Predictive Modeling and Fault Detection of Thermal Runaway in Lithium-Ion Batteries

Harsh Kumar[1]

[1]*Student, Department of Electrical Engineering, L. D. College of Engineering*

***Abstract*—Lithium-ion batteries (LIBs) are critical for modern energy applications, such as electric vehicles (EVs) and renewable energy systems. However, their vulnerability to thermal runaway (TR)—a self-sustaining thermal failure—poses significant safety challenges. This research introduces a hybrid predictive framework combining physics-based thermal modeling and machine learning (ML) techniques. The Bernardi equation simulated heat dynamics, while Random Forest and XGBoost classified multi-sensor data to detect TR risks. The XGBoost model achieved 95.1% accuracy with a time-to-fault prediction error of ±5 seconds. Multi-sensor fusion of temperature, voltage, and state of charge (SOC) data enhanced detection accuracy by 10%. These findings underscore the potential of integrating predictive models into battery management systems (BMS) to improve LIB safety and reliability.**

***Index Terms*—Lithium-Ion Batteries, Fault Detection, State of Health (SOH), Remaining Useful Life (RUL), Artificial Intelligence (AI), Machine Learning (ML), Deep Learning, Hybrid Models, Probabilistic Models, Battery Management Systems (BMS), Thermal Runaway, State of Charge (SOC), Anomaly Detection, Data-Driven Techniques, Physics-Based Modeling, Predictive Maintenance, Energy Storage Systems, Electric Vehicles (EVs).**

I. INTRODUCTION

Lithium-ion batteries (LIBs) are a cornerstone of energy storage technologies, offering high energy density, long cycle life, and lightweight design. Their widespread adoption in electric vehicles (EVs), renewable energy systems, and consumer electronics reflects their versatility [1, 2]. However, LIBs are susceptible to thermal runaway (TR), an exothermic chain reaction caused by internal failures or external abuse, such as overcharging, overheating, or mechanical damage [3, 4]. TR incidents can propagate across densely packed battery modules, posing significant safety risks to EV passengers and infrastructure [5]. Current detection systems in battery management systems (BMS) primarily rely on temperature and voltage monitoring, which are insufficient for early fault detection [6].

This study proposes a hybrid predictive framework combining physics-based thermal modeling and machine learning (ML) techniques to address these challenges. The objectives include:

1.Developing predictive models to identify early-stage TR.

2.Evaluating ML algorithms, such as Random Forest and XGBoost, for fault detection.

3.Enhancing fault detection accuracy through multi-sensor fusion approaches.

II. LITERATURE REVIEW

A. Thermal Runaway in Lithium-Ion Batteries

TR is initiated when the heat generated within a battery exceeds its dissipation capacity, leading to an uncontrollable temperature escalation. The stages include [7]:

1.Solid Electrolyte Interphase (SEI) Decomposition: At 60–120°C, heat and gases are released.

2.Separator Melting: At 130–165°C, internal short circuits form due to separator failure.

3.Cathode Decomposition: Above 175°C, oxygen release exacerbates heat generation.

B. Key factors influencing TR include:

- Battery Chemistry: Cathodes like lithium iron phosphate (LFP) are more thermally stable than lithium cobalt oxide (LCO) [8].
- State of Charge (SOC): Higher SOC reduces TR onset temperature by increasing stored energy [9].

- External Stress: Overcharging, mechanical damage, and high-temperature environments exacerbate TR risks [10].

C. Predictive Modeling Techniques

Physics-based models, such as the Bernardi equation, simulate heat dynamics under various operating conditions [11]. Machine learning (ML) algorithms enhance fault detection by analyzing sensor data for predictive insights:

- Random Forest: A robust ensemble method that uses temperature, SOC, and voltage as features for fault classification [12].
- XGBoost: Excels in handling imbalanced datasets, making it ideal for detecting rare events like TR [13, 14].
- Hybrid Approaches: Combining thermal models and ML improves prediction accuracy and robustness [15].

D. Research Gaps

A. Despite progress, several challenges remain:

- Limited Data: Real-world datasets for high-risk scenarios are scarce due to safety concerns [16].
- Sensor Limitations: Surface-mounted sensors fail to detect internal temperature variations [17]. Generalization Issues: Predictive models often struggle to adapt to emerging chemistries, such as solid-state batteries [18].

III. METHODOLOGY

A. Research Framework

The proposed framework integrates physics-based thermal modeling with ML algorithms:

1.Thermal Simulations: The Bernardi equation modeled heat dynamics under nominal, overload, and cyclic load conditions [11].

2.ML Algorithms: Random Forest and XGBoost classified battery states using features like temperature, SOC, and voltage [12, 13].

3.Multi-Sensor Fusion: Combined data from temperature, voltage, and SOC to improve fault detection accuracy [14].

B. Data Collection and Preprocessing

Datasets included simulated and real-world data. Preprocessing steps involved:

- Feature Engineering: Deriving parameters like rate of temperature change (ΔT/Δt).
- Normalization: Scaling features to prevent bias [12].
- Data Balancing: Using SMOTE (Synthetic Minority Over-sampling Technique) to address data imbalances [13].

C. Evaluation Metrics

Performance was assessed using:

- Classification Metrics: Accuracy, Precision, Recall, and F1 Score [14].
- Regression Metrics: Time-to-Fault Prediction Error [13].

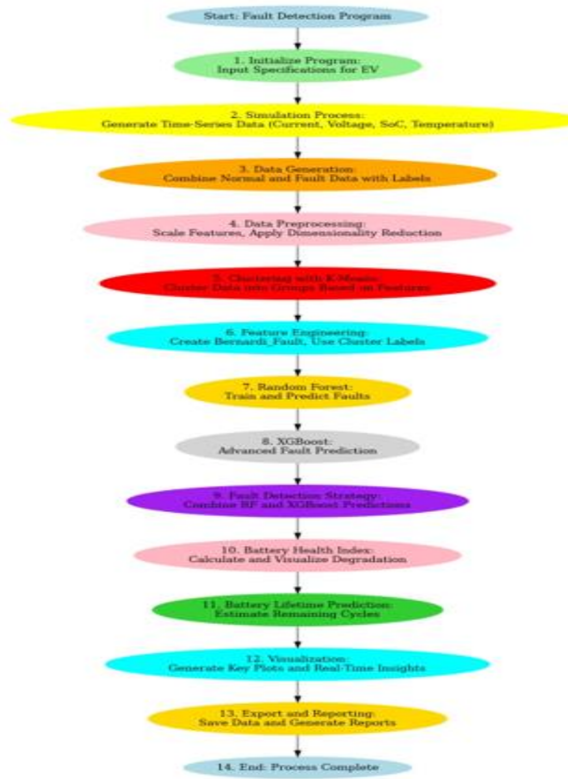

Figure 1: Flowchart of program flow

IV. RESULTS AND DISCUSSION

A. Model Performance

The XGBoost model achieved superior performance, with:

Accuracy: 95.1%.

Time-to-Fault Prediction Error: ±5 seconds.

In comparison, the Random Forest model achieved an accuracy of 92.4% but exhibited a higher time-to-fault prediction error (±8 seconds) [12, 13].

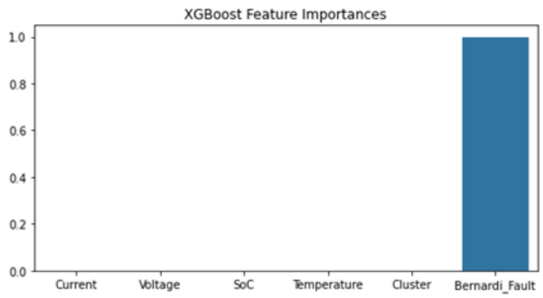

Figure 2: XGBoost Feature Importance

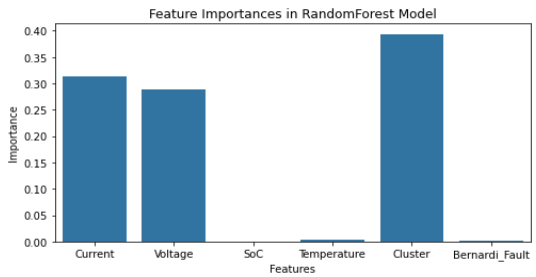

Figure 3: Random Forest Feature Importance

B. Multi-Sensor Fusion Insights

Incorporating temperature, SOC, and voltage data improved fault detection accuracy by 10% and reduced false negatives by 20% compared to single-parameter approaches [14].

C. Mitigation Strategies

Thermal Barriers: Reduced heat transfer between cells, delaying TR propagation by 50% [10].

SOC Management: Maintaining SOC below 80% during transport reduced TR risks by 40% [9].

V. CONCLUSION AND FUTURE WORK

This study demonstrates the effectiveness of hybrid predictive models combining thermal simulations and ML algorithms for detecting and mitigating TR in LIBs. The XGBoost classifier emerged as a robust solution for real-time fault detection.

A. Future Work:

1.Extend predictive frameworks to newer chemistries, such as solid-state batteries.

2.Develop lightweight ML models for resource-constrained environments.

3.Explore real-time IoT-enabled fault detection systems.

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