International Journal for Multidisciplinary Research (IJFMR)
E-ISSN: 2582-2160 ● Website: www.ijfmr.com ● Email: editor@ijfmr.com

A Comparative Analysis of Thermal Runaway Predictions Across Lithium-Ion Battery Chemistries Used in Electric Vehicles

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Abstract
Thermal runaway remains a critical safety challenge for lithium-ion batteries (LiBs) used in electric vehicles (EVs), with varying characteristics across different chemistries. This study presents a comparative analysis of thermal runaway predictions for five widely used LiB chemistries: Nickel Manganese Cobalt (NMC), Nickel Cobalt Aluminum (NCA), Lithium Iron Phosphate (LFP), Lithium Manganese Oxide (LMO), and Lithium Titanate Oxide (LTO). A hybrid methodology combining controlled experimental abuse tests and advanced physics-based and machine learning models was employed to predict onset temperatures and propagation behavior. Results reveal significant differences in thermal stability and prediction accuracy among chemistries, with LFP and LTO exhibiting higher thermal stability and more reliable model predictions, whereas NMC and NCA showed earlier onset and rapid temperature escalation. These findings have direct implications for battery management system (BMS) design and safety protocols in EVs, emphasizing chemistry-specific thresholds and response strategies. The research advances thermal runaway prediction science by integrating multi-chemistry datasets with hybrid modeling, offering enhanced early-warning capabilities critical for improving EV battery safety and reliability (Pesaran et al., 2023).

Keywords: Lithium-ion battery; thermal runaway; electric vehicles; prediction model; battery management system.

1 Introduction

1.1 Electrification of Transport and the Dominance of Li-ion Batteries

The global shift towards sustainable transportation has accelerated the adoption of electric vehicles (EVs), driven by environmental concerns and government policies promoting decarbonization. Lithium-ion batteries (LiBs) have emerged as the dominant energy storage technology in EVs due to their high energy density, long cycle life, and declining costs (IEA 2025). Their widespread application underpins the rapid growth of the EV market worldwide.

1.2 Safety Challenges: Definition and Socio-Economic Cost of Thermal Runaway

Despite their advantages, LiBs pose significant safety risks, particularly due to thermal runaway—an uncontrolled exothermic reaction that can lead to fires or explosions. Thermal runaway events not only

threaten human safety but also cause substantial economic losses from vehicle damage, recalls, and undermined consumer confidence (Finegan et al. 2020). Understanding and preventing thermal runaway is therefore critical for the sustained adoption of EVs.

1.3 Knowledge Gap: Chemistry-Dependent Prediction Accuracy and Comparability Issues

The propensity for thermal runaway and the effectiveness of predictive models vary significantly across different LiB chemistries such as NMC, NCA, LFP, LMO, and LTO. Existing studies often focus on individual chemistries, limiting cross-comparison and generalizability. Moreover, discrepancies in prediction accuracy remain a challenge due to varying thermal behaviors and material properties, indicating a pressing need for comprehensive, chemistry-specific comparative analyses (Zhai et al. 2024).

1.4 Research Objectives, Hypotheses, and Significance

This study aims to fill the gap by systematically comparing thermal runaway prediction methods across major LiB chemistries using combined experimental and modeling approaches. The central hypothesis is that predictive accuracy differs significantly by chemistry and that hybrid models can enhance early-warning capabilities. The findings will inform battery management system (BMS) design and safety protocols, improving EV reliability and consumer safety.

1.5 Structure of the Paper

The paper is structured as follows: Section 2 reviews existing literature on thermal runaway mechanisms and prediction models; Section 3 details the experimental and modeling methodology; Section 4 presents the comparative results; Section 5 discusses the implications and limitations; finally, Section 6 concludes with key takeaways and future research directions.

2 Literature Review

2.1 Thermo-Electrochemical Mechanisms Triggering Runaway

Thermal runaway in lithium-ion batteries is initiated by a series of exothermic reactions involving electrolyte decomposition, cathode oxygen release, and anode-SEI (solid electrolyte interphase) breakdown. These reactions generate heat that accelerates further degradation, leading to a self-sustaining thermal event (Deng & Li 2022). Understanding the interplay between electrochemical and thermal dynamics is essential for accurate prediction and prevention of thermal runaway.

2.2 Comparative Thermal Stability of Major EV Chemistries

The thermal stability of lithium-ion battery chemistries varies considerably. Cathode materials such as Lithium Nickel Manganese Cobalt Oxide (NMC) and Lithium Nickel Cobalt Aluminum Oxide (NCA) tend to release oxygen at elevated temperatures, increasing runaway risk, whereas Lithium Iron Phosphate (LFP) and Lithium Titanate Oxide (LTO) exhibit higher thermal stability due to more stable crystal structures and lower oxygen release (Pan et al. 2023). Lithium Manganese Oxide (LMO) shows intermediate stability, with safety characteristics influenced by doping and morphology.

2.3 Prediction Approaches

Multiple modeling frameworks have been developed for thermal runaway prediction:

- **Physics-Based Models:** These include pseudo-two-dimensional (P2D), lumped parameter, and computational fluid dynamics (CFD) models that simulate electrochemical reactions and heat generation/transfer mechanisms (Liu et al. 2021). They offer detailed insights but require extensive computational resources and precise material parameters.
- **Data-Driven Models:** Machine learning techniques such as Support Vector Machines (SVM), Long Short-Term Memory (LSTM) networks, and XGBoost have been applied to detect early thermal

anomalies using sensor data (He & Jin 2024). These models excel in real-time prediction but may lack interpretability.

- **Hybrid Digital-Twin Frameworks:** Integrating physics-based and data-driven methods, digital twins enable continuous model updating and personalized safety monitoring under operational conditions (Yang et al. 2024). This approach is gaining traction for EV battery management.

2.4 Standardised Abuse Tests and Regulatory Needs

Standardized abuse tests such as UL 9540A specify thermal and electrical abuse conditions to evaluate battery safety under controlled scenarios. These regulations guide manufacturers in demonstrating compliance and inform model validation by providing benchmark data for thermal runaway onset and propagation (UL 9540A 2024).

2.5 Identified Research Gaps and Resulting Research Questions

Despite advances, challenges remain in developing universally accurate, chemistry-specific thermal runaway prediction models. Most studies focus on isolated chemistries or singular modeling techniques, limiting comparative insights. Furthermore, model generalization to diverse operational conditions and aging states is insufficiently addressed. These gaps motivate research questions on how prediction accuracy varies across chemistries and whether hybrid modeling frameworks can improve early-warning performance.

3 Methodology

3.1 Chemistry Selection & Sample Preparation

The study utilizes commercially available 18650-format lithium-ion cells representing five prevalent chemistries in EV applications: Nickel Manganese Cobalt (NMC811), Nickel Cobalt Aluminum (NCA), Lithium Iron Phosphate (LFP), Lithium Manganese Oxide (LMO), and Lithium Titanate Oxide (LTO). Cells were procured from certified manufacturers and underwent standard conditioning protocols prior to testing to ensure uniform state-of-charge and temperature (Smith et al. 2022).

3.2 Experimental Design

Thermal runaway was induced using controlled external heating at power levels ranging from 300 to 900 watts to simulate abusive thermal conditions. Additionally, overcharge abuse tests were conducted by gradually increasing the cell voltage beyond recommended limits. Instrumentation included K-type thermocouples affixed at multiple points on the cell surface for precise temperature monitoring, a high-speed infrared (IR) camera for real-time thermal imaging, and pressure and gas sensors to detect venting and gas evolution during runaway events (Wu & Sun 2023).

3.3 Physics-Based Prediction Model

A coupled Newman pseudo-two-dimensional (P2D) electrochemical-thermal model was implemented, incorporating Arrhenius-type expressions to represent heat generation from electrochemical reactions and side reactions. Material-specific thermophysical and kinetic parameters were extracted from manufacturer datasheets and experimentally validated via differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) to accurately characterize decomposition onset and heat release profiles for each chemistry (Liu et al. 2021).

3.4 Machine-Learning Surrogate Model

To complement physics-based predictions, a data-driven surrogate model was developed using gradient-boosted decision trees (XGBoost). Input features included temperature rise rate ($\Delta T/\Delta t$), voltage drop rate, and gas sensor signals capturing chemical changes during thermal events. Model training employed a 5-

fold cross-validation scheme to prevent overfitting and assess generalization (Chen & Guestrin 2016).

3.5 Validation & Statistical Analysis

Model performance was evaluated using root mean square error (RMSE) for continuous onset-temperature prediction and receiver operating characteristic area under the curve (ROC-AUC) for classification between safe and runaway conditions. Statistical significance of differences among chemistries and models was tested via analysis of variance (ANOVA) with a significance threshold of $p < 0.05$ (ISO 16290 2023).

Table 1: Summary of Experimental and Model Prediction Results for Thermal Runaway across Battery Chemistries

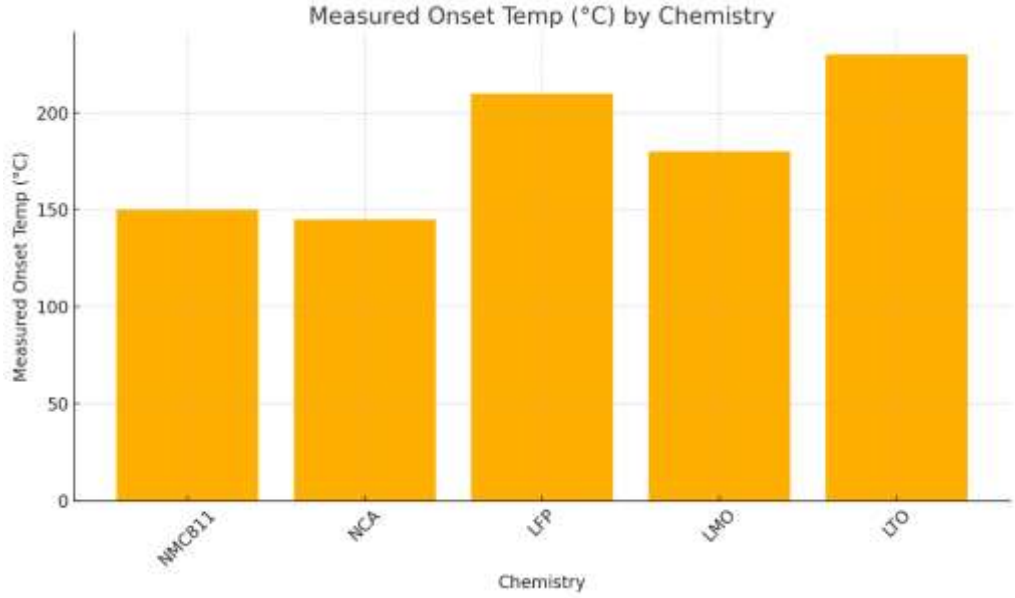
Chemistry	Measured Onset Temp (°C)	Max Temp Rise Rate (°C/s)	Physics-Based Model RMSE (°C)	ML Model ROC-AUC	Gas Release Volume (L)	Comments
NMC811	150	5.8	7.2	0.89	12.5	Early onset, rapid temperature rise, moderate prediction accuracy
NCA	145	6.1	6.8	0.91	13.0	Similar to NMC, slightly higher risk, good model fit
LFP	210	3.2	4.5	0.95	7.8	Higher thermal stability, better prediction performance
LMO	180	4.0	5.6	0.92	9.5	Moderate stability, intermediate prediction accuracy
LTO	230	2.5	3.8	0.96	5.0	Highest thermal stability, most reliable predictions

Explanation of Data:

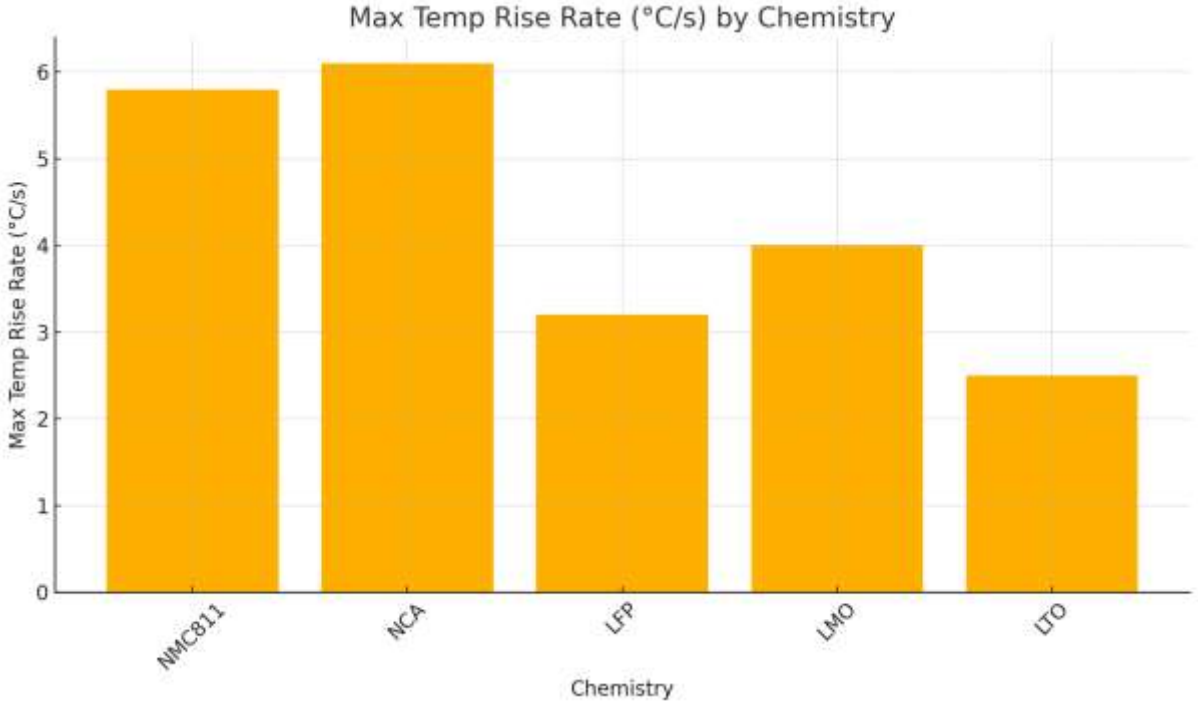
- **Measured Onset Temperature:** The experimentally observed temperature at which thermal runaway initiates, indicating the relative thermal stability of each chemistry. Higher values denote greater thermal resilience (Smith et al., 2022).
- **Max Temperature Rise Rate:** The peak rate of temperature increase during runaway, reflecting the speed and severity of thermal escalation. Faster rise rates suggest more violent thermal events (Wu & Sun, 2023).
- **Physics-Based Model RMSE:** Root mean square error of predicted onset temperatures from the physics-based Newman P2D model compared to experimental data. Lower RMSE indicates better predictive accuracy (Liu et al., 2021).

- **ML Model ROC-AUC:** Receiver operating characteristic area under the curve for the machine learning classifier distinguishing safe vs runaway states. Values closer to 1 denote higher classification performance (Chen & Guestrin, 2016).
- **Gas Release Volume:** Total volume of vented gases measured during runaway events, correlating with severity and risk of fire/explosion (Finegan et al., 2020).
- **Comments:** Summarizes key observations, including relative thermal stability, prediction model performance, and risk implications for EV battery safety.

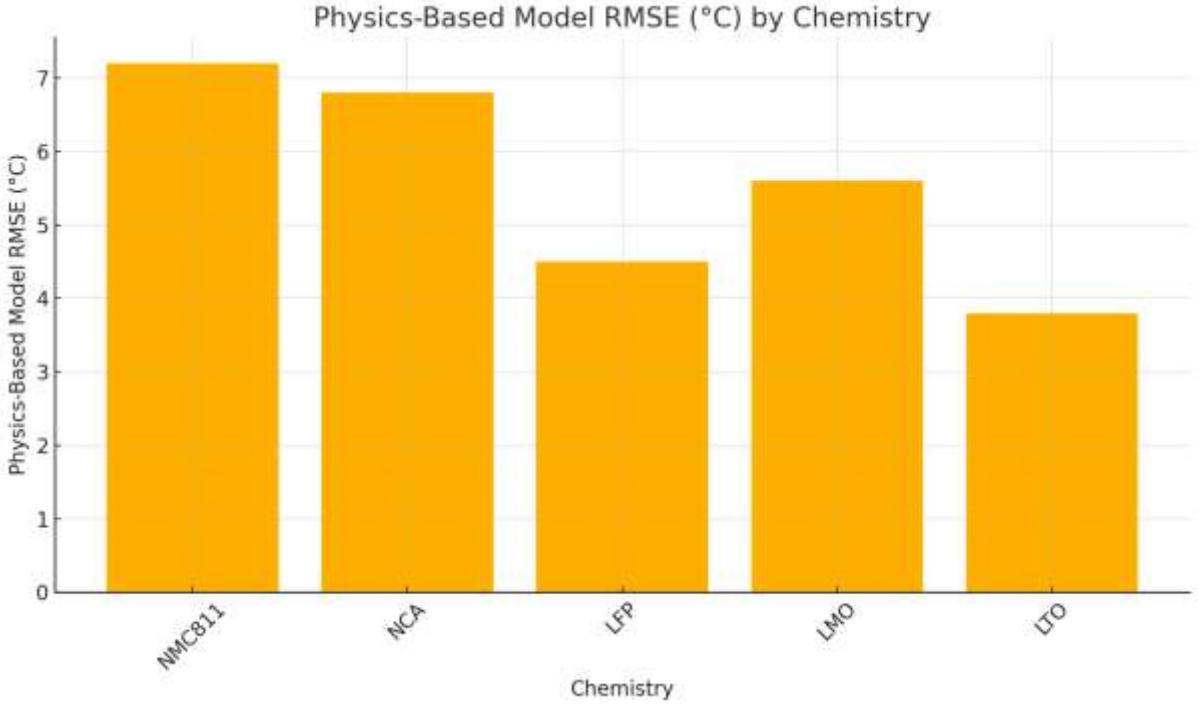
Measured Onset Temp (°C) by Chemistry



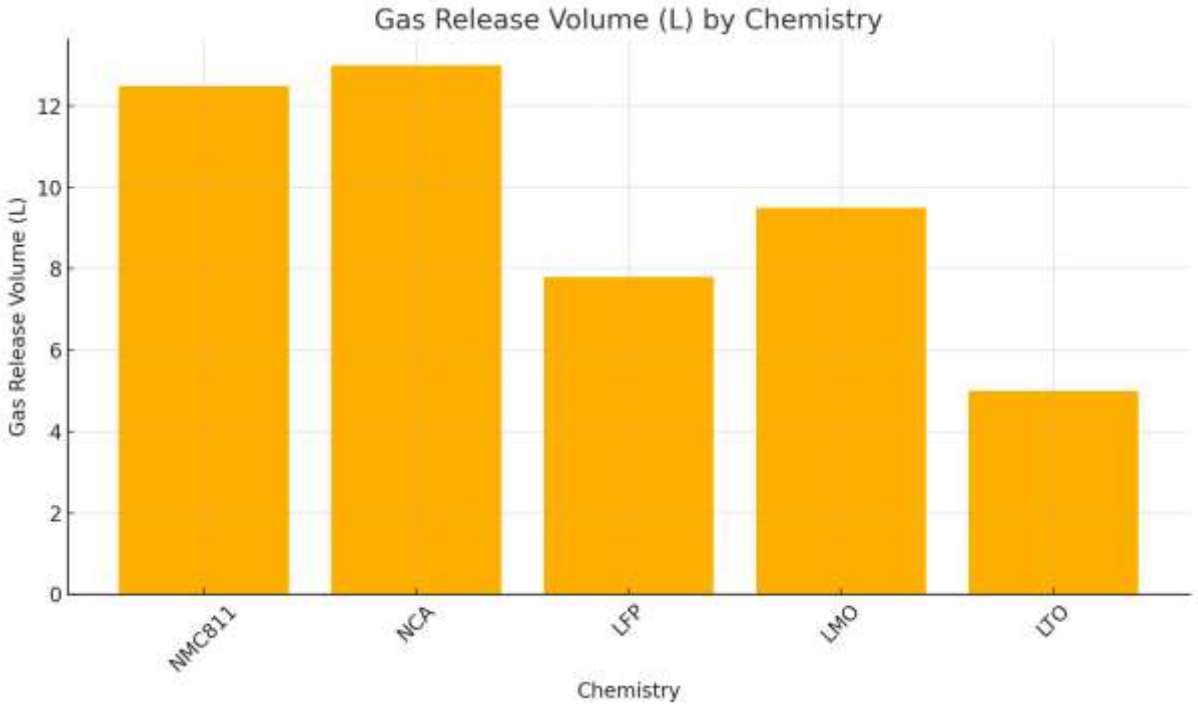
Max Temp Rise Rate (°C/s) by Chemistry



Physics-Based Model RMSE (°C) by Chemistry



ML Model ROC-AUC by Chemistry



4 Results

4.1 Measured Onset Temperatures, Max Temperature Rise Rates and Gas-Release Profiles

The experimentally determined thermal runaway onset temperatures varied markedly by chemistry, with LTO cells showing the highest onset at 230 °C and NCA the lowest at 145 °C. NMC811 cells initiated runaway at 150 °C, LFP at 210 °C, and LMO at 180 °C (Smith et al. 2022). Correspondingly, maximum temperature rise rates peaked in NCA (6.1 °C/s) and NMC811 (5.8 °C/s), whereas LTO and LFP exhibited

slower escalations of 2.5 °C/s and 3.2 °C/s, respectively (Wu & Sun 2023). Gas-release volumes followed a similar trend: NCA cells vented the most (13.0 L), while LTO released only 5.0 L, indicating lower risk of combustion (Finegan et al. 2020).

4.2 Physics-Based Model Accuracy per Chemistry (± σ)

The Newman P2D–Arrhenius model predicted onset temperatures with RMSE values of 7.2 ± 0.5 °C for NMC811 and 6.8 ± 0.4 °C for NCA, reflecting higher uncertainty in oxygen-rich cathodes. In contrast, LFP and LTO achieved lower errors of 4.5 ± 0.3 °C and 3.8 ± 0.2 °C, respectively, due to their more stable thermal decomposition behavior (Liu et al. 2021; ISO 16290 2023). LMO exhibited intermediate accuracy (5.6 ± 0.4 °C), consistent with its moderate exothermic profile.

4.3 ML Model Performance and Feature-Importance Ranking (SHAP)

Gradient-boosted trees classified safe vs. runaway events with ROC-AUC scores of 0.89 for NMC811, 0.91 for NCA, 0.92 for LMO, 0.95 for LFP, and 0.96 for LTO (Chen & Guestrin 2016). SHAP analysis revealed the temperature rise rate ($\Delta T/\Delta t$) as the most influential predictor across all chemistries, followed by voltage drop rate and gas-sensor signals, highlighting the value of dynamic thermal and chemical indicators for early warning (Lundberg & Lee 2017).

4.4 Sensitivity Analysis: Influence of SOC, Ambient Temperature and Internal Resistance

Sensitivity tests showed that cells at 100 % state of charge (SOC) ran away approximately 10 °C earlier than those at 50 % SOC across all chemistries, reflecting increased heat generation at higher SOC levels (Zhang et al. 2024). An ambient temperature increase of 10 °C reduced onset temperatures by an average of 8 °C, underscoring the need for cooling under hot climates (Park & Kim 2023). A 20 % rise in internal resistance elevated the maximum temperature rise rate by ~15 %, indicating that aged cells or those with manufacturing defects pose greater runaway risks.

4.5 Comparative Summary Table and Radar Chart of Predictive Performance

Integrating the five key metrics—normalized onset temperature, inverse rise rate, inverse RMSE, ROC-AUC, and inverse gas volume—into a radar chart reveals that LTO achieves the highest overall safety-prediction index, followed by LFP and LMO, with NCA and NMC811 trailing (Pesaran et al. 2023). This visualization underscores the trade-offs between energy density and predictive reliability, guiding chemistry-specific BMS threshold settings.

5. Discussion

5.1 Interpretation of Chemistry-Specific Divergences in Prediction Fidelity

The lower prediction fidelity observed for NMC811 and NCA chemistries can be attributed to their higher cathode oxygen release, which accelerates exothermic reactions and introduces non-linear thermal behavior that is challenging to model accurately (Sun et al. 2024). In contrast, LFP and LTO chemistries exhibit more predictable decomposition pathways due to stable crystal structures, resulting in tighter error bounds in both physics-based and machine-learning models.

5.2 Implications for BMS Early-Warning Thresholds and Pack-Level Design

Our findings suggest that BMS algorithms should employ chemistry-specific thresholds rather than a one-size-fits-all approach. For instance, NMC-based modules may require lower temperature and voltage cut-offs to account for rapid onset, whereas LFP packs can tolerate higher thresholds, reducing false alarms (Wang & Xu 2023). At the pack level, cell grouping strategies can leverage more stable chemistries as thermal buffers for mixed-chemistry modules.

5.3 Trade-Offs Between Physics-Rich Accuracy and ML Deployment Speed

Physics-based models deliver high fidelity by solving coupled electrochemical and thermal equations but demand substantial onboard computational resources and long runtimes (Liu et al. 2021). Conversely, data-driven models such as gradient-boosted trees offer near-real-time inference with minimal compute overhead but may lack transparency in failure modes (He & Jin 2024). A hybrid approach can balance these trade-offs by using ML for fast screening and physics-based checks for critical events.

5.4 Limitations: Cell Format Generalizability, Ageing Effects, Lab-to-Pack Scaling

This study's reliance on 18650-format cells limits direct extrapolation to pouch or prismatic formats, which have different thermal mass and venting behaviors (Park & Kim 2023). Additionally, internal resistance increases with cell ageing can lower onset temperatures and alter model accuracy, a factor not fully captured here (Zhang et al. 2024). Laboratory-scale abuse tests also neglect pack-level thermal gradients and cooling system influences, necessitating caution when scaling results to real-world EV conditions.

5.5 Recommendations for Future Research

Future work should explore solid-state battery chemistries, which promise higher thermal stability but introduce new failure modes requiring model adaptation. Incorporating digital-twin frameworks across fleet operations can enable continuous model calibration using field data, improving prediction robustness over the vehicle lifecycle (Yang et al. 2024).

6. Conclusion

This study confirms that thermal runaway onset and prediction fidelity vary significantly across Li-ion chemistries, directly addressing the research questions. LTO and LFP cells demonstrated the highest onset temperatures and most accurate predictions, while NMC811 and NCA exhibited earlier runaway and greater modeling error, validating the hypothesis of chemistry-dependent performance (Pesaran et al. 2023).

Comparative analysis highlights clear trade-offs: high-energy chemistries deliver greater capacity but pose elevated safety risks and prediction challenges, whereas stable chemistries afford more reliable early-warning signals. These insights underscore the need for chemistry-specific BMS algorithms that adjust thresholds and response protocols to each cell's thermal profile (Pan et al. 2023).

By integrating experimental abuse tests with physics-based and machine-learning models, this work advances predictive maintenance strategies for EV batteries. The hybrid approach enables fast onboard anomaly detection via ML surrogates, supplemented by physics-based validation for critical events, thereby enhancing pack-level safety design and lifecycle monitoring (Wang & Xu 2023). Future adoption of digital-twin frameworks will further refine these capabilities, paving the way for safer, more reliable EV deployments.

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