# Enhancing Lithium-ion Battery Safety: Analysis and Detection of Internal Short Circuit basing on an Electrochemical-Thermal Modeling

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## Abstract

As the main cause of thermal runaway, the prompt identification of Internal Short Circuit (ISC) occurrences in lithium-ion batteries (LIBs) has emerged as a critical priority for ensuring battery safety. To address this critical need, for a comprehensive understanding of ISC behaviors, an electrochemical-thermal-ISC coupled model has been developed in this work to simulate battery performance across various ISC levels. This model is also utilized to validate the efficacy and robustness of the advanced detection approach proposed. By integrating both thermal and electrical aspects using the Pseudo Two-Dimensional (P2D) and Energy Balance Equation (EBE), our model serves as an efficient surrogate for ISC experiments. Key ISC indicators have been analyzed and integrated into the proposed ISC detection algorithm to enhance its effectiveness. The algorithm utilizes an Equivalent Circuit Model (ECM)-based approach for estimating ISC resistance. This research not only advances our understanding of ISC dynamics but also establishes a robust framework for the timely and reliable detection of ISCs. These advancements significantly enhance the overall safety and reliability of LIBs in electric vehicles (EVs).

## 1. Introduction

With the increasing growth and application of LIBs, particularly in EVs, concerns over battery safety have escalated due to a significant number of car fire accidents Chen et al. (2021). Among the recognized types of battery failure modes, ISC is considered the most significant safety concern for LIBs B. Liu et al. (2018).

While many studies have used mechanical abuse to induce ISC modes and quantify their effects on temperature, State of Charge (SoC), and other measurements, the precise mechanism of spontaneous ISC during the daily use of EVs remains unclear Huang et al. (2021). Therefore, early detection and accurate identification of ISC before it leads to thermal runaway (TR) have become key research areas.

According to Feng et al., generating failure data is a primary objective in developing a comprehensive online ISC detection approach Feng, Weng, Ouyang, and Sun (2016). Various methods have been employed in previous literature to induce ISC experimentally, including mechanical deformation like the nail penetration test Abaza et al. (2018) and crush tests Zhu, Zhang, Sahraei, and Wierzbicki (2016), as well as heating triggers such as inserting ISC devices within cells Orendorff, Roth, and Nagasubramanian (2011) and overheating Spinner et al. (2015). Additionally, dendrite growth and external short circuit (ESC) substitute tests have been used by L. Liu et al. (2020); Feng, He, Lu, and Ouyang (2018). Due to the challenges associated with reproducibility and safety in ISC experiments, researchers also opt to develop battery ISC models to capture ISC effects on main signals Kim, Smith, Ireland, and Pesaran (2012); Feng et al. (2016).

In this study, we generated ISC data by modeling a high-fidelity ISC model. Given that temperature growth and voltage drop are key ISC indicators Lai et al. (2021); Wu et al. (2023), we coupled a thermal and electrochemical model to simulate these responses for ISC detection algorithm development.

Another primary objective is the formulation of the detection algorithm. Achieving online and onboard diagnosis in EVs relies on signals measured by Battery Management Systems (BMS), necessitating a computationally efficient algorithm. Over recent years, several approaches leveraging voltage signals for ISC detection have been proposed, including observing abnormal voltage changes Keates, Otani, Nguyen, Matsumura, and Li (2010); Sazhin, Dufek, and Gering (2016); Seo, Goh, Park, Koo, and Kim (2017), capturing differences between predicted and actual values Yokotani (2014), and applying algorithms utilizing voltage signals Seo, Park, Song, and Kim (2020); Hu, Wei, and He (2020). Regarding another key ISC signal, temperature response, only limited works have utilized it through model-based approaches Feng, Ouyang, et al. (2018); Jia, Brancato, Giglio, and Cadini (2024).

In this study, we implemented the Extended Kalman Filter (EKF) algorithm based on a simplified lumped electrical-thermal model, as proposed in our previous work. Model parameters were estimated from a dataset generated by the high-fidelity plant model. Utilizing both the voltage and temperature signals, the direct indicator, $R_{ISC}$, was set as the state in the algorithm to be estimated to identify ISC levels.

The remainder of this paper elaborates on the detection approach in Section 2, provides a detailed description of the built ISC plant model in Section 3, presents the detection results and validation of the proposed approach in Section 4, and concludes in Section 5 by summarizing the findings and their implications.

## 2. An Overview of ISC Detection Approach

Figure 1 presents the comprehensive framework of the ISC detection approach proposed in this study.

As shown in the upper part of the figure, a coupled electrochemical-thermal model (plant model) is developed to generate a dataset representing the operational behavior of a healthy battery, as detailed in subsequent sections. The Recursive Least Squares (RLS) parameter estimation tool is then employed to derive lumped model parameters, facilitating an accurate representation of battery electrical signals with computational efficiency for online detection algorithms.

The Equivalent Circuit Model (ECM) is chosen as the lumped electrical model due to its simplicity and widespread use in battery State of Charge (SOC) estimation in Battery Management Systems (BMS). The temperature lumped model, represented by Equation 1, incorporates heat generation from internal resistance and ISC resistance, as well as heat dissipation through natural air convection between the battery surface and the environment. To parameterize the ECM, the Hybrid Pulse Power Characterization (HPPC) working profile is applied to the plant model. The HPPC current and voltage simulated from the plant model are utilized for parameter estimation. Details of the estimated parameters applied for the detection algorithm are provided in Table 1.

$$mC_m \frac{dT}{dt} = \frac{V^2}{R_{ISC}} + R_0 I^2 - hA(T - T_{\mathrm{a}}) \quad (1)$$

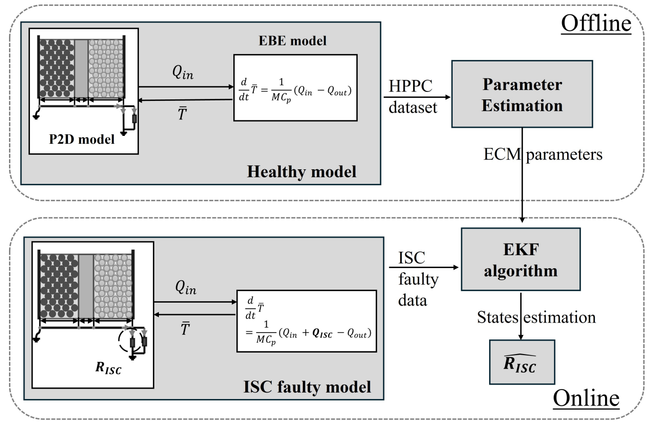


Figure 1. The overall ISC detection approach

Table 1. Battery parameters in lumped model

| Symbol | Value | Unit |
|---|---|---|
| $Q$ | 2.3 | Ah |
| $R_0$ | 0.0249 | Ω |
| $R_1$ | 0.0072 | **m**Ω |
| $R_2$ | 0.3641 | **m**Ω |
| $\dot{\tau_1}$ | 13.18 | s |
| $\dot{\tau_2}$ | 9.66 | s |

Figure 1 shows that, in the lower part (online detection phase), simulated ISC signals are obtained by introducing a parallel resistance as the ISC input for both the electrochemical and thermal models. The ECM-thermal-ISC model integrates parameters generated offline, including an additional item for ISC resistance, as a state to be estimated, into the model-based EKF algorithm for implementation and evaluation.

As highlighted by Hu et al. (2020), the state estimation process in the EKF consists of two primary stages: prediction and update. During the prediction stage, estimated state values are computed using model equations within the algorithm, incorporating the error covariance from the previous estimation step. This stage forecasts the next state based on the current state estimate and system dynamics. In the subsequent update stage, predicted states are refined by integrating measurements from sensors, which in this case are simulated values from the high-fidelity model.

The key aspect of the algorithm employed here involves incorporating the ISC resistance as one of the estimated states by integrating it into the ECM within the framework of the EKF algorithm. The state vector can be expressed as:

$$\mathbf{x} = [z,\ i_{R1},\ i_{R2},\ 1/R_{ISC}]^T, \quad (2)$$

while the input and output vectors are:

$$\mathbf{u} = [i_t,\ v_t]^T, \quad (3)$$

$$\mathbf{y} = [v_t,\ T]^T, \tag{4}$$

For further details regarding the functions and implementation of the algorithm, as well as other parameters applied, please refer to our previous work Jia et al. (2024).

## 3. Model Implementation

In this section, the detail of the electrochemical-thermal-ISC model developed to simulate the battery ISC is further described. The cell we simulated in this research is the A123 LiFePO4 26650.

### 3.1. Coupled Electrochemical-thermal Model

The electrochemical model employed is P2D model, which is based on a set of Partial Differential Equations (PDEs) describing the dynamics of physical processes within the battery electrodes and electrolyte Jokar, Rajabloo, Désilets, and Lacroix (2016). The main equations of the model are shown as below: Mass conservation of Li+ in the spherical active material:

$$\frac{\partial c_s}{\partial t} - \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 D_s \frac{\partial c_s}{\partial r}\right) = 0 \tag{5}$$

where $c_s$ represents the concentration of Li+ in solid phase , $r$ is the particle radius of the electrodes, $D_s$ is the intercalation diffusivity.

Charge conservation in the electrodes:

$$\sigma_{\text{eff}} \frac{\partial^2 \phi_s}{\partial x^2} = j_f \tag{6}$$

where $\sigma_{\text{eff}}$ is the effective elective electrical conductivity, $\phi_s$ is the electrical potential in solid phase, $j_f$ is the electrode current density $(I/A_s)$ and $A_s$ is the specific interfacial area.

Mass conservation in the electrolyte phased:

$$\frac{\partial(\varepsilon_e c_e)}{\partial t} = \frac{\partial}{\partial x}\left(D_e^{\text{eff}} \frac{\partial c_e}{\partial x}\right) + \frac{1 - t_+^0}{F} j_f \tag{7}$$

where $\varepsilon_e$ is the volume fraction of phase in electrolyte phased, $c_e$ is the concentration of Li+ in electrolyte, $D_e^{\text{eff}}$ is the elective electrolyte diffusivity, F is the Faraday's constant, $t_+^0$ is the transference number.

Charge conservation in electrolyte:

$$\frac{\partial}{\partial x}\left(\kappa^{\text{eff}} \frac{\partial \phi_e}{\partial x}\right) + \frac{\partial}{\partial x}\left(\kappa_{\text{D}}^{\text{eff}} \frac{\partial \ln c_e}{\partial x}\right) + j^{\text{Li}} = 0 \tag{8}$$

where $\kappa^{\text{eff}}$ is the effective electrolyte conductivity, $\phi_e$ is the potential of the eletrolyte phase, $j^{Li}$ is the reaction flux.

Over-potential and cell voltage:

$$\eta = \phi_s - \phi_e - U = \phi_s - \phi_e - (U_{\text{ref}} - (T - T_{\text{ref}})\frac{dU}{dT}) \tag{9}$$

where the T is the temperature of the battery cell.

The detail equations and the specific parameters used in this P2D model are sourced from the research by Prada et al. (2012). The temperature of this model is obtained from the output of the thermal model.

The thermal model is built based on the energy balance theory proposed by Bernardi et alBernardi, Pawlikowski, and Newman (1985). The temperature change with time can be described as Eq. 10

$$mC_m \frac{dT}{dt} = I(U - V - T\frac{dU}{dT}) - hA(T - T_{\text{a}}) \tag{10}$$

In this equation, the first part of the right side is the heat generation while it can be outputted from the electrochemical model, while $I$ is the overall current, U is the open circuit voltage (OCV), V is the terminal voltage and $-T\frac{dU}{dT}$ is the reversible entropy change. The second part of the right is the heat dissipation while $h$, 10 $W/m^2/K$ is the heat transfer coefficient, $A$, 0.00634 $m^2$ is the inner surface area of the battery cell and $T_{\text{a}}$, 298 $K$ is the environmental temperature. In the left side, $m$, 0.07 $Kg$ is the mass of the battery cell and $C_m$, 1100 $J/kg/K$ is the heat capacity. These data are extracted from the battery data-sheet and other literature A123 Systems (2012); Song, Hu, Choe, and Garrick (2020); Bernardi et al. (1985).

The P2D electrochemical model and the thermal model can be coupled as shown in the figure 1, similar with Feng et al. (2016). As demonstrated in Eq.9 and Eq.10, the coupling achieved by considering the temperature dependent OCV. To be specific, the average temperature generated from the thermal model based on the heat generation and dissipation is timely converted to the electrochemical model by effecting the OCV.

### 3.2. ISC Model

As we illustrate in the figure 1, by paralleled the extra ISC resistance to the P2D, the ISC can be simulated. Therefore, the total current will be described as bellow:

$$I = I_{\text{t}} + I_{\text{ISC}} = I_{\text{t}} + \frac{V}{R_{\text{ISC}}} \tag{11}$$

At the same time, the heat generated from ISC counted from the Eq 12. should be added into the overall thermal equation.

$$Q_{\text{ISC}} = I^2 R_{\text{ISC}} \tag{12}$$

### 3.3. Simulation Result

By setting different values of the $R_{ISC}$ value, various levels of ISC can be simulated based on the P2D-thermal-ISC model implemented here. Lower the $R_{ISC}$ correspond to more se-

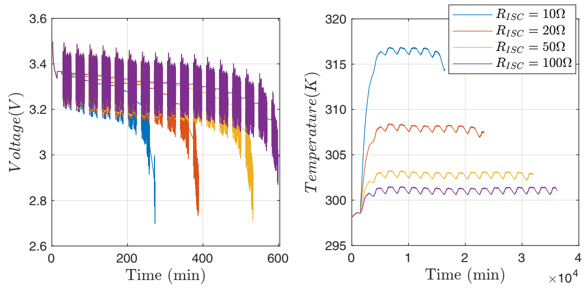


Figure 2. ISC simulation results

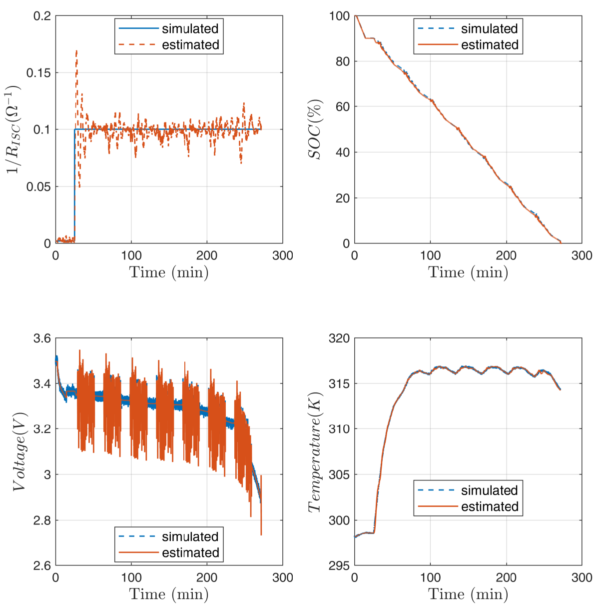


Figure 3. ISC detection results for $R_{ISC} = 10\Omega$

vere ISC conditions. The corresponding measurements simulated from the model are shown in figure 2 . Consistent with the findings in Feng, Ouyang, et al. (2018), the continual loss of SOC and the increase in heat generation are two main indicators of ISC occurrences. This is demonstrated by the quicker voltage drop and higher temperature rise observed with more severe ISC levels.

## 4. ISC Detection Results

To validate the proposed approach, measurements including voltage and temperature were generated from the built model using the Urban Dynamometer Driving Schedule (UDDS) profile. These signals were utilized by the algorithm to estimate the $R_{ISC}$ online, with ISC simulated by specifying the $R_{ISC}$ profile. The covariance of the measurement noises was set to be 0.1 mV and 2.5 mK, respectively.

For evaluating the performance of the early detection approach,

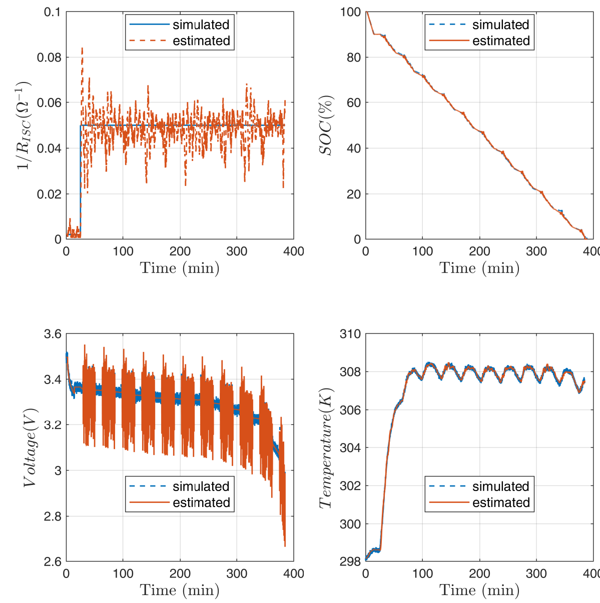


Figure 4. ISC detection results for $R_{ISC} = 20\Omega$

we set $R_{ISC}$ to a moderate level by dropping its value from a relatively high value (representing no ISC) to 10 Ω and 20 Ω, which are considered moderate ISC levels in other research studies (Feng, He, et al., 2018; Hu et al., 2020; Seo et al., 2020). The comparison between the algorithm's estimated states and simulated states from the built model is depicted in the top two sub-figures of Figure 3 and 4. Despite some fluctuations observed in the estimated $R_{ISC}$, these are attributed to measurement noise and the simplified model used within the EKF algorithm. Nonetheless, the estimated $R_{ISC}$ closely and promptly tracks the simulated ISC value after its occurrence, demonstrating rapid and accurate detection of early ISC.

Specifically, from the results, it can be observed that after ISC is triggered, the estimated value converges to the true value within two minutes, while the temperature rises to 299 K for both cases. This implies that the approach can provide an alarm for severe ISC levels based on the estimated value of $R_{ISC}$ before the temperature reaches a critical threshold, thereby preventing further thermal runaway or loss of battery capacity. Moreover, the SOC estimation displays good consistency with the real value. Furthermore, the voltage drop and temperature rise observed in the simulated results after ISC occurrence, as depicted in the figure, illustrate the primary ISC responses. These indicators demonstrate good consistency between the simulated data and the calculated data generated from the built-in model in the algorithm and the estimated states.

## 5. Conclusion

In this research, an electrochemical-thermal-ISC model was constructed in COMSOL to simulate ISC events and validate the proposed model-based ISC detection algorithm. This model combines the P2D model for electrical signals with the EBE for the thermal model, coupling them through temperature changes and the relationship between OCV and temperature.

The ECM-based algorithm demonstrated promising performance in early ISC detection. The ECM parameters utilized in the algorithm were derived through parameter estimation using a dataset generated from the high fidelity model under healthy battery conditions. .

In conclusion, the proposed method holds potential for application in BMS for early ISC detection, owing to its simplicity and efficiency. However, future research will focus on developing a more comprehensive battery model that considers the temperature response of physical electrochemical parameters to better capture dynamic responses and temperature distribution within the battery cell. Furthermore, enhancements to the algorithm will aim to incorporate temperature response and achieve precise localization of ISCs.

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