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Advanced thermal modeling of lithium-ion batteries: foundations for advanced capacity prediction

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ABSTRACT

Thermal modeling of lithium-ion batteries is crucial for optimizing their performance and reliability in applications such as electric vehicles and energy storage systems. This study introduces a novel thermal modeling framework to predict internal battery temperature as a function of current and ambient temperature. Three advanced methodologies, NN-LM, NN-BR, and GPM, were evaluated using drive cycle data across temperatures that vary from -20 °C to 25 °C. Among these, Gaussian process modeling (GPM) demonstrated the highest accuracy with an RMSE of 0.034%, while NN LM achieved an RMSE of 0.083%, offering a computationally efficient alternative suitable for real-time applications. The developed thermal model establishes a foundation for future research aimed at predicting battery capacity by incorporating the effects of internal temperature. Furthermore, accurate monitoring of internal temperature is critical for preventing thermal runaway by enabling early detection of unsafe thermal conditions. This work establishes a robust foundation for future research, aiming to develop real-time capacity prediction models, ultimately enhancing battery management systems under diverse operating conditions.

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1. INTRODUCTION

Technologies for energy storage play a major role in achieving the worldwide goal of net-zero emissions [1]. Because of high energy and power densities, LIBs constitute the most widely used energy storage options for personal electronics, mobility, and power tools [2]. The efficiency and electrical/thermal performance of LIBs must be improved in order to further lower the financial and environmental costs related to LIBs. The discharge capacity efficiency and battery longevity for the electric vehicle (EV) and battery energy storage system (BESS) industries are directly impacted by the temperature profile inside cells [3]-[5]. Battery safety issues [6] like thermal runaway can be caused by several factors as high internal temperatures [7], [8] or penetration [9]. The internal temperature may serve as a sign in the rapid detection of internal short circuits [10], [11]. Inside LIB, thermal gradients are easily produced, and a uniform temperature might be harmful to the life of the battery. According to experimental research, a pouch cell's internal temperature gradient can triple the rate of disintegration [12]. Because cylindrical cells are less effective at dissipating heat than pouch cells, thermal gradients are more likely to occur [13]. The temperature differential throughout the surface cell can exceed 5 °C when galvanostatic EIS is used with a peak-to-peak current of 10 °C and convective boundary conditions [14]. This implies that there might be notable temperature gradients inside the jellyroll and that the cell's core may be substantially different in temperature from a location on the cell’s surface [15]. As a result, real-time internal temperature estimation during operation greatly enhances battery system performance, longevity, and safety. It is somewhat simple to monitor the temperature directly on the surface [16], but it’s much less feasible to place a temperature sensor within a cell for commercial use. Even though the in-cell thermocouple technology [17] has shown promise in research, the thermocouple's chemical stability and additional expense make it unsuitable for large-scale battery manufacture [18]. To simulate and forecast the internal temperature distribution of a battery, distributed thermal models have been created; however, this sort of prognostic method suffers from error accumulation, particularly when simulating over a long duration. The data-driven approach has demonstrated efficacy in accurately estimating the interior temperature of batteries [19]. The incredibly high volume of training data needed, however, is a major disadvantage. Finding the internal temperature in real time has been made easier with the use of the virtual thermal sensor (VTS) technique [20]-[22]. The variations of Kalman Filters were put into practice inside the thermal model to estimate the internal temperature [23]. Built on the kind of model they are built on, VTS temperature estimation techniques can be broadly divided into three categories: fundamental continuum, reduced-order, and two/three-node thermal models [24].

The cylindrical cell's two-node model is built on the kind of model they are built on; VTS temperature estimation techniques can be broadly divided into three categories: fundamental continuum, reduced-order, and two/three-node thermal models. The battery's simplified two-node thermal model [20] and prismatic cells [21] were suggested for the estimation of internal temperature. Along the direction of electrode thickness, only two nodes are positioned. If the model projections are to be believed, the C rate is limited to below 1 °C due to the low computing cost and limited accuracy of these two-node thermal models. Taking electrical-thermal coupling into account increased the two-node thermal model's accuracy [20], but the models were still only applicable to modest electrical loads. for the second VTS type, the thermal model with reduced order has demonstrated efficacy in estimating temperature variations within the cell as well as volume-averaged temperature [25]. A simple EIS could be used to estimate core temperature [26]. These effective reduced-order modeling techniques, however, are only applicable to 2D simplification and mild discharge current circumstances. Due to the latter limitation, these techniques are not appropriate for practical, application-relevant thermal limit conditions like bottom and side cooling. The third VTS type uses continuum models based on physics to estimate temperature [27]. The average temperature of the bulk cell is estimated based on an extended Kalman filter (EKF) on a lumped electrochemical thermal model. However, because of their relatively high computing cost, such continuum models are not appropriate for estimating temperature at widely distributed locations [21]. Tools for effectively estimating the interior distribution of temperatures with application-relevant thermal limits and a spectrum of electrical loads have been few until now.

In order to forecast the interior temperatures of LIBs under various current and ambient temperature circumstances, this research presents a novel thermal modeling framework. Each of the three sophisticated approaches included in the framework, NN-LM, NN-BR, and GPM, is intended to maximize the trade-off between computational resources and forecast accuracy [28]. The model's dependability has been extensively validated through trials done over a wide variety of ambient temperatures, from -20 °C to 25 °C. Notably, the GPM shows an exceptionally low RMSE of 0.034%, making it the most accurate model among those examined. Furthermore, the NN-LM approach turns out to be a computationally efficient substitute, especially useful in situations when quick computing results are crucial, in addition to being highly effective at predicting temperature [29]. the created thermal model is also used to assess variations in battery capacity. This important development successfully connects theoretical understanding with real-world applications by combining heat modeling and capacity assessment.

The structure of this manuscript is organized as follows: i) Section 1 offers a comprehensive review of the literature, examining existing approaches to lithium-ion battery thermal modeling and their limitations; ii) Section 2 presents the experimental setup and provides a detailed description of the dataset, including drive cycle profiles and thermal chamber conditions across a range of ambient temperatures; iii) Section 3 outlines the proposed methodology, focusing on the development and implementation of three thermal modeling approaches: neural networks using Levenberg-Marquardt (NN-LM) and Bayesian regularization (NN-BR), as well as Gaussian process modeling (GPM) also reports the simulation and validation results, including a comparative analysis of model performance based on RMSE metrics and parity plots , and explores the application of the thermal model for predicting battery capacity under varying thermal conditions; and iv) Section 4 concludes the study by summarizing the key findings and proposing future research directions for enhanced battery management systems.

2. METHOD

This section presents the methodology used to model the internal temperature of lithium-ion batteries as a function of current and ambient temperature. It begins with data collection from realistic drive cycles followed by preprocessing and analysis. Three modeling techniques are applied neural networks (NN), Gaussian process modeling (GPM), and optimization algorithms (Levenberg-Marquardt and Bayesian regularization) also, the overall modeling strategy and the integration of these methods are illustrated in the accompanying flowchart.

2.1. Flowchart

The thermal modeling process, as illustrated in Figure 1, begins with data collection from realistic drive cycles. These data include current (I) and ambient temperature (Ta), which are essential for characterizing the internal thermal behavior of LIB. The collected data is then organized for further processing and analysis, ensuring a structured approach to model development and evaluation. Three distinct methods are employed for thermal modeling: the NN method, the PGM method, and two variants of the LM and BR optimization techniques. The NN method utilizes machine learning techniques to establish a relationship between current, ambient temperature, and battery temperature (Ti). This approach iteratively adjusts the model by evaluating the RMSE. If the RMSE is not sufficiently minimized, the hidden neuron (HN) count is incremented by a constant (n), refining the network structure until an optimal model is achieved.

The GPM method uses Gaussian processes to model battery thermal dynamics with built-in uncertainty estimation, making it robust for nonlinear relationships Unlike NN methods, GPM doesn't require iterative tuning LM and BR are optimization techniques within the NN approach LM minimizes error via gradient descent, while BR improves generalization through regularization, all models are evaluated using RMSE, and the most accurate is selected GPM was implemented using MATLAB's MBC Toolbox and NN with the neural network fitting toolbox.

To estimate the internal temperature of a lithium-ion battery cell as a function of current and ambient temperature, a Gaussian process model (GPM) was developed using the model-based calibration (MBC) toolbox in MATLAB/Simulink.

- Input data preparation: The Signal builder block was used in Simulink to generate realistic input profiles.
- Construction of the training dataset: The training dataset was constructed using the tuples [I,Ta]→Ti.
- Model fitting with GPM (MBC toolbox): Using the MBC toolbox, the training dataset was first imported into the MBC environment. The input variables were defined as current and ambient temperature, while the output variable was set as internal temperature. A Gaussian process model was then fitted using either the default kernel functions or optimized configurations selected through cross-validation, and the model's performance was evaluated using diagnostic tools such as RMSE calculation. Finally, the trained GPM was exported as a Simulink-compatible block using the generate Simulink block feature for integration into the simulation environment.

NN-LM and NN-BR were developed following the same steps using the model fitting features of the neural network toolbox.

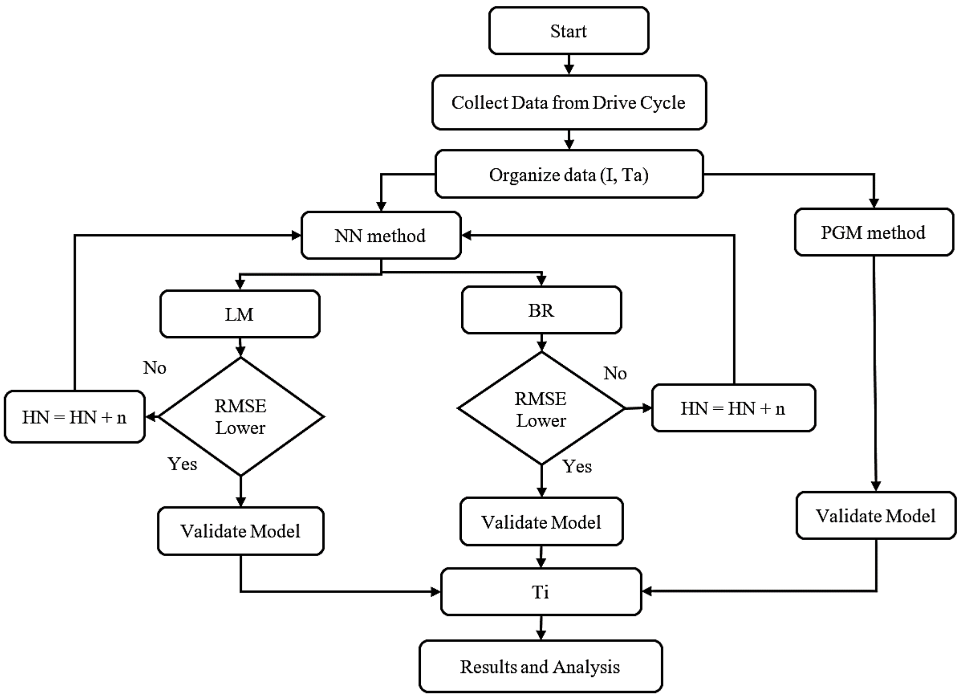

Figure 1. Development of a thermal modeling strategy using three methods

2.2. Data description

This study uses data Figure 2 from tests on a Panasonic 18650PF (2.9 Ah) battery conducted at the University of Wisconsin-Madison in a thermal chamber (-20 °C to 25 °C) under Dr. Phillip Kollmeyer, Key parameters voltage, current, power, and case temperature were recorded using a Digatron tester, Among nine drive cycles, "Cycle 4" was chosen for its consistent 0.1 s sampling rate and realistic power profile of a scaled-down electric Ford F150, ensuring accurate and uniform battery behavior representation.

At lower temperatures (-20 °C, -10 °C, and 0 °C), Figure 3, the current exhibits less pronounced variations, potentially due to the reduced electrochemical activity and higher internal resistance of the battery under cold conditions. The distinction between these profiles, although subtle, emphasizes the importance of high-resolution data visualization in understanding the thermal and electrical behavior of lithium-ion batteries. These findings validate the approach of analyzing current as a function of temperature to model internal battery temperature under realistic drive conditions.

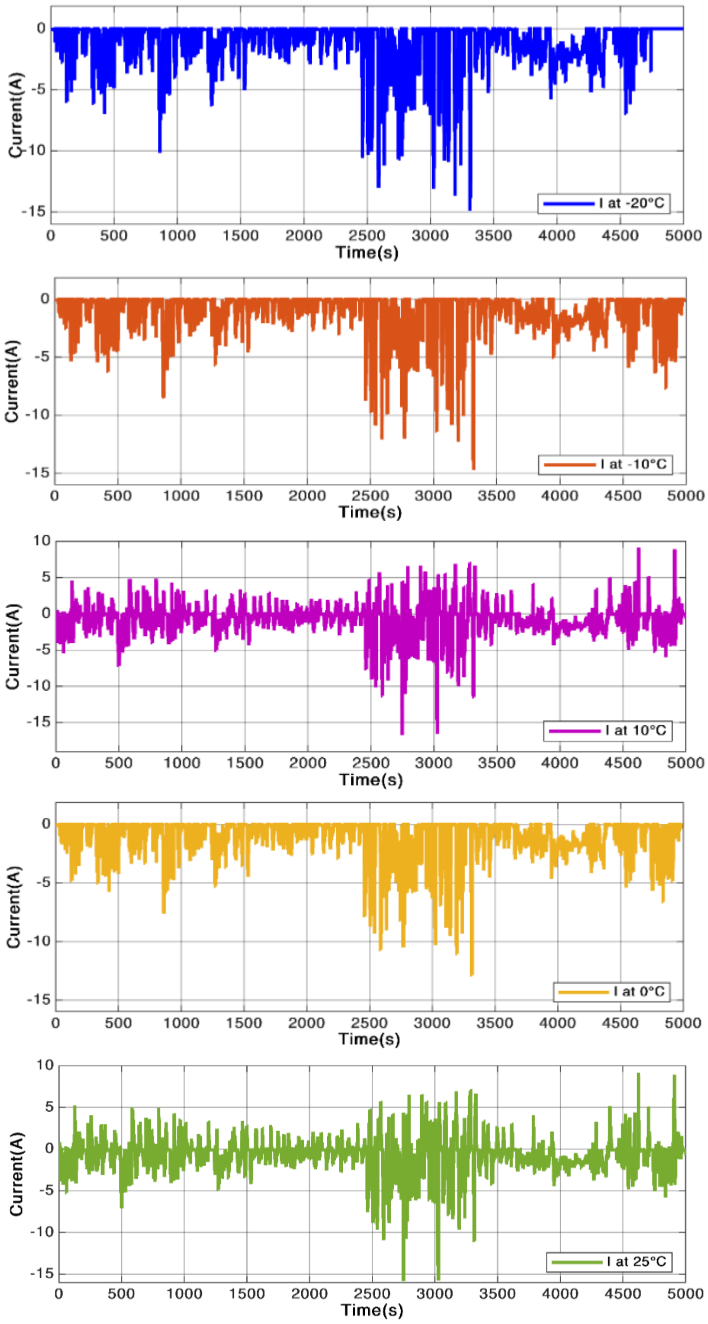

Figure 2. Current profiles at the TR

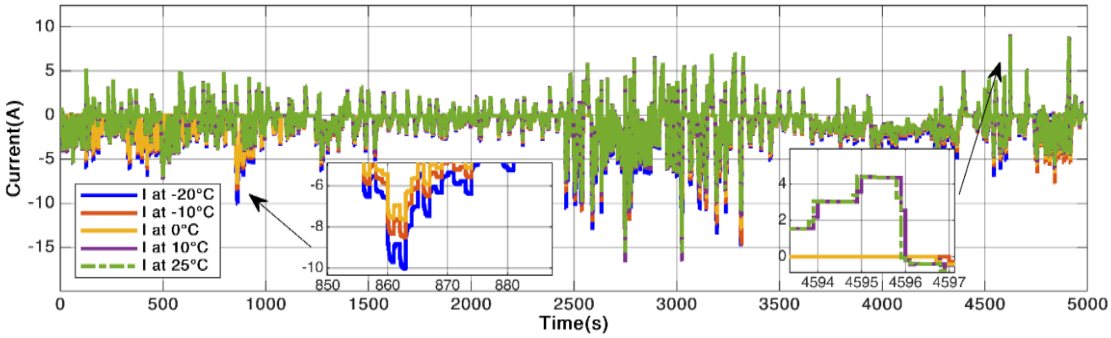

Figure 3. Comparison of various current profiles at different TR

2.3. Neural network method

The neural network (NN) approach is used to model the relationship between the input parameters, current (I) and ambient temperature (Ta)—and the output which is the internal battery temperature (Ti). The network typically consists of multiple layers, including one or more hidden layers, with (1) as the mathematical representation for a single hidden layer.

$$Ti = \emptyset\left(\sum_{j=1}^{Nh} W2_j * \sigma\left(\sum_{i=1}^{Ni} W1_{ij} * xi + b1_j\right) + b2\right) \tag{1}$$

Where:
- xi Represents the inputs (I and Ta).
- $W1_{ij}$ and $W2_j$ are the weights connecting the input and the hidden layer, and the hidden layer to the output, respectively.
- $b1j$ and $b2$ are bias terms.
- σ is the activation function for the hidden layer.
- $\emptyset$ is the output activation function (commonly linear for regression tasks).
- Nh Is the number of neurons in the hidden layer.

2.3.1. Optimization algorithms

Two commonly used optimization algorithms in neural network training are:
- Levenberg-Marquardt (LM): This algorithm is a combination of gradient descent and the Gauss-Newton method. It optimizes the network parameters to minimize the cost function, which is generally the mean squared error, as in (2).

$$\mathrm{E}(\theta) = {}^{1}/_{2}\left(\sum_{k=1}^{N}\left(Ti^k - \widehat{Ti}^k\right)^2\right) \tag{2}$$

  Where Ti^k and $\widehat{Ti}^k$ are the measured and predicted temperatures, respectively, and θ represents the model's parameters.
- Bayesian regularization (BR): This method introduces a regularization term into the cost function to balance accuracy and generalization. The modified cost function is as (3).

$$\mathrm{E}(\theta) = {}^{\beta}/_{2}\left(\sum_{k=1}^{N}\left(Ti^k - \widehat{Ti}^k\right)^2\right) + {}^{\alpha}/_{2}\,\|\theta\|^2 \tag{3}$$

  Where α and β control the trade-off between fitting the data and model complexity.

2.4. PGM method

The PGM offers a probabilistic perspective to the modeling problem. It assumes a prior distribution over functions that relate I, Ta, and Ti. This relationship can be expressed as (4).

$$\mathrm{Ti} \sim \mathrm{GP}\left(m(x), k(x, \acute{x})\right) \tag{4}$$

Here:
- $m(x)$ is the mean function, often initialized to zero for simplicity ($m(x) = 0$).

– $k(x,\acute{x})$ is the covariance (or kernel) function that quantifies the similarity between any two data points x and $\acute{x}$ A commonly used kernel is the squared exponential:

$$K(x,\acute{x}) = \sigma_f^2 \; exp\left(\frac{\|x-\acute{x}\|^2}{2\rho^2}\right) \tag{5}$$

Where x = [I, Ta], ρ is the length scale, and σ_f^2 is the signal variance. When provided with training data $\{X, Ti\}$, the model computes the posterior distribution of Ti for new inputs X_*, as in (6).

$$p(Ti : X, X_*, T_*) = N(\mu_*, C_*) \tag{6}$$

Where: μ_* is the posterior mean; C_* is the posterior covariance matrix.

3. RESULTS AND DISCUSSION

The thermal modeling framework was developed using MATLAB/Simulink Figure 4, leveraging its graphical programming environment to integrate and compare three advanced modeling approaches. The model processes input parameters, including current (I) and ambient temperature (Ta), to predict the internal battery temperature (Ti). These predictions are achieved through three distinct methodologies: NN-LM, NN-BR, and the PGM. Each method is implemented within dedicated Simulink blocks, enabling a seamless comparison of their performance.

3.1. Validation with NN-LM

Initially, Table 1, the model was tested with 10 HN, yielding an MSE of approximately 0.0406 for training and validation, with a correlation coefficient (R) value of 0.99991, indicating excellent correlation. As the number of hidden neurons was increased to 30, the MSE significantly decreased to 0.00851 for training, with a corresponding R value of 0.99998. The best results were obtained with 50 hidden neurons, where the training MSE reached a minimum of 0.00673 and an R value of 0.99999, demonstrating near-perfect correlation.

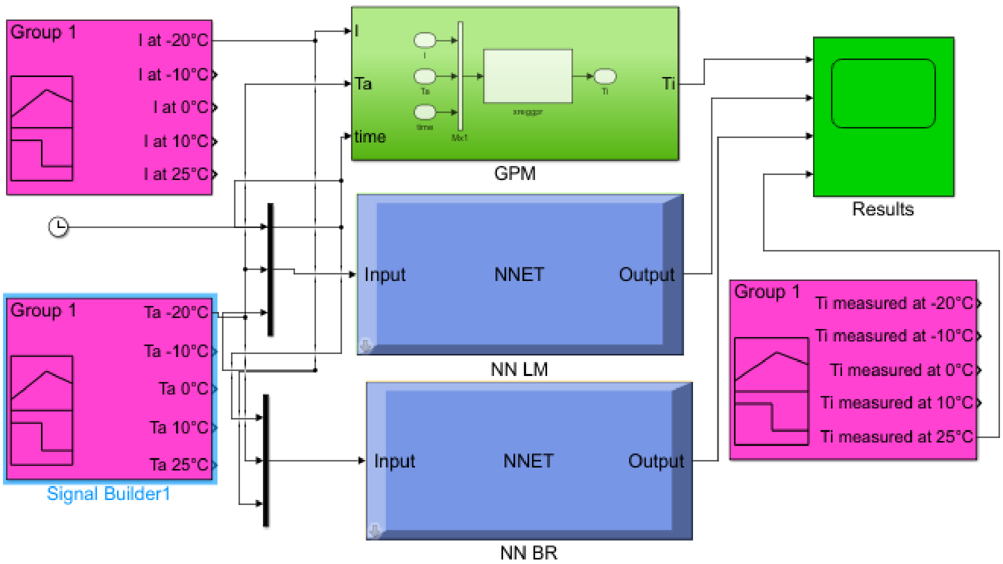

Figure 4. MATLAB/Simulink thermal model

Table 1. NN-LM performance metrics-MSE and regression (R) for different hidden layer configurations

Indicators	Levenberg-Marquardt algorithm performance					
	Hidden 10		Hidden 30		Hidden 50	
	MSE	R	MSE	R	MSE	R
Training	0.0406	0.99991	0.00851	0.99998	0.00673	0.99999
Validation	0.04	0.99991	0.00879	0.99998	0.00672	0.99999
Testing	0.0404	0.99991	0.00894	0.99998	0.00698	0.99999

To confirm the optimality of the model, additional testing was conducted with 70 hidden neurons. However, the MSE increased slightly compared to the configuration with 50 hidden neurons, indicating overfitting or diminishing returns with a larger network size. Based on these results, the NN model with 50 hidden neurons was selected as it achieved the lowest MSE while maintaining excellent generalization. Figure 5 illustrates the performance of the neural network (NN) trained with the Levenberg-Marquardt (LM) algorithm in predicting the internal temperature (Ti) of the battery across different ambient conditions: TR. These results provide valuable insights into the model's accuracy and reliability, as evidenced by the strong correlation between predicted and measured temperatures. These results highlight the strength of the NN-LM model in accurately representing the thermal behavior of the battery. The consistently high performance validates the architecture and optimization method, establishing this approach as a reliable tool for thermal modeling in battery management systems.

3.2. Validation with NN-BR

The results Table 2 of the neural network Bayesian regularization NN-BR model highlight its exceptional ability to accurately predict battery thermal behavior. With 10 hidden neurons, the model achieves an MSE of 0.0217 and an RRR value of 0.99995, indicating strong predictive accuracy. Increasing the hidden neurons to 30 significantly reduces the MSE to 0.00713, with an RRR value of 0.99998, showing enhanced performance. The best results are obtained with 50 hidden neurons, where the model achieves its lowest MSE of 0.00708 and an RRR value of 0.99998, demonstrating near-perfect correlation. These findings confirm that 50 hidden neurons strike the optimal balance between accuracy and generalization, showcasing the robustness and reliability of the Bayesian regularization method for battery thermal modeling.

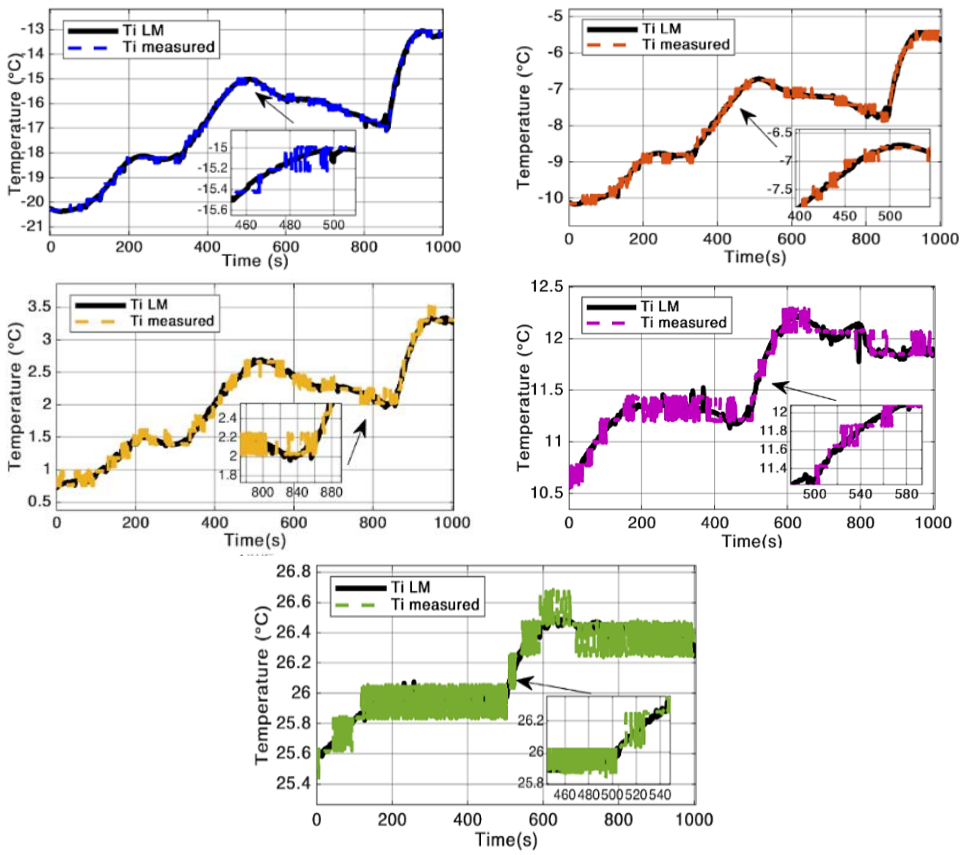

Figure 5. NN-LM model validation for different temperatures TR

Table 2. NN-BR performance metrics - MSE and regression (R) for different hidden layer configurations

Indicators	Bayesian regularization algorithm performances					
	Hidden 10		Hidden 30		Hidden 50	
	MSE	R	MSE	R	MSE	R
Training	0.0217	0.99995	0.00713	0.99998	0.00722	0.99998
Testing	0.0217	0.99995	0.00715	0.99998	0.00708	0.99998

Figure 6 obtained with the NN Bayesian regularization (BR) model illustrate its strong predictive performance across various ambient temperatures, including -20 °C, -10 °C, 0 °C, 10 °C, and 25 °C. The parity plots for each temperature show a clear alignment of data points along the diagonal line, indicating a close match between the predicted and actual battery temperatures. This alignment demonstrates the model's ability to capture the underlying thermal behavior of the battery accurately. These visual results provide a clear and intuitive representation of the accuracy and reliability of the BR model, alongside its comparison with the LM approach. While both methods demonstrate strong predictive capabilities.

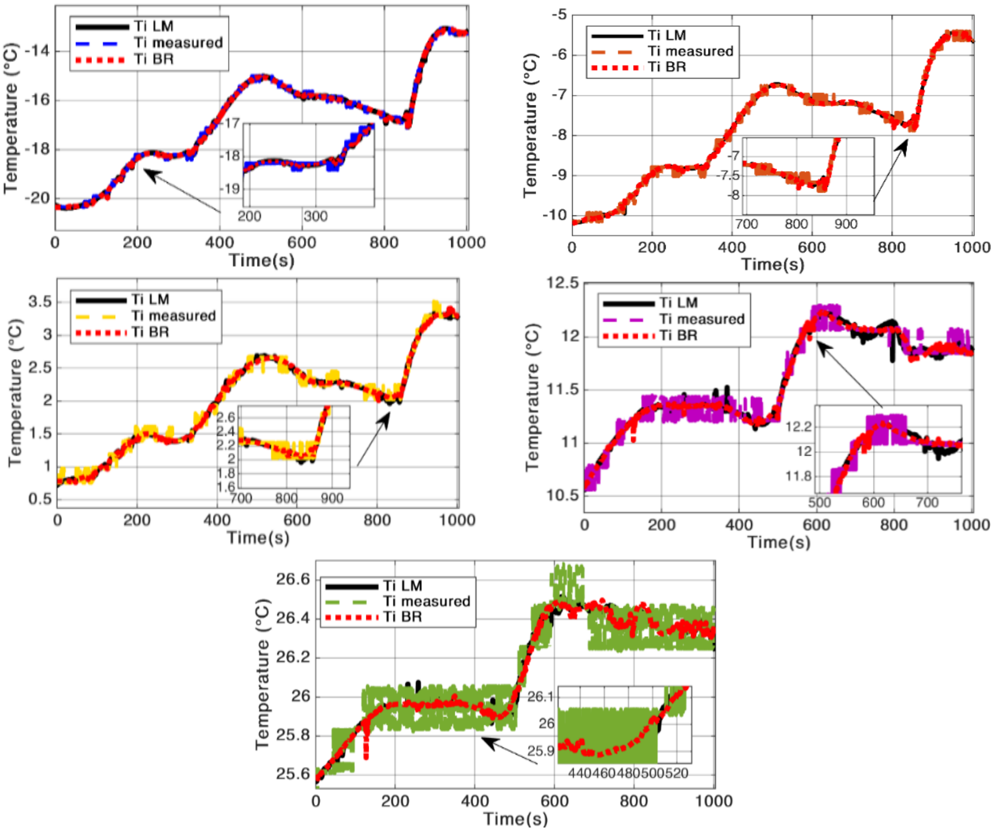

Figure 6. NN-BR model validation for different temperatures TR

3.3. Validation with GPM

The GPM Figure 7 delivers exceptional accuracy in predicting the internal temperature (Ti) of the battery under varying ambient conditions, including -20 °C, -10 °C, 0 °C, 10 °C, and 25 °C. The parity plots show an almost perfect match between the predicted and actual values, with the data points closely following the diagonal line, highlighting the model's ability to capture the intricate thermal dynamics of the battery. Achieving an RMSE of 0.034%, GPM stands out as the most accurate method among those tested, providing unparalleled precision.

Although GPM offers superior accuracy and achieves lower RMSE than NN-LM, it comes with higher computational cost due to its probabilistic framework and reliance on covariance functions. This makes GPM ideal for applications where precision outweighs efficiency, such as critical battery performance simulations. Overall, GPM sets the benchmark for accuracy, particularly in applications where precision is non-negotiable. Yet, its higher complexity highlights the importance of balancing accuracy requirements with computational resources.

3.4. Application of the thermal model to battery capacity prediction

Battery capacity, a fundamental parameter for assessing energy storage systems, is commonly calculated using the Coulomb counting formula. This method integrates the current drawn from or supplied to the battery over time, providing a measure of the available capacity. Mathematically, it is expressed as (7).

$$C = \int I(t)\, dt \tag{7}$$

Where I(t) is the instantaneous current. However, capacity is not solely a function of the current; it is influenced by several external and internal factors, including ambient temperature, which impacts the battery's electrochemical activity and energy storage efficiency.

In this study, the Coulomb counting formula was applied to compute the battery capacity at various ambient temperatures: -20 °C, -10 °C, 0 °C, 10 °C, and 25 °C. The results, illustrated in Figure 8, demonstrate a clear dependency of capacity on temperature. At lower temperatures, the capacity decreases significantly due to the reduced mobility of lithium ions within the electrolyte and increased internal resistance. Conversely, as the temperature rises, the capacity improves, reaching its peak at 25 °C. This analysis underscores the strong influence of ambient temperature on battery performance, highlighting the need for accurate thermal modeling to predict capacity under diverse operating conditions

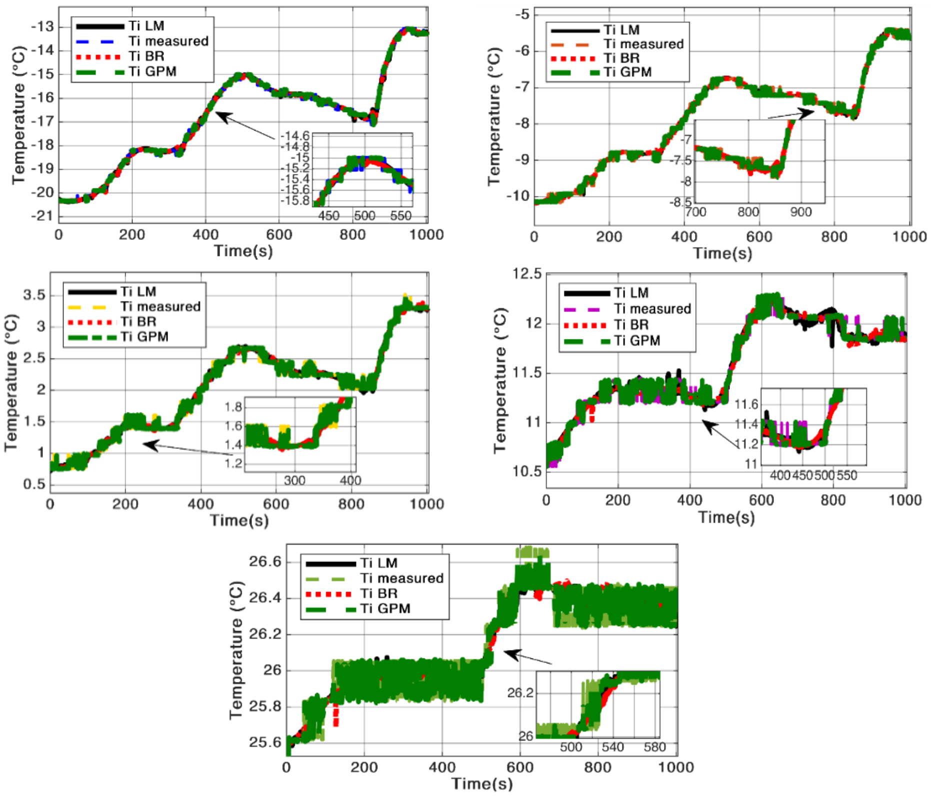

Figure 7. GPM model validation for different temperatures TR

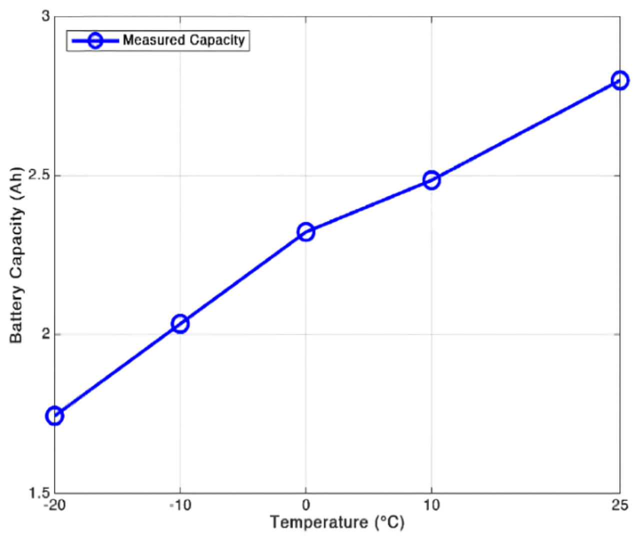

Figure 8. Capacity in function of temperatures

Furthermore, interior temperature, which fluctuates dynamically when in use, has an impact on battery capacity in addition to external temperature. The battery's internal temperature fluctuates as a result of chemical processes, heat production during cycles of charge and discharge, and resistance-related energy losses. These variables further affect the battery's capacity by changing the electrochemical kinetics and the availability of active material. This article's thermal model offers the framework required to include internal temperature in capacity prediction models, allowing for a thorough examination of battery behavior in practical settings, in the future work capacity will be predicted using current, ambient temperature and battery internal temperature that is obtained with the thermal model.

4. CONCLUSION

This study addresses important issues with battery management systems by introducing a novel thermal modeling framework created especially for lithium-ion batteries. The suggested framework uses advanced techniques, including NN-LM, NN-BR, and GPM, to accurately forecast internal battery temperature while accounting for the impacts of both current and ambient temperature. The GPM achieved an outstanding RMSE of 0.034%, confirming its position as the most accurate method. Extensive validation across a range of operational conditions, from -20 °C to 25 °C, has shown the stable performance of these models. On the other hand, NN-LM proved to be a computationally effective substitute, making it appropriate for real-time deployment.

A comprehensive understanding of battery behavior is fostered by the combination of thermal modeling and efficient battery management, which improves safety, dependability, and efficiency. The findings of this study have important implications for future studies on sophisticated capacity prediction models that incorporate derating and thermal dynamics. Thus, our work has the potential to significantly influence the development of next-generation battery management systems, especially in crucial fields where efficient control of thermal dynamics and capacity is essential, such as electric vehicles and renewable energy storage.

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AUTHOR CONTRIBUTIONS STATEMENT

This journal uses the Contributor Roles Taxonomy (CRediT) to recognize individual author contributions, reduce authorship disputes, and facilitate collaboration.

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C : **C**onceptualization	I : **I**nvestigation	Vi : **Vi**sualization
M : **M**ethodology	R : **R**esources	Su : **Su**pervision
So : **So**ftware	D : **D**ata Curation	P : **P**roject administration
Va : **Va**lidation	O : Writing - **O**riginal Draft	Fu : **Fu**nding acquisition
Fo : **Fo**rmal analysis	E : Writing - Review & **E**diting	

CONFLICT OF INTEREST STATEMENT

The authors declare that they have not received any funding, benefits, or personal relationships that could have influenced the work reported in this paper.

DATA AVAILABILITY

The data supporting the findings of this study are available from https://data.mendeley.com/datasets/wykht8y7tg/1.

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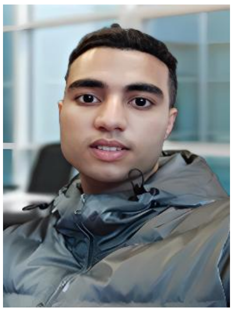

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