of lithium-ion batteries in critical systems.

This paper introduces an innovative approach to model and predict the complex thermal runaway propagation for a pack composed of 12 cylindrical Lithium-ion battery cells. First, a pyrolysis-based model was introduced to simulate the 18650-type battery flames in thermal runaway of battery packs, providing a detailed understanding of the underlying mechanisms. Then, a database is constructed through numerical simulations for different cathode chemistries, ambient temperatures, and heat release rates (HRRs). After training the database, the deep learning models are utilized to predict both the thermal runaway time and the evolution of temperature fields over time, showcasing their potential for accurate and efficient predictions. These numerical models and AI models deepen our understanding of dynamic thermal-runaway behaviours, facilitate the safety management of battery storage system, and fosters the development of adaptive control systems. Additionally, this study explores the feasibility of using AI for analyzing battery thermal runaway behaviours and provides insights for future research directions in this field.

2. Methodology

The foundation of this research lies in the generation of a comprehensive dataset through the utilization of advanced simulation tools. Fire Dynamics Simulator (FDS) is employed to simulate a fixed geometry (4 × 3) of thermal runaway scenarios. The simulations, capturing variations in cathode chemistries, ambient temperatures, and HRRs, form the bedrock upon which the subsequent deep learning models are constructed, see Figure 1. In AI model training, the input variables encompassing battery pack conditions, namely battery chemistry, ambient temperature, and HRRs, are leveraged to facilitate the training of two distinct models. One model is dedicated to predicting battery failure time, and the other model focuses on forecasting the temperature distribution of a battery pack. The overall objective is to imbue the models with the ability to generalize across these diverse conditions, thereby enhancing their applicability to real-world scenarios.

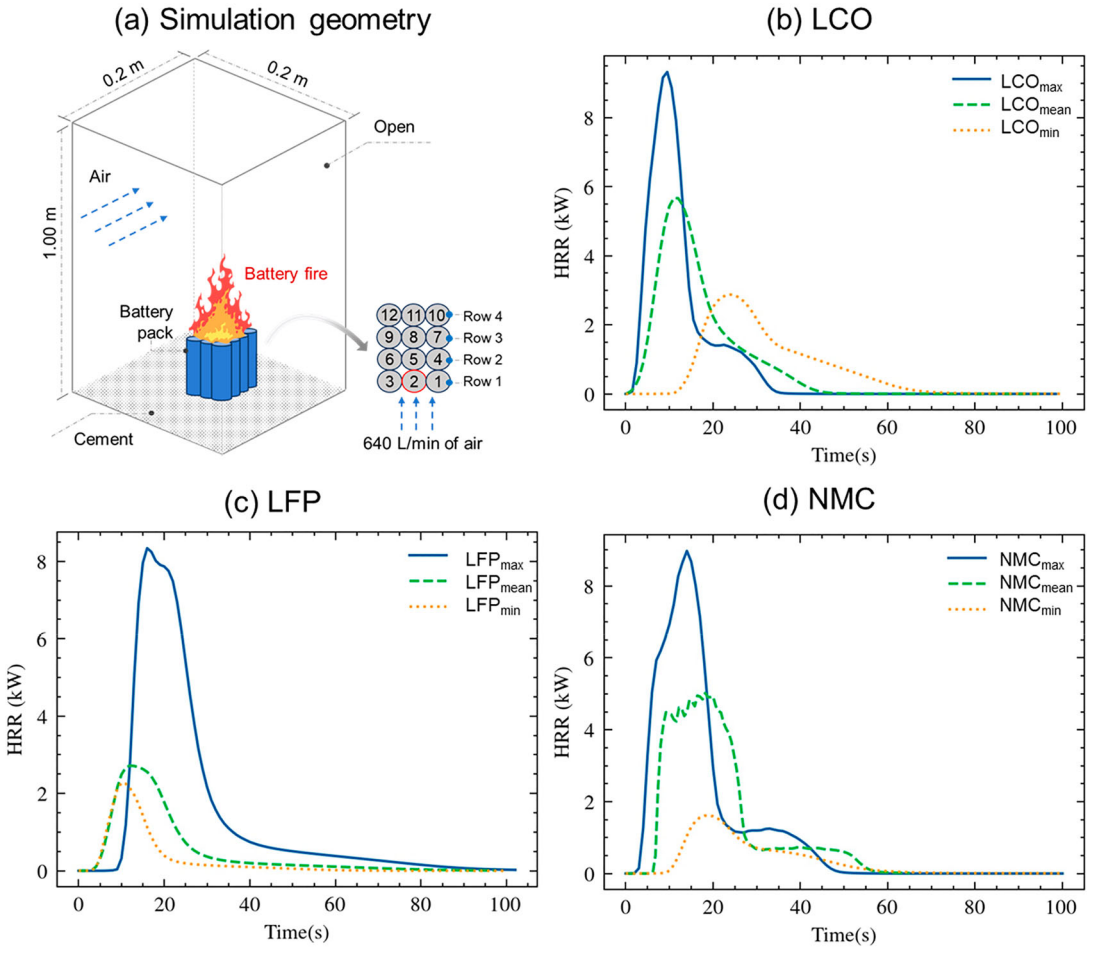

Figure 2. (a) Simulation geometry including the dimensions and boundaries, the minimum, mean, and maximum HRR of (b) LCO, (c) LFP, (d) NMC cell.

Within this context, the forthcoming sections delve into the intricate details of the methodology, beginning with an elucidation of the simulation process using FDS. Subsequently, the architecture and training of the deep learning models are expounded upon, outlining the detailed process by which the models learn and generalize from the simulated thermal runaway data. The results obtained from the application of these models to diverse scenarios are then presented, furnishing insights into the models' efficacy and reliability.

2.1. CFD model set-up

In the endeavour to establish an extensive thermal runaway database for battery fires, 18650-type lithium-ion battery cells are chosen to construct the pack model, as depicted in Figure 2(a). For simplicity, all cylindrical cells in the model are closely packed and have direct contact with the nearby cells. All simulations are carried out in FDS 6.8.0 (McGrattan et al., 2020) as the computational tool, which is an open-source CFD code with Large Eddy Simulation (LES) turbulence solver. The computational domain, comprising a cube measuring $0.2 \times 0.2 \times 1.0\ m^3$, was specifically designed to capture the flame effectively. To ensure computational independence, a grid resolution of 2 mm was employed, based on our previous work (Hosseini & Maghrebi, 2021).

Boundary conditions were set to reflect an open environment at the top and sides of the computational domain, allowing free flow of gases and heat, while the bottom boundaries were treated as walls with no-slip conditions. The initial conditions assumed an ambient temperature and atmospheric pressure, ensuring uniform initial conditions across all simulation scenarios. The material properties of the cells, such as thermal conductivity, specific heat, and density, were defined according to the typical characteristics of 18650-type lithium-ion batteries, as sourced from the literature (Sadeghi & Restuccia, 2024).

Figure 2(a) illustrates a top view schematic of the cell packs tested. A battery pack matrix with 12 cells was simulated in an environment with a 640 L/min air flow. The

airflow was modelled using a uniform inlet velocity at the domain's inlet boundary, ensuring a controlled convective environment consistent with experimental setups.

The initiation of battery thermal runaway was postulated to commence through a complex electrochemical reaction process inside the cell (Ditch & Zeng, 2023), yielding and injecting flammable gases and particles to form a flame. The underlying degradation and gas-generation process inside the battery is very similar to the 'pyrolysis' of a common combustible solid, except that such a process is self-sustained without the flame heating and intensive enough to form a jet flame. Sadeghi and Restuccia (2024) proposed a single-step pyrolysis model to simulate fires in thermal runaway, in which a solid lumped substance is used to represent the battery components and degrades into volatiles to form flame. A kinetic analysis is performed using FDS to estimate the activation energy (E) and pre-exponential factor (A). The remaining parameters, including the material thermal properties, were estimated by fitting the HRR to experimental data for 18650-type batteries with LCO, LFP, and NMC cathodes. The same model is used in this work. The single-step pyrolysis model incorporates a reaction rate that is dependent on temperature, following an Arrhenius-type expression with parameters calibrated to replicate the experimentally observed thermal runaway behaviour.

For each battery, 8 temperature sensors are strategically positioned along the surface of each cell across the vertical direction to continually monitor the temperature distribution. Cell 2 (marked in red) was heated by setting an internal heat generation to trigger the thermal runaway propagation, based on the experimental measurement (Coman et al., 2016; Sadeghi & Restuccia, 2024). This internal heat generation was applied uniformly across the cell volume and activated initially to mimic the onset of thermal runaway. The onset of thermal runaway in the remaining batteries is set by an average temperature of 180 °C (He et al., 2024; Niu et al., 2020; Said & Stoliarov, 2021; Wang et al., 2019). Once this threshold is reached in any of the other batteries, the internal heat generation is dynamically activated to simulate the exothermic reactions typical of thermal runaway. This setup ensures that thermal runaway propagation is accurately modelled by simulating the heat transfer between cells and the subsequent reaction to the elevated temperatures. Thus, for these other cells, the propagation of thermal runaway is driven by the combined heating effects from both the internal cell reactions and external flame intensity, which is simulated by internal heat flux and the single-step pyrolysis model.

To encompass diverse battery types, the initial simulation setup was designed to capture the diversity in cathode materials, environmental conditions and HRRs. Specifically, Lithium Nickel Manganese Cobalt Oxide (NMC), and Lithium Iron Phosphate (LFP) were selected as the cathode materials due to their widespread usage and distinct thermal behaviours during thermal runaway. The technical specification of battery cells used in this study is shown in Table 1. The charging protocol follows the constant-current (CC) mode, as the focus was on investigating the thermal runaway and temperature field evolution under controlled simulation conditions rather than specific charging or discharging behaviours. The chosen CC mode provides a consistent input parameter for numerical simulations and AI model training. These materials allow for a comprehensive understanding of how different chemistries influence the propagation of thermal runaway in battery packs.

Table 1. Technical specification of battery cells used for HRR fitting (Said, 2020).

Specification	LCO	NMC	LFP
Cathodes	LCO	NMC	LFP
Anode	Carbon	Carbon	Carbon
Nominal voltage (V)	3.7	3.6	3.2
Nominal capacity (mAh)	2600	3000	1500
Discharging current (A)	1.3	0.6	≤ 0.7
Charging current (A)	1.3	1.5	≤ 0.7
Diameter (mm)		18	
Height (mm)		65	

In the battery pack, the batteries are connected without any gaps or tabs, ensuring direct thermal contact between them. Ambient temperatures were set at 20°C, 30°C, 40°C, and 50°C to reflect a range of real-world operating and storage conditions(Fu et al., 2015; Jin et al., 2021; Said et al., 2019). These values were chosen to investigate the impact of environmental factors on thermal runaway propagation, as higher ambient temperatures can accelerate battery degradation and increase fire risks. To evaluate fire risks comprehensively, the SoC was fixed at 100%, given that fully charged batteries present significantly higher risks of thermal runaway compared to partially charged batteries. Additionally, the pyrolysis parameters for the simulations were derived using three distinct heat release rates (HRRs): minimum, mean, and maximum, capturing a broad spectrum of fire dynamics under different scenarios, as shown in Figure 2(b–d). The minimum and maximum HRRs were selected based on the values in the literature (Chen et al., 2015; Fu et al., 2015; Liu et al., 2015; Wang et al., 2021), and the mean HRR was calculated from available experimental measurements for a specific cathode. Consequently, a comprehensive numerical database comprising 36 thermal runaway scenarios was established for subsequent artificial intelligence (AI) training, as listed in Table 2.

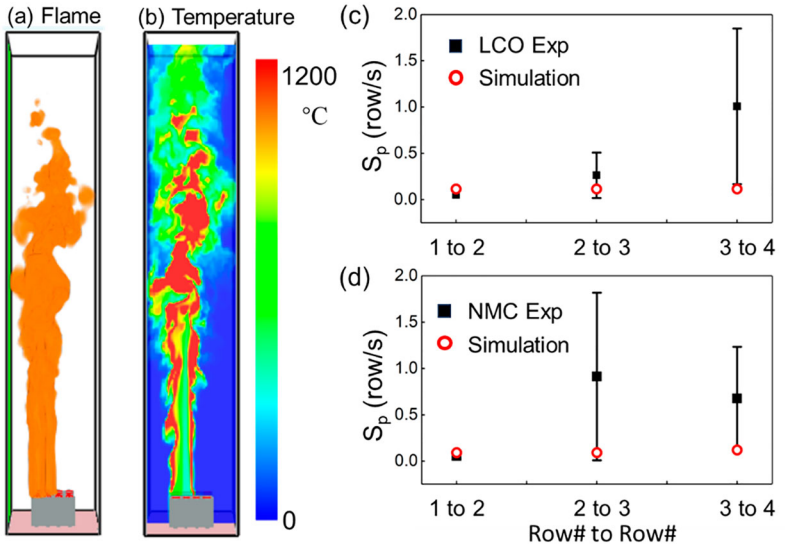

Figure 3. Thermal runaway of the LCO battery pack with the maximum HRRs under the ambient temperature condition of 20 °C: (a) Flame behaviour; (b) Temperature field; Row-to-row thermal runaway propagation speeds (Said, 2020) for (c) LCO cell, (d) NMC cell.

Table 2. Simulation parameters of battery thermal runaway propagation.

Parameter	Value or range	Number of variations
Cathodes	LCO, LFP, NMC	3
Ambient temperatures (°C)	20, 30, 40, 50	4
HRRs	Min, mean, max	3
Initiation temperature of thermal runaway (°C)	180 (He et al., 2024; Niu et al., 2020; Said & Stoliarov, 2021; Wang et al., 2019)	1 (fixed)

In the simulations, LES turbulent solver incorporating with a single-step and mixing-controlled flaming combustion model is employed to address the phenomena of jet flame and combustion heat originating from thermal runaway in lithium-ion batteries. The simulation captures the complex interaction between the turbulent flow and chemical reactions, which are essential to accurately predict the flame dynamics and heat transfer. A standardized simulation duration of 40 seconds is chosen for each scenario, deemed adequate for capturing the thermal propagation of a battery pack fire.

2.2. CFD model validation

By varying cathode materials and HRRs, diverse thermal runaway scenarios in the battery pack are observed under varying ambient temperatures. The battery pack composed of LCO cells with the maximum HRRs (Said, 2020) under the ambient temperature condition of 20 °C is taken as an example to show the simulation results, as shown in Figure 3(a–b). The detailed evolution of thermal runaway is also presented in Video S.1. For all scenarios used, thermal runaway is initiated by the second cell in the first row. Upon ignition, the released heat from this battery elevates the temperature of its immediate neighbours. When the surrounding batteries reach their failure temperature, a cascading effect occurs, leading to thermal runaway propagation until all batteries fail in succession.

Figure 3 also presents the simulation outcomes of row-to-row thermal runaway propagation speeds for LCO and NMC cells under ambient temperature, juxtaposed with experimental results (Said, 2020). Given the non-reproducibility of thermal runaway onset times for individual cells, the onset time from one row to the next is adopted for propagation characterization. This is computed by averaging onset times of all cells in the relevant row, subsequently utilized to calculate a row-to-row propagation speeds (SP) in units of row/s as illustrated in Figure 3(c–d).

The simulation outcomes affirm the effectiveness of simulating thermal runaway processes, particularly in capturing the propagation speeds between the first and second rows and between the second and third rows, which align closely with the experimental data. Notably, regardless of LCO or NMC simulations, discrepancies appear in the propagation rates from the third to fourth row, where simulated speeds consistently lie at the lower limit of experimental results. This discrepancy arises from variations in the experimental and simulation setups. In the experiment, thermal runaway in the third row was initiated using a surface electric heater, necessitating approximately 168 seconds of pre-heating for the entire battery pack. However, in the simulation, thermal runaway in battery 2 was triggered directly by an

internal heat source, simulating the heat generated by an internal short circuit within the battery. The pre-heating step, which is not replicated in the simulation, introduces additional thermal energy that accelerates propagation in the experiment. In addition, the experiment was conducted in a confined space, enhancing thermal radiation across the battery pack, unlike the open space considered in the simulation. These factors contribute to the faster propagation observed experimentally. Despite these differences, the simulation still effectively replicates key aspects of the experimental outcomes and provides additional fire parameters that are essential for AI model training.

2.3. Dataset pre-processing

Given the dynamic nature of battery pack thermal runaway, the surface temperature of individual cells was extracted every 0.1 seconds in the vertical direction for each scenario. This process aimed to capture the dynamic thermal runaway evolution and collect diverse behavioural characteristics. Consequently, a comprehensive database was compiled, consisting of 172,800 temperature data points and 432 instances of battery failure times. Each thermal runaway scenario is characterized by 4800 temperature data points and 12 battery failure times.

Upon compilation of the thermal runaway database, data preprocessing (refer to Figure 4(a)) becomes imperative to optimize it for training the AI model predicting thermal runaway behaviours. Initially, the average surface temperature in the vertical direction was computed for each cell, representing battery temperature. These temperatures were then amalgamated into a new matrix depicting the instantaneous temperature distribution of the pack. Each moment under varying electrode materials, ambient temperatures, and HRRs corresponds to an instantaneous pack temperature distribution, while diverse electrode materials, ambient temperatures, and HRRs correspond to the thermal runaway time of the cell. The ultimate goal is to construct AI models facilitating predictions of battery thermal runaway time and transient temperature distributions during the failure process based on electrode material, ambient temperature, and HRR parameters.

Subsequently, the entirety of processed data constitutes the training set for the artificial AI model. This dataset is subsequently partitioned into two subsets: a 90% portion allocated for model training and a 10% subset designated for assessing model performance during training. An analogous procedure is replicated for arbitrary battery thermal runaway scenarios, serving to evaluate the model's post-training efficacy.

2.4. Deep learning algorithm

Since there are two targets to be predicted: (1) battery thermal runaway time, (2) temperature field prediction during the thermal runaway, two separate AI models are developed, an artificial neural network (ANN) for predicting battery thermal runaway time and a convolutional neural network (CNN) for predicting the temperature field. Both models were designed and tuned through a systematic process to ensure optimal performance, as described below.

The theoretical foundation for using machine learning methods in this study lies in their ability to efficiently model complex, non-linear relationships in high-dimensional data. Traditional numerical simulation approaches, while accurate, are computationally intensive and time-consuming, particularly for dynamic phenomena like thermal runaway and temperature field propagation. Machine learning provides a data-driven alternative, enabling the models to learn patterns from a large dataset of simulations and generalize to unobserved scenarios. Specifically, ANNs excel in solving regression problems involving continuous outputs, such as thermal runaway time, due to their capacity to approximate intricate non-linear functions. Likewise, CNNs are highly effective for spatial data analysis, making them well-suited for predicting the temperature field by capturing spatial dependencies through convolutional layers.

For predicting the time of battery thermal runaway, an ANN (Chen et al., 2023) is employed, featuring an input layer, two hidden layers, and an output layer, where the cathode type, ambient temperature, and the level of HRR are input parameters, as shown in Figure 4(b). The input layer takes three parameters: cathode type, ambient temperature, and the level of HRR. The output layer provides 11 parameters representing the predicted battery thermal runaway times at different cells in the pack, as extracted from simulations. The hidden layers consist of two layers each with 10 neurons, and the output layer contains 11 parameters representing the battery thermal runaway time extracted from simulations. Key hyperparameters, including the learning rate (0.001) and batch size (1), were selected through grid search and evaluated on validation data to ensure the best performance. The ANN was trained using backpropagation with the Adam optimizer on thermal runaway time database split into 90% for training and 10% for validation. Battery 2 was designated as the ignition source with a failure time of 0. This design enables the ANN to model the relationships between input parameters and thermal runaway times effectively.

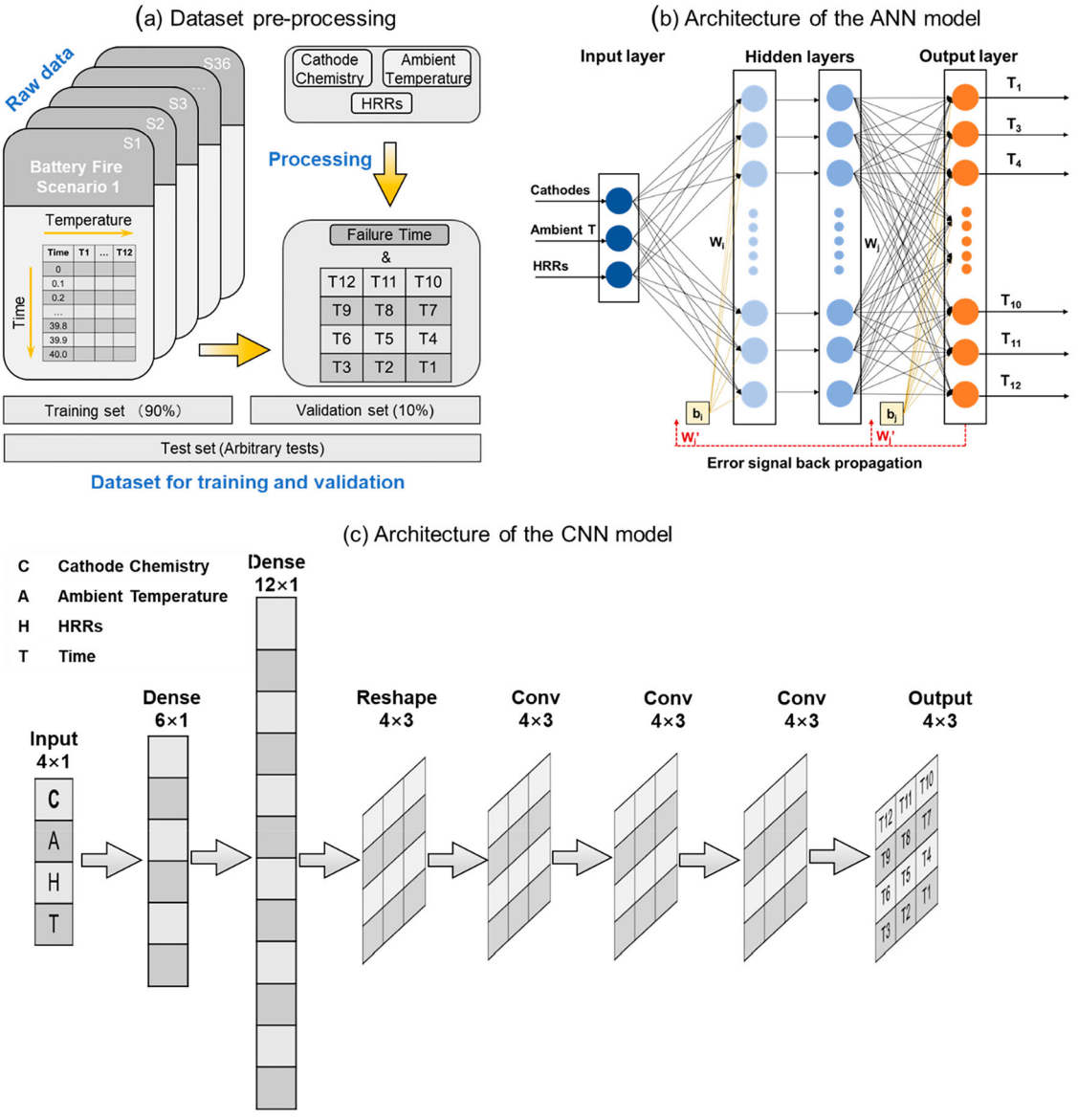

Figure 4. (a) Dataset pre-processing and division for training, validation, and test, (b) ANN model for battery thermal runaway time prediction, (c) CNN model for temperature field prediction.

For temperature field prediction, a convolutional neural network (CNN) is employed for regression analysis (Figure 4(c)). The input parameters for this model include cathode chemistry, ambient temperature, level of HRR, and time. The grid search method was also used here to determine the best structure of the model. Finally, the CNN structure comprises an input layer, two fully connected networks, a reshaping layer, and three convolutional layers with 3 × 3 convolution kernels followed by an output layer representing a 4 × 3 grid corresponding to the average temperature of each battery. The convolutional layers utilize a stride of 1, and same padding, with ReLU activation. The CNN is also trained on the temperature database split into 90% for training and 10% for validation. The network is optimized using the Adam optimizer with a learning rate of 0.01 and trained using a batch size of 36, ensuring accurate predictions for temperature distributions.

Both neural networks employ Rectified Linear Unit (ReLU) as the activation function to introduce nonlinearity, enhancing their ability to capture complex relationships in the data. Their performance is evaluated using metrics such as mean square error (MSE), mean absolute error (MAE), and R^2 (Wang, Zhang, Wu, et al., 2022), as shown in Eqs.(1)-(3), where y_i is the predicted thermal runaway time or battery temperature, and $\widehat{y_i}$ is the simulated thermal runaway time or battery surface temperature. By employing these machine learning methods, this study addresses the limitations of traditional numerical simulations, delivering efficient,

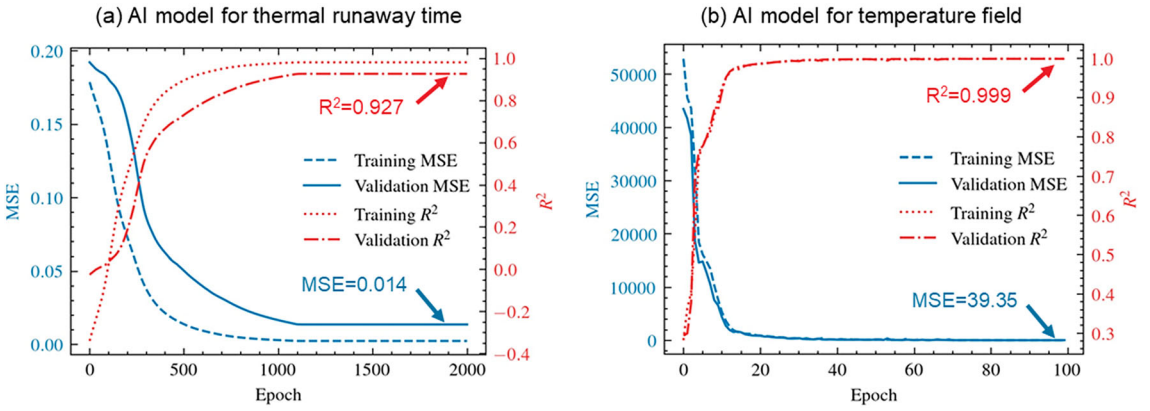

Figure 5. MSE (blue) and R^2 (red) of training (dashed) and validation (solid) during the training process: (a) AI model for battery thermal runaway time prediction, (b) AI model for temperature field prediction.

real-time predictions for thermal runaway time and temperature fields while maintaining high accuracy and reliability.

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \widehat{y_i}| \tag{1}$$

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \widehat{y_i})^2 \tag{2}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \widehat{y_i})^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} \tag{3}$$

3. Results and discussion

3.1. Model training

Following the model training, the performance evaluation of these models is depicted in Figure 5. After 100 steps of iterations, the AI models exhibit convergence, demonstrating minimal MSE losses of 0.014 and 39.346, and maximal R^2 coefficients of 0.927 and 0.999. These results underscore the proficient ability of the deep learning models to precisely forecast the thermal runaway time and transient temperature field of the battery pack within the boundaries of the training dataset. The learning curves for both the ANN and CNN models (Figure 5) indicate stable convergence, suggesting that the selected hyperparameters and network architectures are well-suited for this application. Further details on the training process, including hyperparameter tuning and validation strategies, are provided in are provided in Appendix A.

3.2. Predicting battery thermal runaway time

After training, the AI model is applied to novel battery fire scenarios. Two additional battery scenarios, encompassing complete thermal runaway stages (from row 1 to row 4), are simulated to affirm the model's efficacy. The scenarios involve a battery pack comprising LCO cells with maximum HRRs at an ambient temperature of 35 °C and a battery pack comprising NMC cells with mean HRRs at an ambient temperature of 55 °C. Notably, these scenarios fall within (35 °C) and beyond (55 °C) the database scope, aiming to assess the model's performance within and beyond its established domain.

Figure 6 illustrates a comparison between the deep-learning model's predicted battery thermal runaway time and the time simulated by FDS. Notably, a close agreement is observed in the LCO battery pack with maximum HRRs at 35 °C ambient temperature, displaying an MSE of 2.28 s^2, MAE of 1.38 and an R^2 of 0.97. However, for the NMC battery pack with mean HRRs at 55 °C ambient temperature, the AI model demonstrates suboptimal predictive accuracy, yielding an MSE of 29.27 s^2, MAE of 4.53 s and an R^2 of 0.75. Furthermore, the predictions consistently precede the thermal runaway time of each cell. The elevated MSE and MAE in the NMC battery pack case can be attributed to scenarios beyond the database scope, which reflect the model's difficulty in predicting thermal runaway time for cases beyond its training data. This highlights the model's limitations in generalization and provides insights into the prediction error for out-of-scope cases.

The results suggest that the proposed AI model effectively predicts the thermal runaway time of batteries in the context of a progressing battery fire. The model demonstrates commendable accuracy within the confines of the database, showcasing a relative error below 10%. Moreover, its efficacy extends to scenarios outside the database, maintaining a relative error below 30%. This underscores the model's potential for generalization, emphasizing the prospect of extrapolating the established mapping relationship between battery operating

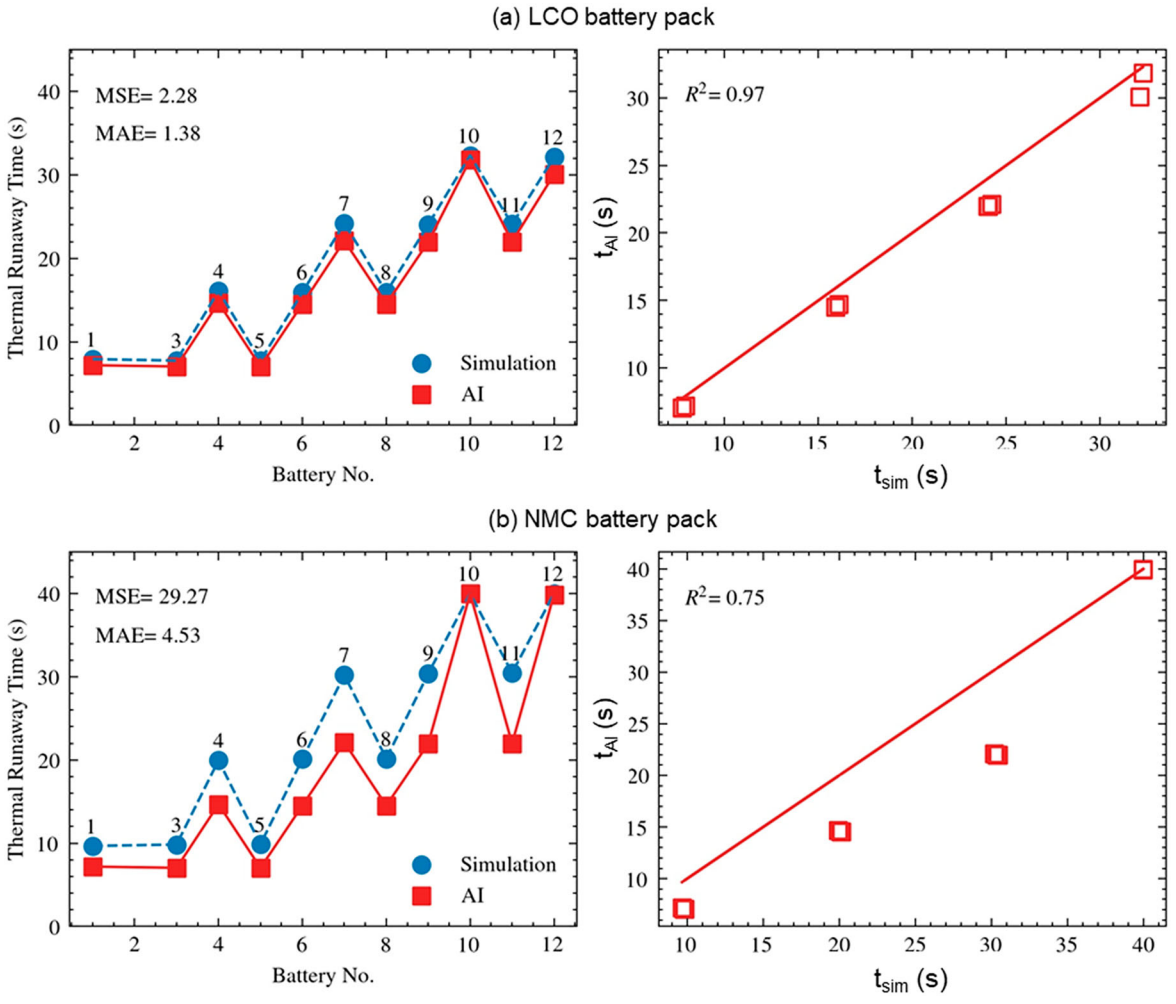

Figure 6. Comparison of battery thermal runaway propagation time from FDS simulation and AI prediction of (a) LCO battery pack, (b) NMC battery pack.

conditions and thermal runaway time to scenarios not explicitly covered in the training dataset.

3.3. Predicting temperature field

By understanding the evolution of temperature distributions during the thermal runaway process, engineers and researchers can make informed decisions and design more efficient and reliable systems. While the operational conditions of a battery enable the prediction of individual cell failure times during thermal runaway, obtaining the temperature evolution throughout this process remains a challenge. To address this, a new AI model was trained to predict the temperature field during the thermal runaway process.

In Figure 7(a), a comparative analysis is presented between simulated and AI predicted temperature fields for battery packs, comprising LCO with maximum HRRs (ambient temperature: 35 °C). The transient prediction results are shown in Figure 8(a) at 10 s, 20 s, and 30 s, where the time is also used as the input for the AI model. Details of this prediction can be seen in Video S.2. We compared the average temperature field of the battery pack in the top view, with the battery arrangement shown in Figure 2(a), where each square represents the average temperature of a battery. Notably, the battery pack with LCO cells and maximum HRRs exhibits close agreement between simulation and prediction, characterized by an MAE less than 4.89 °C and R^2 of 0.999. The error histogram further substantiates the performance of our AI models, with most errors concentrated within a small range, thereby reinforcing the robustness of our approach.

Conversely, the battery pack with NMC cells and medium HRRs, at 55 °C ambient temperature (Figure 7(b) and Video S.3), shows a larger MAE below 9.15 °C and R^2 of 0.998. The transient prediction results compared with simulation results are shown in Figure 8(b). It can be seen that compared with the previous case, there is a certain error between the prediction result

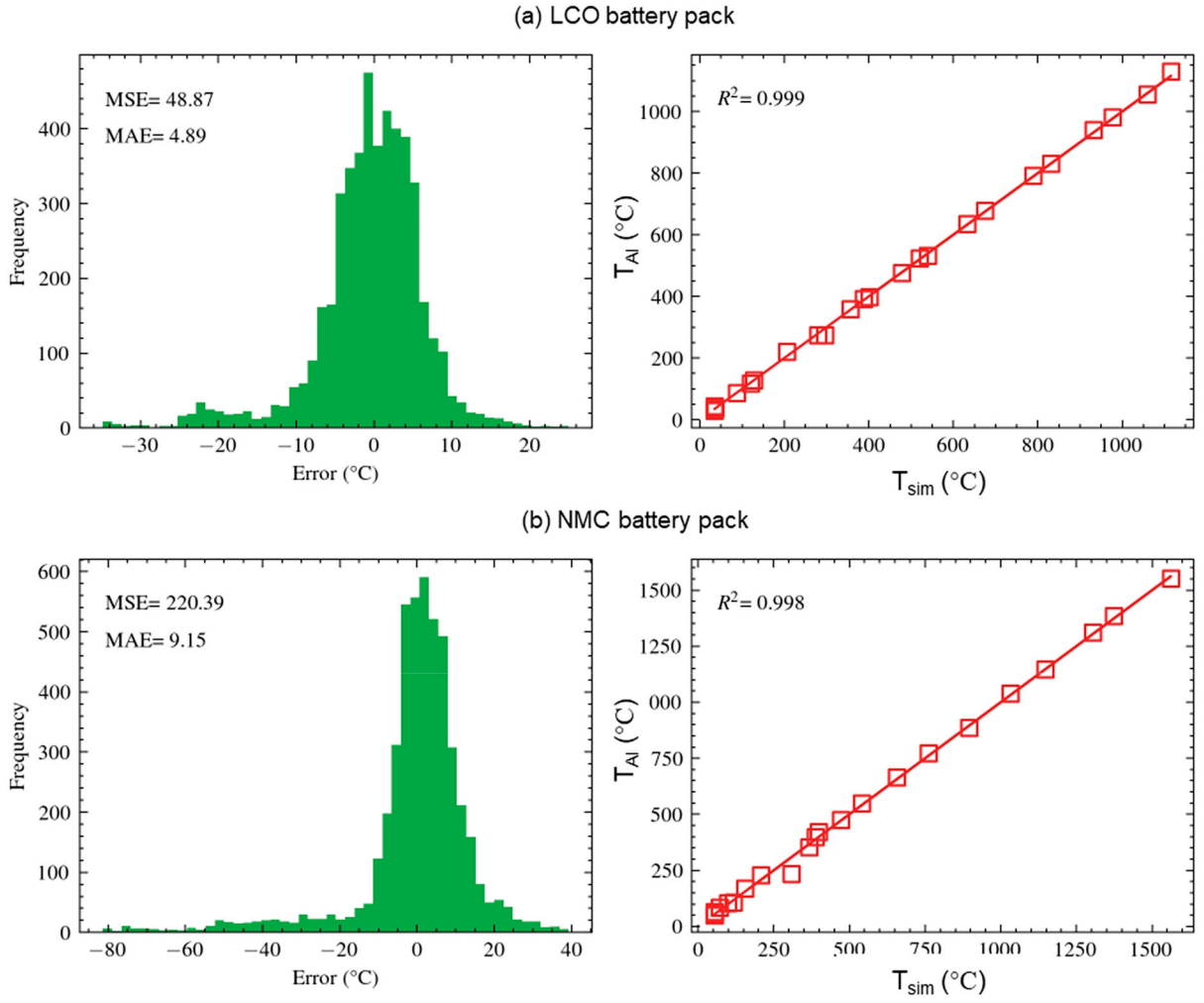

Figure 7. Overall performance of AI model in predicting temperature field compared with simulation results: (a) LCO battery pack, (b) NMC battery pack (Ambient temperature: 35 °C and 55 °C). See Video S.2 and S.3.

and the simulation result. However, this discrepancy is deemed acceptable given the wide-ranging fire-induced temperature variations within practical battery scenarios. In summary, the presented AI model consistently predicts temperature fields in the context of thermal runaway scenarios for both considered cases. This forms a foundational step for subsequent temperature predictions in real-world thermal runaway scenarios involving battery packs.

3.4. Application in battery thermal and safety management

The burgeoning demand for efficient and safe battery management systems has prompted the exploration of AI integration, offering substantial potential for advancing battery management capabilities. Specifically, AI holds promise in predicting critical moments pertinent to battery health, safety, thermal runaway, and the risk of fire and explosion.

Traditional methodologies predominantly rely on predefined thermal models and simplified assumptions, often lacking the requisite precision to capture the intricate dynamics of thermal phenomena within batteries. In contrast, AI methodologies leverage extensive datasets encompassing diverse operational conditions and usage scenarios. Through the utilization of vast amounts of historical data, AI models can discern intricate patterns and hidden flaws within the system. Once adequately trained and furnished with real-time measurements, these AI models can accurately forecast critical health indicators and safety events for individual cells within battery packs. Consequently, this enables the implementation of proactive measures aimed at averting catastrophic events.

One key area where AI can revolutionize battery management is the prediction of temperature distribution in a single battery and the battery pack. Then, the predicted battery temperature field can further forecast the critical events of battery fire, such as the decomposition of SEI membrane, the evaporation of electrolyte solvent,

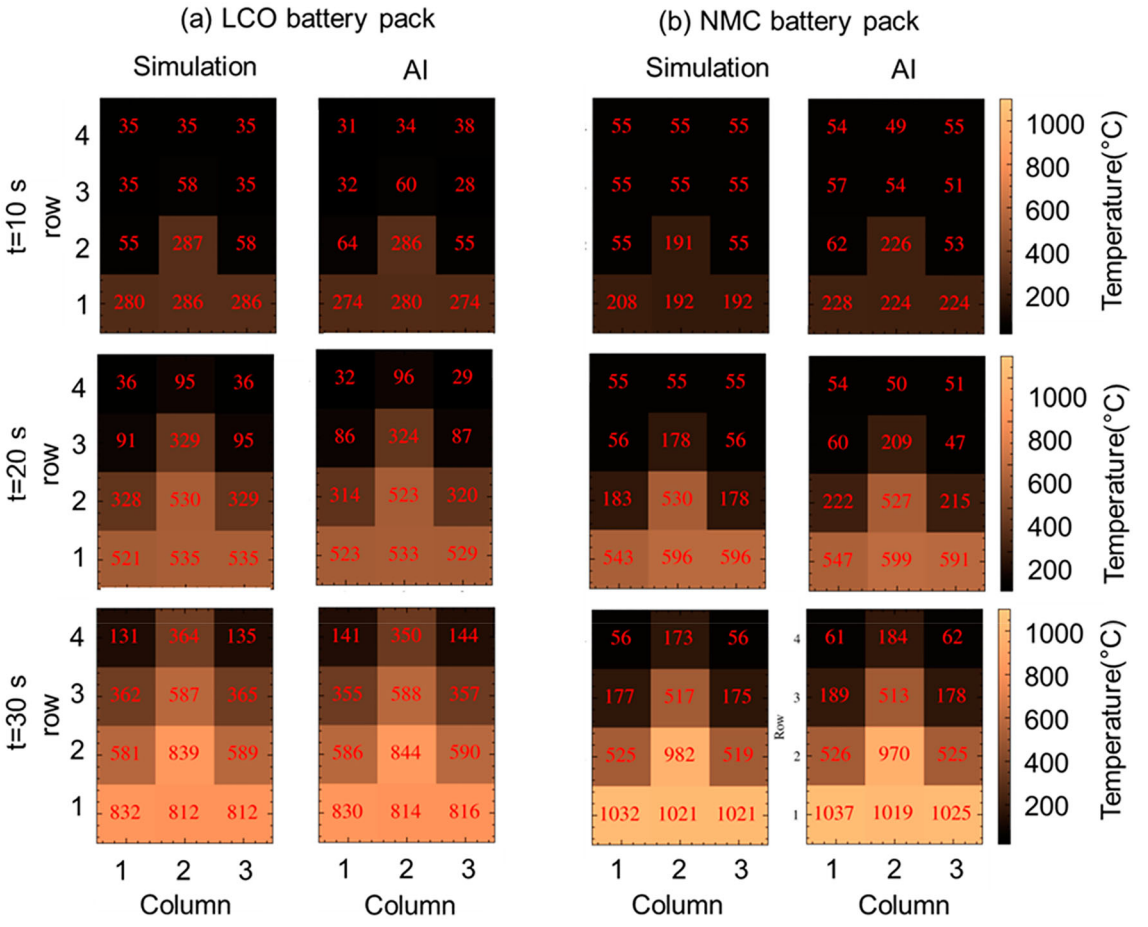

Figure 8. Comparison between the simulated and AI predicted temperature fields (top view schematic of the cell packs) of (a) LCO battery pack, (b) NMC battery pack at 10 s, 20 s, and 30 s (Ambient temperature: 35 °C and 55 °C). See Video S.2 and S.3.

venting, thermal runaway, flaming, and fire propagation. For instance, Feng et al. (2014, 2018) divided the thermal runaway process into 6 stages with 3 critical temperature. Many studies (Liu et al., 2024; Tao et al., 2020; Wang et al., 2012; Wang et al., 2019) experimentally measured the surface temperature of 18650 cells, for which the battery safety valve ruptures at approximately 120 °C (i.e. the venting temperature). Table 3 summarizes the critical temperatures for Li-ion battery safety. Knowing when the temperature reaches critical levels can trigger automatic cooling mechanisms or activate emergency shutdown procedures to prevent further escalation of the situation. Thus, the process of predicting temperature fields is crucial in battery thermal and safety management systems.

In light of the aforementioned critical temperature thresholds, our study further predicts the critical moments of SEI membrane decomposition, safety valve rupture (venting), and gas-fuel self-ignition in individual battery cells within a battery pack. The prediction is based on temperature field simulations and predictions derived from AI models. Figure 9 presents a comparative analysis between the forecasted critical events generated by the deep-learning model and the corresponding time simulated using FDS.

Significantly, a close concurrence is observed in the LCO battery pack scenario, characterized by maximum heat release rates (HRRs) at an ambient temperature of 35 °C. The MSE is recorded at a maximal value of 0.06 s^2, with a maximum MAE of 0.19 s. Conversely, in the NMC battery pack context, featuring mean HRRs at an ambient temperature of 55 °C, the AI model exhibits suboptimal predictive accuracy. Notably, the maximum MSE and MAE are notably higher, at 1.52 s^2 and 0.86 s, respectively.

Moreover, it is observed that the forecasts consistently anticipate the simulated critical events of each cell. Since these predicted times are based on predictions of the temperature field as well as the critical temperature, the increased MSE and MAE observed in the NMC battery pack scenario can be attributed to instances falling outside the scope of the database, indicating challenges in extrapolating thermal runaway time beyond the expertise of the AI model. While these predictions provide an

Table 3. Critical temperatures for Li-ion battery failure, thermal safety, and risk of fire and explosion.

Critical event	Initiation/critical temperature (°C)	References
SEI membrane decomposition	~ 69	(Wang, Zhu, Gao, et al., 2022; Wu et al., 2018; Zheng et al., 2022)
Boiling point of electrolyte solvent	90 (DMC), 110 (EMC)	(Feng et al., 2019; Lamb et al., 2015; Ströbel et al., 2023; Zhang et al., 2022)
$LiPF_6$ decomposition	~ 100	(Ryou et al., 2012; Wang, Feng, et al., 2023; Yang et al., 2006)
Venting	120 (18650 cell)	(Feng et al., 2014; Feng et al., 2018; Liu et al., 2024; Tao et al., 2020; Wang et al., 2012; Wang et al., 2019)
Thermal runaway	~ 180	(He et al., 2024; Niu et al., 2020; Said & Stoliarov, 2021; Wang et al., 2019)
Gas-fuel self-ignition temperature	400–500	(Quintiere, 2006)
Peak cell temperature	700–1100	(He et al., 2024; Jia et al., 2022; Niu et al., 2020; Said & Stoliarov, 2021; Wang et al., 2019)

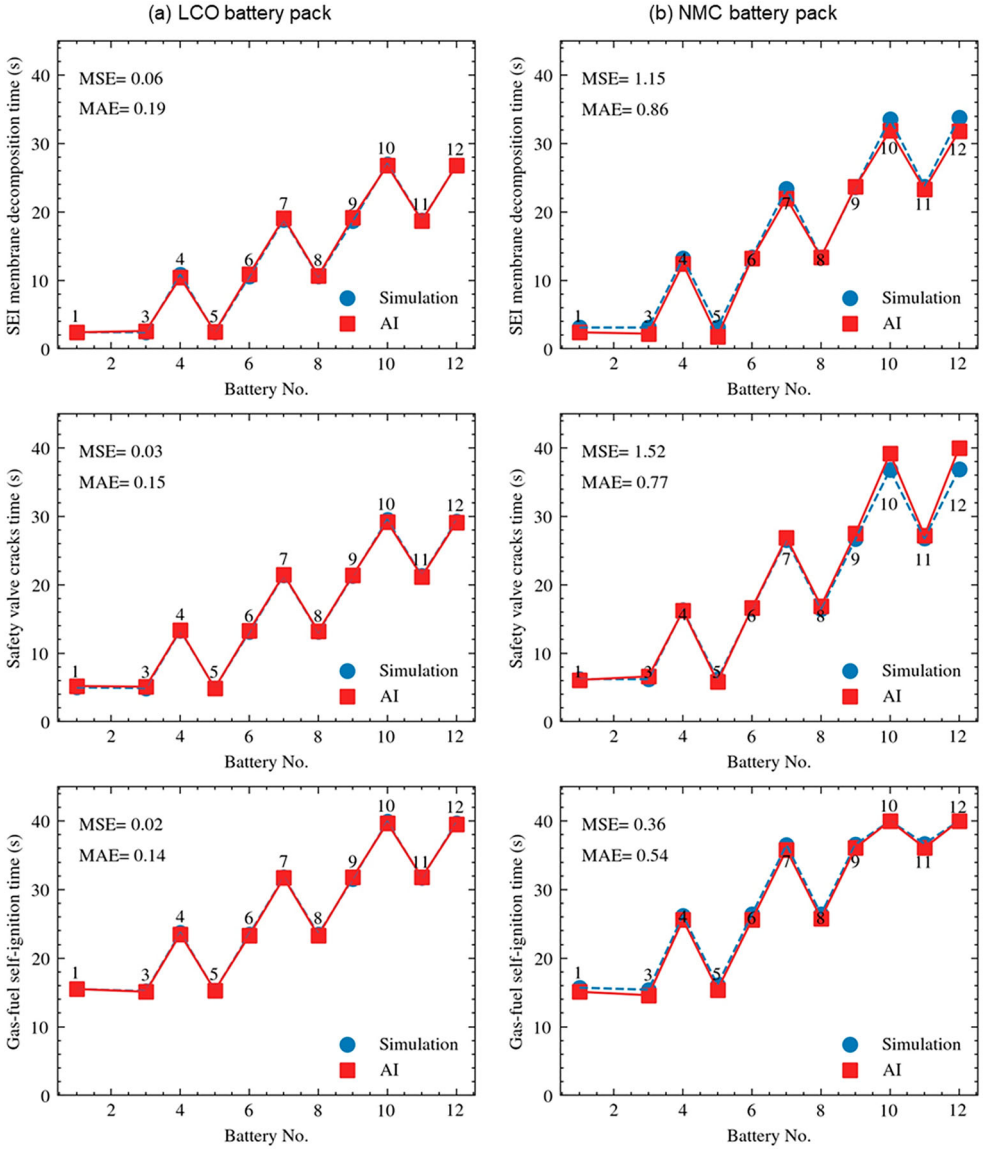

Figure 9. Comparison of safety valve cracks time from FDS simulation and AI prediction of (a) LCO battery pack, (b) NMC battery pack.

initial avenue for pre-emptively addressing battery thermal runaway, enhancing prediction accuracy is imperative. This can be achieved through the augmentation of database diversity and quantity, facilitating a broader and more comprehensive understanding of battery thermal behaviour.

3.5. Discussion

In summary, the current AI models, trained on diverse battery thermal runaway scenarios, demonstrated precision in predicting both battery thermal runaway time and temperature distribution during thermal runaway.

If the simulation is used to study the thermal runaway behaviour of a battery under a specific condition, it would typically require several days or weeks of computation. However, with the trained AI model, it is possible to predict the thermal runaway time and the temperature distribution of the battery at each moment in real-time, with the prediction time for thermal runaway and temperature distribution for a given scenario being less than 1 s. Specifically, the deep learning model significantly reduces computation time compared to traditional simulation methods, making it suitable for real-time applications in battery safety management systems.

While the model designed for thermal runaway time prediction excels within the database's boundaries but falters in cases beyond, the model specialized for temperature distribution exhibits commendable performance in cases within and beyond the database scope. The results show that the thermal runaway time predictions are highly sensitive to the initial training database. Differences between model predictions and actual outcomes can arise due to variations in these conditions that are not fully captured by the training data, e.g. for the NMC battery pack in Figure 6, the prediction error is higher than that of LCO pack because its test environment is not within the database range. However, the prediction of the temperature field can still give a reasonable result even if the initial state of the target scene is not within the range of the training database, e.g. for the NMC battery pack in Figures 7 and 8.

To address potential biases and uncertainties, it is essential to consider the limitations of the simulation data used for training. For instance, this study employs a fixed ignition source (battery 2 in Figure 2), but real-life scenarios may involve greater complexity and ignition in different locations. The assumption of a fixed ignition source may not fully represent the stochastic nature of thermal runaway initiation in practical settings, potentially introducing bias into the model's predictions. Additionally, the simulations rely on simplified assumptions regarding the uniformity of the battery pack and boundary conditions, which may not capture real-world variations in cell geometry, material properties, or operational conditions. These limitations suggest that while the models perform well under controlled conditions, they may not fully capture the complexity and variability of real-world scenarios, highlighting the need for further refinement and validation. Future studies will incorporate batteries with different SoC, various topologies, and larger-scale battery packs to improve the model's applicability to more realistic settings and better reflect the diverse conditions encountered in practice.

Augmenting the database size is recognized as a means to enhance predictive accuracy for both thermal runaway time and temperature distribution models. However, the simulation's accuracy is pivotal in determining the model's precision, as deviations from real thermal runaway scenarios can occur. Therefore, refining the accuracy of battery thermal runaway simulations is crucial to curbing prediction errors in thermal runaway time and temperature distribution. This involves improving the fidelity of the simulations to better reflect the actual physics of battery thermal events, ensuring that the AI models are trained on data that closely mirrors real-world conditions.

Another strategy involves incorporating both experimental and simulated data for AI model training, assigning greater weight to authentic experimental data. This approach enables the AI model to acquire substantial a priori knowledge from simulated data while rectifying inaccuracies through real experimental data, significantly reducing the requisite number of experiments for model training. Additionally, understanding the uncertainties in model predictions is crucial to mitigate the risk of erroneous predictions in critical safety scenarios. This involves analyzing the variability in experimental data and assessing how it impacts the training process, thereby ensuring that the model is robust and reliable under diverse conditions. By quantifying this uncertainty, we can better gauge the confidence level of our predictions and identify areas where further refinement is necessary. This comprehensive data-driven approach ensures that the AI models are robust and adaptable to varying operational environments.

Although this work is only a preliminary study on the application of AI to battery thermal safety, the implications of our findings are significant for advancing battery safety research. Our results provide a foundation for developing more sophisticated predictive tools that can enhance the design of battery management systems and safety protocols. By improving our models and expanding the training data, we aim to better predict and mitigate risks associated with battery thermal runaway, ultimately contributing to safer battery technologies and more reliable energy storage solutions. Furthermore, these models can be seamlessly integrated into existing battery management systems to provide real-time predictions and preventive measures, thereby enhancing overall battery safety and performance. Our approach also provides guidance for the applications of AI in battery systems, reinforcing the potential of AI-driven insights in addressing complex thermal phenomena in energy storage devices. This integration has the potential to transform battery safety management, enabling predictive maintenance and proactive risk mitigation in real-world applications.

4. Conclusions

In this study, an innovative AI-based methodology for predicting thermal runaway time and temperature fields in battery management systems is introduced based on experimentally verified pyrolysis models. By analyzing simulated thermal runaway data, the AI model achieves high accuracy in thermal runaway time prediction, with a relative error below 10% for database-contained scenarios and below 30% for scenarios outside the database range. The model also demonstrates exceptional performance in predicting temperature field distributions and critical events, achieving an R⊃2 value above 0.99 and a maximal MSE of 1.52 s⊃2. These findings underscore the potential of integrating advanced simulation techniques with deep learning for proactive safety measures and improved battery management.

Despite these achievements, limitations remain. The model's accuracy diminishes for scenarios significantly outside the training database, highlighting the need for more extensive and diverse training datasets. Future work will focus on expanding the database, integrating additional physical phenomena, and exploring real-time applications to further enhance model robustness and scalability.

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