

ABSTRACT

The growing integration of renewable energy sources and the electrification of transport systems have increased the demand for efficient and reliable energy storage technologies. Lithium-ion batteries (Li-ion) are at the forefront of this transition due to their high energy density, long cycle life, and efficiency. However, their performance and safety are susceptible to temperature fluctuations. In electric vehicles (EVs), elevated or non-uniform temperatures can cause degradation, efficiency loss, and thermal runaway, posing safety risks.

This thesis presents a multi-level framework combining experimental characterization, electrothermal modelling, deep learning-based prediction, and advanced thermal management strategies. Temperature- and state of charge (SoC) dependent parameters such as open-circuit voltage, internal resistance, and entropic heat were extracted through experiments. These parameters inform the development of electrothermal models for two chemistries: LFP (prismatic) and NMC (cylindrical). The modelling includes resistance-based approaches and equivalent circuit models with inductive elements, enabling accurate prediction of temperature and voltage behaviour across varied discharge conditions. To enhance prediction under variable operating environments, data-driven models including Long Short-Term Memory (LSTM), Gated Recurrent Unit (GRU), and Transformer were trained on datasets collected at 4 °C, 24 °C, and 43 °C. These models estimate SoC, voltage, and temperature while capturing electrothermal dynamics and ageing indicators such as capacity fade and resistance growth. This integration of machine learning supports real-time monitoring and decision-making for battery management systems.

Thermal management solutions are then explored through a detailed numerical investigation of passive cooling with Phase Change Materials (PCMs). The effect of discharge rate, melt fraction, and PCM layer thickness (1.25 mm, 2.50 mm, and 5.00 mm) is analyzed to identify optimal configurations that maintain thermal safety without overdesign. Performance

metrics such as the Cell Cooling Coefficient and PCM Cooling Enhancement Factor are introduced. Building on this, an AHP-TOPSIS framework is applied to rank over 110 commercially available PCMs based on ten thermophysical and safety attributes. The simulation results guide the selection to ensure compatibility between PCM thermal properties, discharge-dependent heat loads, and optimal thickness configuration. The study also compares PCM-based cooling with passive immersion techniques using dielectric liquids like water-glycol, silicone, and mineral oil. A hybrid battery thermal management system is developed by integrating PCM with a liquid cooling jacket to improve thermal regulation beyond passive methods. A vehicle-level hybrid framework is also constructed in MATLAB Simulink to simulate coupling between an electric vehicle's battery and cabin thermal systems, allowing analysis of shared thermal loads and energy consumption.

Overall, this research delivers a scalable and technically rigorous strategy for improving the safety, thermal stability, and performance of Li-ion batteries. The work offers actionable insights for real-time diagnostics and future battery system development by integrating electrothermal modelling, machine learning, and advanced cooling design. It also contributes to sustainability by supporting clean energy technologies aligned with the UN Sustainable Development Goals (SDG 7 and SDG 13) and India's FAME and National Electric Mobility Mission.

Keywords: Electrothermal modelling; Lithium-ion battery; Phase Change Materials; Deep learning; Hybrid thermal management systems