Multiphysics-informed DeepONet of a lithium-ion battery to predict thermal runaway

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ABSTRACT

This study proposes a multiphysics-informed deep operator network (MPI-DeepONet) to predict the thermal runaway of lithium-ion batteries (LIBs) under a variety of thermal operational and abuse conditions. Specifically, this study aims to address the functional mapping from a heating curve to predict the evolution of the temperature of a LIB and dimensionless concentration of dominant components of the LIB including an anode, cathode, electrolyte, and solid electrolyte interphase. The proposed method has two key characteristics. First, the MPI-DeepONet is supervised by using ordinary and partial differential equations, which govern highly complex and nonlinear phenomena of thermal runaway of a LIB, including the chemical reaction degradation of the dominant four components and thermodynamics. This feature enables to train of the proposed neural network with a small amount of data available, suggesting that the proposed neural network is accurate and robust even though the proposed method is trained even with limited data. Second, the proposed neural network is trained with the data that is generated from high-fidelity finite element analysis under a variety of thermal operational and abuse conditions because measurements for the thermal runaway of a LIB are limitedly available. Hence, the MPI-DeepONet does not require actual measurements, which is extremely difficult in field experiments. Finally, the accuracy and robustness of the proposed architecture are verified through actual measurements and other scenarios, which are different from the data trained. The analysis of results reveals that the MPI-DeepONet secures higher accuracy and robustness than purely data-driven DeepONet. The proposed surrogate model, which is faster than existing surrogate models, suggesting that this model contributes to developing a digital twin model of a LIB, which can be deployed on a battery thermal management system and provides sufficient information for effective power and energy management.

1. METHODOLOGY

The thermal runaway phenomenon in batteries involves a complex interplay of factors and chain reactions, encompassing aspects like thermodynamics, chemical reaction decomposition, and the aging of individual components. Traditionally, methods such as the finite element method and finite difference method have been employed to simulate thermal runaway while considering multiphysics considerations. However, it's important to note that when using numerical analysis techniques to calculate intricate multiphysics phenomena like thermal runaway, significant computational time and substantial computational resources are necessary. Consequently, the traditional numerical analysis approaches face limitations when it comes to real-time simulation of thermal runaway under diverse battery operating conditions.

To tackle this challenge, this study introduces a multiphysics-informed deep operator network (MPI-DeepONet) aimed at developing a predictive model for the thermal runaway of lithium-ion batteries (LIBs) under various thermal operational and abuse conditions. The methodology involves several steps. Firstly, the data required for the training of the proposed neural network was generated through high-fidelity finite element analysis (FEA) simulations of the thermal runaway of LIBs under various thermal operational and abuse conditions. The simulations were performed using COMSOL Multiphysics software. Specifically, the main mechanism of thermal runaway is a chain reaction in which chemical decomposition of battery elements occurs depending on temperature, and to analyze

this, chemical reaction models and thermodynamic models must be repeatedly calculated. These calculated data consisted of the heating curve and the evolution of the temperature of a LIB and dimensionless concentration of dominant components of the LIB including an anode, cathode, electrolyte, and solid electrolyte interphase. Next, the generated data was pre-processed to ensure its quality and consistency. The pre-processing steps included normalization, and splitting of the data into train, validation, and test sets. After data generation and preprocessing, the proposed MPI-DeepONet architecture consists of a deep operator network that is supervised by using ordinary and partial differential equations. Specifically, the network comprises five hidden layers situated between the input and output layers. A hyperbolic tangent function serves as the activation function for the input and hidden layers, while the output layer employs a sigmoid function. Furthermore, the chemical degradation of the dominant four components was modeled using the Arrhenius equation. Additionally, to elucidate the thermodynamics underlying the thermal runaway phenomenon, the energy balance equation was employed as follows:

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

where ρ, c_p, T, t, k and $\dot{Q}_{exo}$ denote the cell density, heat capacity, temperature, time, thermal conductivity coefficient and chemical heat generation, respectively. The neural network is trained to predict the evolution of temperature and dimensionless concentration of dominant components of a LIB, given the heating curve. Then, the proposed neural network is trained using the pre-processed data generated from FEA simulations. The training is performed using stochastic gradient descent optimization with backpropagation. The trained neural network is validated using actual measurements and other scenarios that are different from the training data. Finally, the performance of the proposed MPI-DeepONet is evaluated by comparing it with purely data-driven DeepONet in terms of accuracy and robustness. The accuracy is measured using root mean squared error metrics, while the robustness is evaluated by testing the neural network on scenarios that are different from the training data.

2. RESULT AND DISCUSSION

The proposed MPI-DeepONet was trained and evaluated using the data generated from high-fidelity FEA simulations of the thermal runaway of LIBs under various thermal operational and abuse conditions. The performance of the proposed neural network was compared with that of a purely data-driven DeepONet. The results of the evaluation are discussed below.

The performance of the proposed MPI-DeepONet was evaluated by measuring its accuracy and robustness. The accuracy was measured using the root mean squared error (RMSE) metrics. The RMSE values for temperature and dimensionless concentration of dominant components of a LIB are shown in Table 1. The RMSE values for temperature and dimensionless concentrations of the dominant components of the LIB for DeepONet were found to be 10.25 °C, 0.058, 0.038, 0.057, and 0.008, respectively. On the other hand, the MPI-DeepONet achieved better performance with RMSE values of 7.54 °C, 0.047, 0.031, 0.036, and 0.006 for temperature and dimensionless concentrations of the anode, cathode, electrolyte, and solid electrolyte interphase, respectively. These results indicate that the proposed MPI-DeepONet achieved lower RMSE values than the DeepONet, indicating that the proposed neural network has higher accuracy than the DeepONet. In Figure 1, the predicted values of temperature and dimensionless concentrations of anode and cathode by both DeepONet and MPI-DeepONet are shown. It can be observed that the MPI-DeepONet predictions are closer to the simulation results, indicating better performance than DeepONet. This can also be confirmed by the RMSE values of the test dataset, where MPI-DeepONet achieved lower values than DeepONet for all variables. Overall, the results suggest that MPI-DeepONet can be a promising approach for predicting the behavior of LIBs.

Table 1. RMSE values of test dataset for temperature and dimensionless concentrations

	Temp. [°C]	Cpe	Cne	Ce	Csei
DeepONet	10.25	0.058	0.038	0.057	0.008
MPI-DeepONet	7.54	0.047	0.031	0.036	0.006

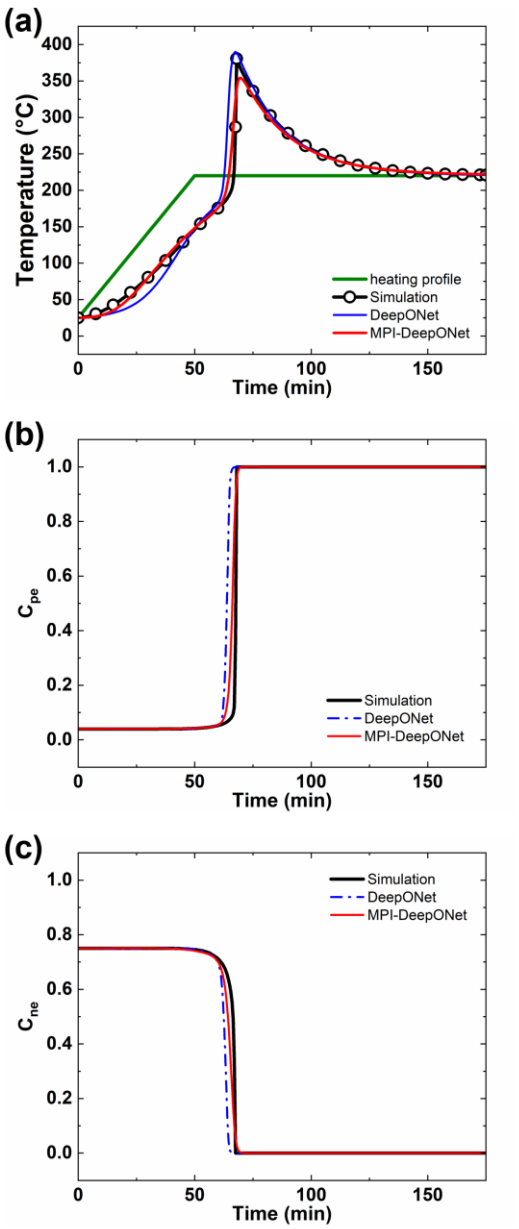

Figure 1. Comparison of thermal runaway prediction results from DeepONet and MPI-DeepONet test data

The proposed MPI-DeepONet was also tested on scenarios that are different from the training data to evaluate its robustness. Specifically, the predicted results are for an extrapolation of the heating target temperature to 260 °C, considering that the maximum heating target temperature of the training data was 240 °C. The results of the robustness evaluation are shown in Table 2. The RMSE values for temperature and dimensionless concentrations using DeepONet are 23.41 °C, 0.126, 0.021, 0.143, and 0.017, while those using MPI-DeepONet are 20.22 °C, 0.094, 0.064, 0.122, and 0.013, indicating better performance by MPI-DeepONet. Additionally, in Figure 2 showing the temperature prediction results using DeepONet and MPI-DeepONet, it is clear that MPI-DeepONet performs better, confirming its superior performance.

Table 2. RMSE values of scenarios other than training data for temperature and dimensionless concentrations

	Temp. [°C]	Cpe	Cne	Ce	Csei
DeepONet	23.41	0.126	0.021	0.143	0.017
MPI-DeepONet	20.22	0.094	0.064	0.122	0.013

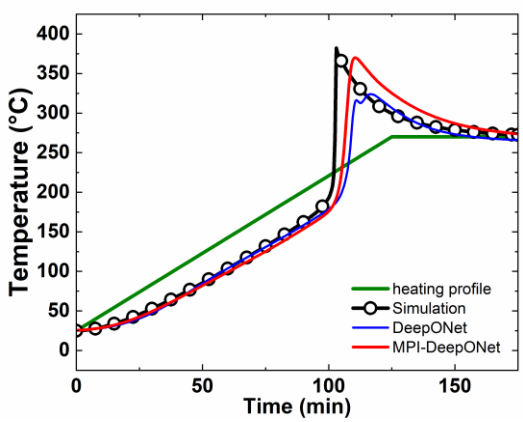

Figure 2. Comparison of thermal runaway prediction results from DeepONet and MPI-DeepONet test data for scenarios other than training data

The proposed MPI-DeepONet is a multiphysics-informed neural network that is capable of predicting the thermal runaway of LIBs under various thermal operational and abuse conditions. The proposed neural network was supervised by using ordinary and partial differential equations, which govern highly complex and nonlinear phenomena of thermal runaway of a LIB, including the chemical reaction degradation of the dominant four components and thermodynamics. The proposed neural network achieved higher accuracy and robustness than the DeepONet. The proposed surrogate model can be used to develop a digital twin model of a LIB, which can be deployed on a battery thermal management system and provides sufficient information for effective power and energy management. In summary, the proposed MPI-DeepONet provides faster than FEA simulations and more accurate than purely data-driven DeepONet for predicting the thermal runaway of LIBs under various thermal operational and abuse conditions. The proposed model can be used to develop a digital twin model of a LIB, which can be used to optimize the power and energy management of LIBs.

3. CONCLUSIONS

In conclusion, this study the proposed MPI-DeepONet to predict the thermal runaway of lithium-ion batteries under a variety of thermal operational and abuse conditions. The proposed method has two key characteristics: it is supervised by using ordinary and partial differential equations, and it is trained using data generated from high-fidelity finite element analysis simulations of the thermal runaway of LIBs. The results showed that the MPI-DeepONet outperformed the purely data-driven DeepONet in terms of accuracy and robustness. The proposed surrogate model provides an efficient and accurate way to predict the evolution of temperature and dimensionless concentration of dominant components of a LIB, given the heating curve. Given that these predictions were corroborated through comparison with FEM results, the subsequent step in future research involves conducting actual experiments to further validate and compare accuracy. The proposed MPI-DeepONet has the potential to significantly improve the safety and reliability of LIBs by predicting thermal runaways under various thermal operational and abuse conditions. It can also contribute to the development of efficient battery thermal management systems that can improve the power and energy efficiency of LIBs. Future research can explore the integration of the proposed model with other models to enhance the accuracy and robustness of the predictions. Additionally, the proposed model can be extended to other types of batteries and energy storage systems for a wide range of applications.

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