Real-time Thermal Runaway Prognosis of a Lithium-ion Battery via Physics-informed Latent Ensemble DeepONet with Synthetic Data

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ABSTRACT

This study proposes a novel architecture of physics-informed latent ensemble deep operator network with synthetic data. The proposed neural network aims to predict thermal runaway of a lithium-ion battery through prior temperature responses in real-time. The proposed neural network introduces three key features to provide an advanced control-enabling solution for battery thermal management systems (BTMS). First, the proposed neural network addresses the architecture of DeepONet as a surrogate model to effectively learn the internal temperature, chemical component concentration, and gas formation under supervision of complex and nonlinear multiphysics representing thermal runaway of lithium-ion batteries. This approach enables accurate and robust virtual sensing capability even with limited data by constraining the prognostic responses to follow the governing equation of the underlying multiphysics. Second, a dual-network architecture is introduced to extract valuable features from prior temperature responses, which inherently contain limited information in real-time scenarios. The network comprises two sub-networks; the first network extracts latent features from decomposed temporal domains across diverse local domains, and the second network ensembles these features to original features to mitigate concerns on overfitting and generalization. This approach ensures effective supervision by stiff governing equations in both local and global domains. Third, novel methods are employed to reduce the training complexity associated with integrating multiphysics equations including separate DeepONet, stan activation function, adaptive weights, and encoders. These methods enhance the expressiveness of temporal and spatial gradients that play an important role in physics-informed neural networks. Hence, this feature not only ensures convergence through a balanced learning but also improves the overall capability of the neural network. Extensive ablation studies validate the contribution of each feature, and thereby confirm the effectiveness of novel architecture and strategies in addressing failure issues in physics-informed neural networks. The proposed method enables real-time prognosis through prior thermal responses, offering a promising pathway toward artificial intelligence transformation in BMS to ensure the safety and efficiency of lithium-ion batteries.

NOMENCLATURE

Symbols	
A	*Frequency factor*
c	*Dimensionless concentration*
c_p	*Heat capacity*
E_a	*Activation energy*
$\dot{Q}_{exo}$	*Volumetric heat generation rate*
R_c	*Gas constant*
R_g	*Gas constant of product*
m_g	*Mass of the gas formation*
P	Pressure
T	Cell temperature
k	Thermal conductivity coefficient
V	Control volume

1. METHODOLOGY

Thermal runaway (TR) in lithium-ion batteries poses a critical safety challenge, leading to rapid temperature escalation, gas formation, and potential catastrophic failure (Feng X et al., 2015). Accurate and timely prognosis of TR is essential for ensuring the safe operation of batteries in electric vehicles and energy storage systems. However, predicting TR in real time is difficult due to the coupled thermal, chemical, and mechanical processes involved (Guo G et al., 2010, Kwak, E. et al., 2022), as well as the limited availability of internal measurements. Recent advances in physics-informed neural networks (Guan H et al., 2023) and operator learning (Wang, S. et al., 2022, Jeong, J. et al., 2024) provide new opportunities to address these challenges by integrating governing equations with data for reliable state prediction.

This study proposes PILE-DeepONet, a physics-informed latent ensemble DeepONet, for accurate and efficient real-time thermal runaway prognosis in lithium-ion batteries under various thermal abuse conditions using prior temperature responses. The proposed framework enables virtual sensing of internal states such as temperature, equivalent chemical concentration, gas formation, and pressure after 900 seconds, based on currently monitored surface temperatures and environmental conditions. This approach provides a foundation for the proactive safety management of batteries.

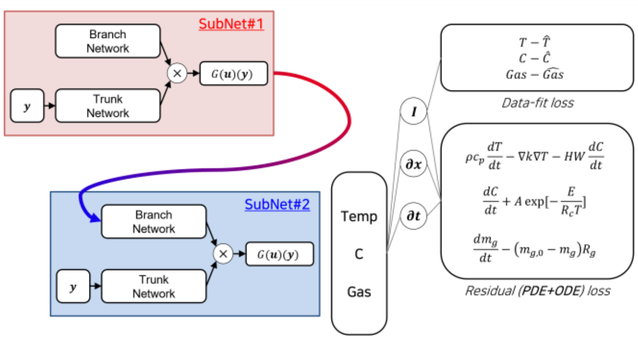

Figure 1 The architecture of PILE-DeepONet

The framework incorporates three essential strategies to achieve high-fidelity real-time TR prognosis. First, it introduces a time-based segmentation method to address the inherent challenges of learning long-term temporal responses under physics intelligence within neural networks. PILE-DeepONet decomposes the entire time domain into smaller regions, enabling the capture of fast local dynamics and preserving the global temporal evolution of the TR phenomenon. This segmentation effectively mitigates the stiffness issues encountered during normalization, allowing for improved stability and learnability during training while preserving the consistency of governing physical laws within each local domain. Second, PILE-DeepONet employs a two-stage neural operator architecture with embedded physics intelligence to efficiently extract and utilize meaningful information from limited monitoring data (Figure 1). The first neural operator acts as a latent feature extractor, capturing diverse information such as cooling performance, slow thermal trends prior to TR onset, and rapid thermal variations across different temporal windows. These latent features from diverse information are then combined with original input data in the second neural operator, which functions as a predictive model to estimate internal TR states. This sequential approach enables accurate internal state inference, reduces overfitting risk, and improves generalization, supporting network robustness under diverse operational and abuse conditions. Both operators are trained under the supervision of the governing multiphysics partial differential and ordinary differential equations describing TR phenomenon, with these equations directly embedded into the loss function. The heat transfer within the lithium-ion battery during TR is governed by the energy conservation equation (Kwak, E. et al., 2022):

$$\rho c_p \frac{\partial T}{\partial t} = \nabla(k\nabla T) + \dot{Q}_{exo}, \tag{1}$$

where ρ, c_p, k, T, and $\dot{Q}_{exo}$ denote the cell density, heat capacity, thermal conductivity coefficient, cell temperature, and volumetric heat generation rate, respectively. This equation describes the temperature distribution of a lithium-ion battery (LIB) by accounting for the propagation of heat throughout the LIB and the generation of heat due to several heat sources. The chemical decomposition associated with TR is described by (Kwak, E. et al., 2022):

$$-\frac{dc}{dt} = A\,exp\left[-\frac{E_a}{R_c T}\right]c, \tag{2}$$

where c, A, E_a, and R_c denote the concentration of chemical component, frequency factor, thermal activation energy, and gas constant, respectively. This equation indicates a significant increase in the decomposition rate of the chemical component with rising temperature, resulting in exponential heat generation in TR. Moreover, this coupling of thermodynamics and chemical reactions results in a pressure increase, originating from rising temperature and gas formation as follows (Hewu W et al., 2019):

$$P = \frac{m_g R_g T}{V}, \tag{3}$$

$$\frac{\partial m_g}{\partial t} = -\left(m_{g,0} - m_g\right)\frac{dc}{dt}, \tag{4}$$

where P, m_g, R_g, V, and $m_{g,0}$ denote the pressure, the mass of the gas formation, gas constant of product, control volume, and the available mass of gas reactant. By incorporating these governing equations during training, PILE-DeepONet ensures that its predictions remain consistent with the underlying conservation laws, even in regions where direct measurements are unavailable. Third, the proposed framework integrates advanced training methodologies to manage the complexity associated with incorporating physics intelligence. The separation of trunk networks, inspired by the mathematical separation of variables, is employed to enhance the expressiveness of derivatives during the optimization of physics-based loss functions. The Stan activation function is utilized to increase the variability and magnitude of derivatives, allowing the network to capture stiff and nonlinear behaviors characteristic of TR phenomena. Adaptive weighting using the neural tangent kernel dynamically adjusts the contributions of each loss term, ensuring that data fitting, physics residuals, boundary conditions, and initial conditions are properly scaled and effectively influence the overall training. Additionally, the normalization of spatial, temporal, and physical variables ensures consistent scaling across different units and magnitudes, promoting stable convergence during training.

The proposed neural network minimizes a composite loss function that integrates data fitting, residuals of the governing physics equations calculated via automatic differentiation, and relevant boundary and initial conditions during the training phase. The adaptive weighting mechanism updates these contributions at each iteration, allowing the network to learn physically consistent and accurate solutions while maintaining computational efficiency.

2. EXPERIMENTS

Comprehensive synthetic data were generated to support the training of PILE-DeepONet under a range of thermal abuse conditions through the multiphysics finite element model (FEM) using COMSOL Multiphysics 6.1 (COMSOL Inc., USA). These data allow PILE-DeepONet to capture key aspects of the TR phenomenon such as internal temperature distribution, concentration of chemical component, gas formation, and pressure.

The multiphysics FEM addressed a simple 1D radial geometry comprising 31 nodes from center to the surface. This geometry was rotated 360 degrees to form the cross-section of a cylinder cell, effectively illustrating radial thermal variations. The outer edge of the node representing the LIB surface was exposed to a heating curve to replicate thermal abuse from external temperature conditions. The thermal abuse condition induces thermal runaway, resulting in complex and nonlinear changes in temperature, concentration of chemical component, gas formation, and pressure. Note that these results reflect the behavior of the LIB cell, with key parameters adjusted based on experimental data, particularly the measured surface temperature and pressure.

The various heating curves used to generate the synthetic data are summarized in Table 1. These thermal conditions were defined by differences in the heating ramp-up time of the heating curve and cooling performance of the surrounding system. These modifications represent various scenarios in which LIBs may be exposed to extreme thermal abuse conditions. Specifically, the heating ramp-up time reflects both slow and rapid temperature increases, while the cooling performance indicates the ability of the thermal management system to dissipate heat. These synthetic data were randomly divided into training, validation, and test sets. The training set comprised 84 TR scenarios, designed for improved accuracy and robustness. The validation set included 10 scenarios from the same distribution of training set to assess generalization and prevent overfitting. The test data were categorized into three different groups. Test Set 1 comprised 11 scenarios similar to the training conditions to evaluate the in-distribution performance of PILE-DeepONet. Test Set 2 is an actual TR experiment scenario, aligning with the distribution of Test Set 1 but offering measured values for surface temperature and pressure. This dataset enables a feasibility analysis of TR prognosis using actual measured surface temperature as input. Test Set 3 comprised 36 unseen synthetic scenarios representing out-of-distribution conditions, where the classification of out-of-distribution was determined based on gradient criteria, aimed at validating the capability of PILE-DeepONet.

Table 1. Heating conditions for generating synthetic data.

	Initial temperature [ºC]	Target temperature [ºC]	Ramp-up time [s]	cooling performance [W/(m^2·K)]
Training set / Validation set / Test set 1	[35]	[270]	[2100 : 45 : 3000]	[7 10 13 16 19]
Test set 2	[35]	[270]	[2600]	[7]
Test set 3	[35]	[270]	[1800 : 40 : 2000] [3100 : 40 : 3300]	[7 13 19]

PILE-DeepONet was implemented using JAX and trained on a server equipped with an AMD EPYC 7542 CPU, 512 GB of memory, a Tesla A100 GPU, and Ubuntu 18.04.6 LTS. The proposed neural network was trained for up to 300,000 iterations using the Adam optimizer, starting with an initial learning rate of 0.001, which decayed exponentially by a factor of 10 every 2,000 iterations. The loss function was computed with adaptive weights, updated at each iteration using the neural tangent kernel to balance the contributions of each loss term. Additionally, training was terminated early if the root mean squared error on the validation set failed to improve over 40,000 consecutive iterations.

3. RESULT AND DISCUSSION

A comprehensive comparative analysis was performed against experimental measurements and multiphysics FEM simulation results to evaluate the effectiveness and practical applicability of PILE-DeepONet for TR prognosis under thermal abuse conditions.

Figure 2 illustrates the temporal evolution of the surface temperature in a lithium-ion battery under thermal abuse conditions, comparing experimental measurements, multiphysics FEM simulation results, and predictions obtained from PILE-DeepONet. The proposed neural network accurately captures TR phenomenon, aligning well with the experimental measurements despite the presence of noise in the monitored data. The shaded yellow region highlights the period during which the input temperature, shown in the inset, increases and serves as the monitored input for predicting the TR peak. PILE-DeepONet successfully predicts the timing and magnitude of the rapid temperature escalation, demonstrating excellent agreement with the experimental and FEM results even in the highly nonlinear TR regime.

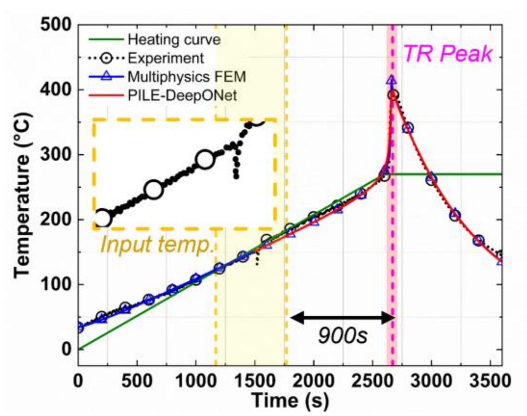

Figure 2. Comparative analysis with actual temperature measurements during TR of multiphysics FEM and PILE-DeepONet.

Figure 3 presents the pressure evolution, where PILE-DeepONet accurately predicts the onset and peak of the pressure rise associated with gas generation during TR. The proposed neural network aligns well with FEM predictions and captures the timing and magnitude of the experimental peak pressure with high fidelity. The effective encoding of multiphysics laws governing the TR phenomenon enables reliable prediction of dynamic pressure behavior under thermal abuse conditions.

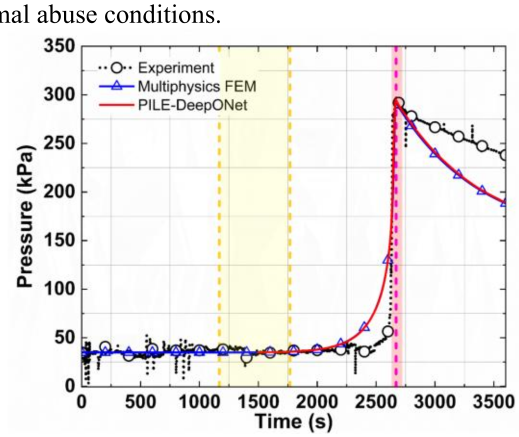

Figure 3. Comparative analysis with actual pressure during TR of multiphysics FEM and PILE-DeepONet.

Figure 4 verifies the feasibility of using PILE-DeepONet for real-time safety management by comparing a cooling simulation with active cooling applied at the precisely predicted TR peak against the uncontrolled scenario. The predicted peak point, indicated by the vertical dashed yellow line around 1750 s, was identified in advance using PILE-DeepONet. This approach reduces the rapid temperature increase and pressure increase by initiating cooling at the predicted critical point, which prevents the system from reaching the TR peak seen in the uncontrolled experimental scenario. This result demonstrates the practical utility of predictive TR prognosis using PILE-DeepONet for real-time safety management. Accurate identification of the intervention point enables active cooling to be applied proactively to suppress the progression into thermal runaway, thereby enhancing battery safety under thermal abuse conditions.

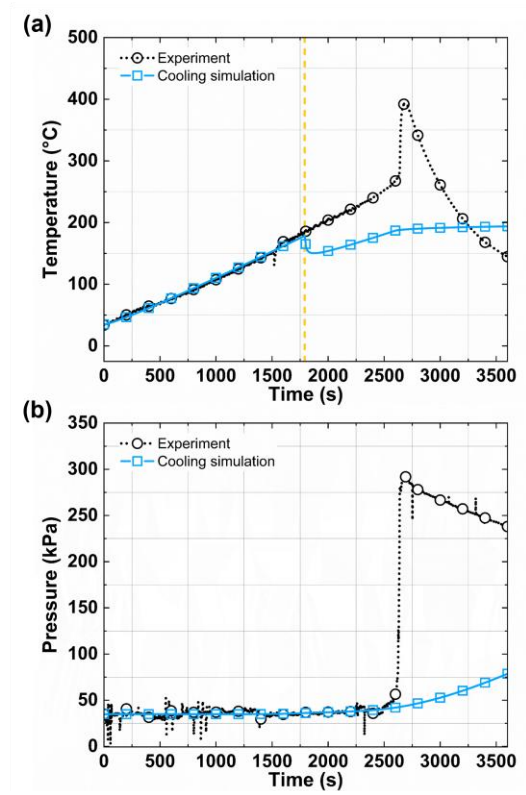

Figure 4 Feasibility of PILE-DeepONet for mitigating TR under thermal abuse

These results collectively demonstrate that PILE-DeepONet enables reliable, accurate, and computationally efficient TR prognosis under various thermal abuse conditions. The ability to utilize noisy monitored data while maintaining prediction accuracy further underscores the robustness of PILE-DeepONet for deployment in real-world battery management systems, supporting proactive TR prevention and enhancing the operational safety of lithium-ion batteries under challenging conditions.

4. CONCLUSIONS

This study introduced PILE-DeepONet as an effective framework for real-time TR prognosis in lithium-ion batteries subjected to various thermal abuse conditions. Extensive analysis confirmed that PILE-DeepONet reliably captures the spatiotemporal progression of TR events, accurately predicting the timing and magnitude of rapid temperature and pressure increases under nonlinear thermal conditions. In addition, the framework successfully identified critical intervention points, enabling timely application of cooling strategies to suppress rapid temperature rise and prevent the system from entering TR. These outcomes underscore the practical viability of PILE-DeepONet for enhancing the safety of lithium-ion batteries through real-time monitoring and proactive intervention. PILE-DeepONet provides a reliable and computationally efficient solution for early TR prediction, delivering valuable insights to support advanced thermal management and safety strategies in electric vehicles and energy storage applications. The demonstrated capability of the framework to maintain accurate performance under practical monitoring conditions highlights potential for seamless integration into battery management systems, advancing the safe and stable operation of lithium-ion batteries across a range of demanding scenarios.

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