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Numerical simulation of Li-Ion battery using ECM method: A case study

Contents

Abstract

Thermal modeling facilitates the understanding of the thermal behavior of the Lithium-Ion (Li-Ion) battery, providing a study for exploring thermal management methods to enhance the battery's efficiency. This study aims to develop the thermal model using numerical methodology with Equivalent-Circuit Model (ECM) in Ansys Fluent. Thermal modeling estimating the total heat generation rate, which is the ohmic heat source percentage in total heat loss. The total heat generation rate value is further utilized for system-level numerical simulations. Furthermore, ambient temperature plays a crucial role in the battery's heat generation and battery performance. Therefore, a parametric study should be conducted with different temperature conditions from 0°C to 45°C and different discharge currents (1C-3C rate) to predict the thermal behavior (heat generation rate) of the battery at different state of charge (SoC) conditions.

Keywords: Computational Fluid Dynamics (CFD), Li-Ion battery, battery thermal management system (BTMS), heat generation, ECM method, numerical simulation, Temperature measurement

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Introduction

Li-Ion batteries are widely used in electrical vehicles (EVs) and consumer electronic devices due to their higher energy and power density and superior durability compared to lead-acid and nickel-metal hydride batteries. However, operating temperature significantly influences Li-Ion battery performance. At lower temperatures, the battery's internal resistance increases while the available capacity decreases, leading to a reduction of the available energy of the battery and maximum power, which in turn affects the performance of electronic devices and EVs. Conversely, high temperatures can cause safety issues and accelerate battery aging. Consequently, it is crucial to study battery performance across different ambient temperatures. Additionally, internal heat generation during charging and discharging plays a vital role in battery performance. Accurate battery temperature prediction requires a detailed analysis of heat generation, including joule heat and reaction heat. These factors are influenced by ambient temperature and the battery's state of charge (SoC) and must be considered for accurate performance assessment.

Previous methods for determining battery heat generation have been largely experimental and primarily suited for laboratory conditions, making them difficult to implement in practical scenarios. Recently, numerical modeling has emerged as a more effective approach for capturing heat generation in batteries. Among various types of numerical models, such as electrochemical models, reduced order models and data-driven black-box models, ECMs have gained popularity due to their balance of accuracy, ease of parametrization and implementation, have been widely used for real-time battery management applications, including battery parameters prediction [1]. Based on physical principles, ECM can accurately calculate heat generation, including joule heat and reaction heat, with clear interpretations. SoC and temperature, both of which influence the parameters of the ECM, have been successfully integrated into these models [2]. This paper investigates the effects of SoC, discharge current, and ambient temperature on the ECM parameters.

Methodology

Heat generation rate in battery

The primary two components in the heat generation process in Li-Ion batteries are reversible heat generation due to entropic changes in the battery and irreversible heat generation due to ohmic losses, charge-transfer overpotentials and mass transfer limitations. The commonly used equation for the volumetric heat generation rate within the battery, $q^{\cdot m}$ (Wm^{-3}), is given as follows,

$$q^{\cdot m} = i(V_{oc} - V) - i\left(T\frac{\partial V_{oc}}{\partial T}\right) \qquad \text{Eq.1}$$

where i (Am^{-3}) is the volumetric current density, which is positive for discharge and negative for charge, Voc and V (V) are the open circuit voltage and the instantaneous voltage of the battery, respectively, and T (K) is the temperature of the battery.

The extreme current densities at the current collectors create further Joule heating. This additional Joule heating is not an issue for smaller batteries like coin and cylindrical types commonly used in consumer electronics but is more apparent in batteries of larger form, such as the prismatic type used in EVs and hybrid electric vehicles [3]. An equation describing volumetric heat generation in larger batteries has been developed, accounting for this additional Joule heating due to higher current densities at the current collectors,

$$q^{\cdot m} = aJ\left[V_{oc} - V - T\frac{\partial V_{oc}}{\partial T}\right] + a_p r_p \vec{i_p}^{-2} \quad \text{Eq.1}$$

$$\vec{i_p} = -\frac{1}{r_p}\nabla V_p \quad \text{Eq.2}$$

$$\vec{i_n} = -\frac{1}{r_n}\nabla V_n \quad \text{Eq.3}$$

Where,
a (m^{-1}) is the specific area of the battery;
J (Am^{-2}) is the current density;
$\vec{i}_p$ and $\vec{i}_n$ (Am^{-1}) are the current density vectors in the positive and negative electrodes;
r_p and r_n (Ω) are the resistances of the positive and negative electrodes;
V_p and V_n (V) are the potentials of the positive and negative electrodes;
a_p and a_n (m^{-1}) are the specific areas of the positive and negative electrodes, respectively.
The addition of the third and fourth terms account for the additional Joule heating of the positive and negative electrodes due to the increased current densities at those sites.

ECM Model

The ECM model for Li-Ion battery is a widely adaptive model that uses multiple parallel combinations of capacitance, resistance and other circuit components to build an electric circuit to replicate the similar properties of Li-Ion batteries. The most widely used electrical equivalent models are Time domain analysis models. The simplest model equation for battery models can be represented by Open Circuit Voltage (OCV)

$V(t) = OCV$

The SoC of a cell is 100% when cell is fully charged and 0% when fully discharged. The amount of charge removed from 100%–0% is the total capacity measured in Ah or mAh.

In this ECM model, the circuit consists of three resistors and two capacitors:

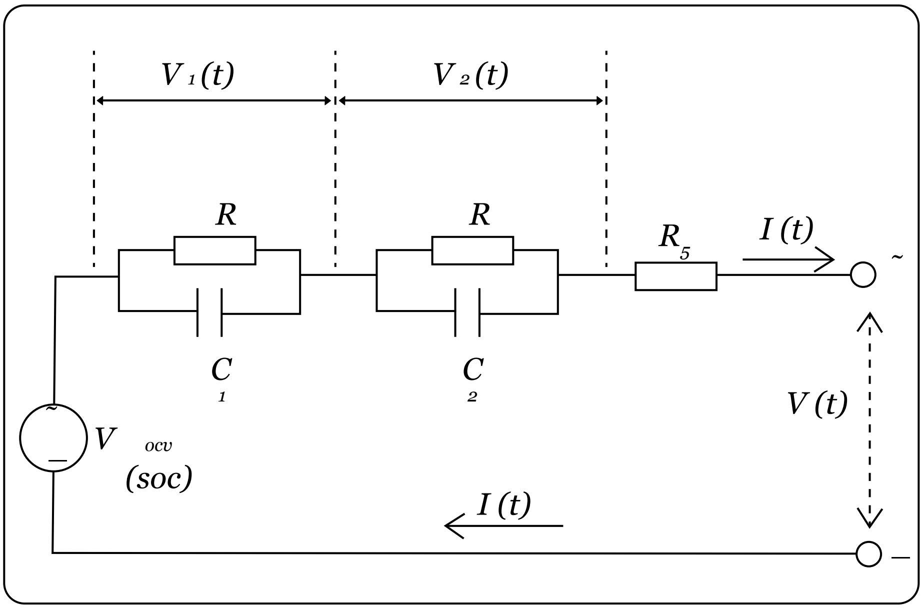


Figure 1: ECM Model

The electric circuit equations can solve to obtain the voltage current relation:

$$V = V_{OCV}(soc) + V_1 + V_2 - R_s(soc)I(t)$$

$$\frac{dV_1}{dt} = \frac{1}{R_1(soc)C_1(soc)}V_1 - \frac{1}{C_1(soc)}I(t)$$

$$\frac{dV_2}{dt} = \frac{1}{R_2(soc)C_2(soc)}V_2 - \frac{1}{C_2(soc)}I(t)$$

$$\frac{d(soc)}{dt} = I(t)/3600Q_{ref}$$

Here, V is the battery cell voltage that can be either obtained directly from the circuit solution in the Circuit Network solution method or calculated as from the MSMD solution method. The battery SoC and temperature are dependent on open circuit voltage, capacitor capacitance and resistor resistance within the battery.

CFD approach

Ansys Fluent was used to perform electro-thermal cell modeling. MSMD model with the equivalent circuit model (ECM) approach helps in dealing with different physics in the solution domain.

Governing equations

In this approach, within the CFD domain, the battery thermal and electrical fields are resolved at the battery cell's scale using the cited differential equations

Mass Conversation

$$\frac{\partial \rho}{\partial \tau} + \nabla . (\rho \hat{u}) = 0$$

Energy equations coupled with electro-chemistry, short circuit,

$$\frac{\partial \rho C_p T}{\partial t} - \nabla . (k \nabla T) = \sigma_+ |\nabla \emptyset_+|^2 + \sigma_- |\nabla \emptyset_-|^2 + \dot{q}_{ECh} + q_{short} \dot{+} \dot{q}_{abuse} \nabla .$$

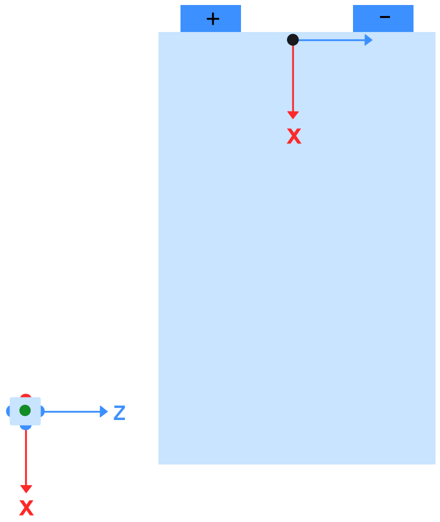
$$(\sigma_+ \nabla \emptyset_+) = -(j_{ECh} - j_{short})$$

$$\nabla . (\sigma_+ \nabla \emptyset_+) = -(j_{ECh} - j_{short})$$

$$\nabla . (\sigma_- \nabla \emptyset_-) = (j_{ECh} - j_{short})$$

Where σ_+ and σ_- are the effective electric conductivities for the positive and negative electrodes, φ_+ and φ_- are phase potentials for the positive and negative electrodes; j_{ECh} and q_{ECh} are the volumetric current transfer rate and the electrochemical reaction heat due to electrochemical reactions, respectively; j_{sho^-} and q_{sho^-} are the current transfer rate and heat generation rate due to battery internal short-circuit, respectively; in this case not needed.

Boundary conditions



Dimensions:

Length	48mm
Thickness	6mm
Height	77.5mm

Figure 2: CAD Model

MSMD model with the ECM approach is used for CFD analysis of the Li-Ion cell.

The details of cell,

battery model: Li-Ion cell

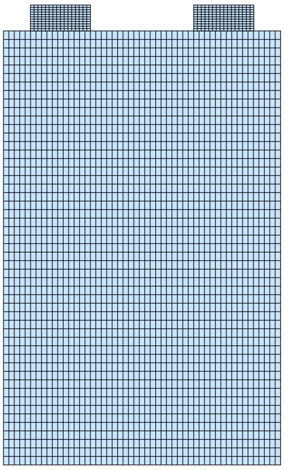
Nominal cell capacity: 460 mAh

initial SoC = 1

C-rate: 1

Meshing

Meshing has been done using Finite Volume Method with Tetrahedral mesh as the CAD model is the simple rectangular block, i.e., not detailed battery cell layer model. For Ansys battery model simulation, a simple rectangular block with the exact dimensions will be enough to run the battery simulation by giving proper battery parameters. The total element count is 45,000 with a very finer mesh. Below picture shows the mesh details of the battery rectangular block.



Results and discussion

This section presents a detailed comparative study of total heat generation rate under different discharge rates (1C - 3C discharge) and different ambient temperature conditions.

Firstly, the temperature graph in Figure 3 shows the transient results of battery model with 1C discharge rate, 100% SoC and 25°C ambient temperature conditions. The graph represents the gradual increase in the maximum temperature of the cell over time.

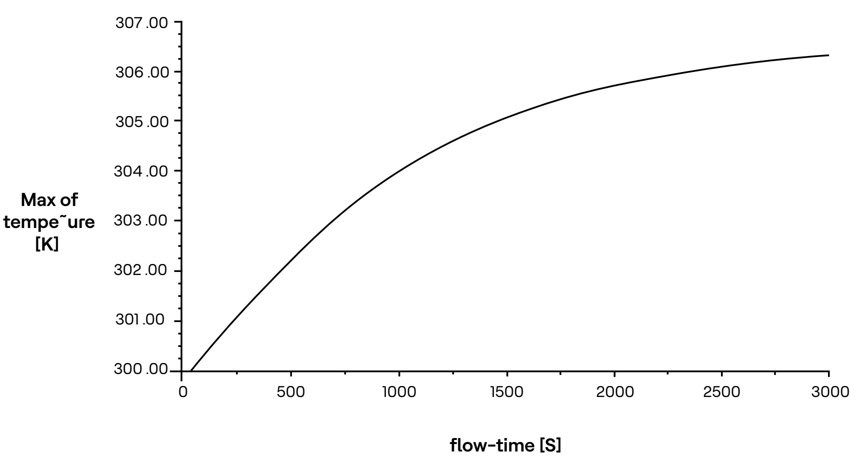


Figure 3: Temperature graph

Figure 4 shows the temperature distribution contour of the battery cell. As seen from the figure, the maximum temperature is obtained at the center of the battery cell versus the cell edges.

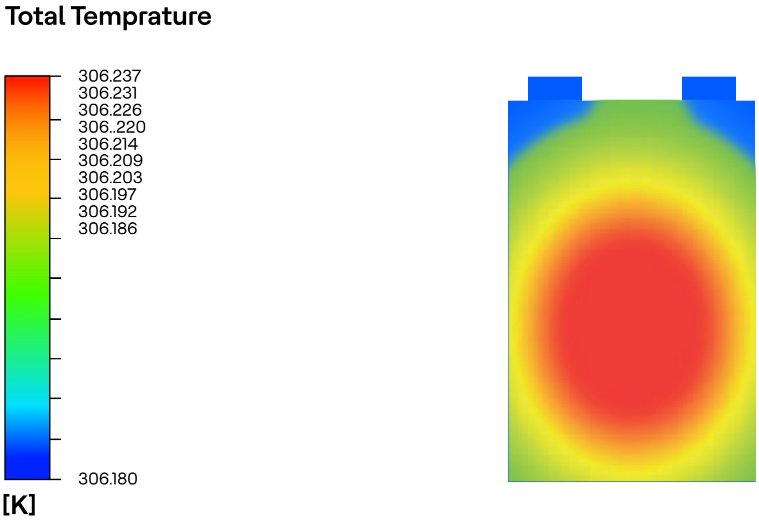


Figure 4: Temperature graph

Figure 5 shows the total heat generation rate contour of the battery. From the figure we can observe that the total heat generation rate is almost equal for the entire cell except on the tabs. The percentage of Joule heat source is 10% of the total heat generation rate.

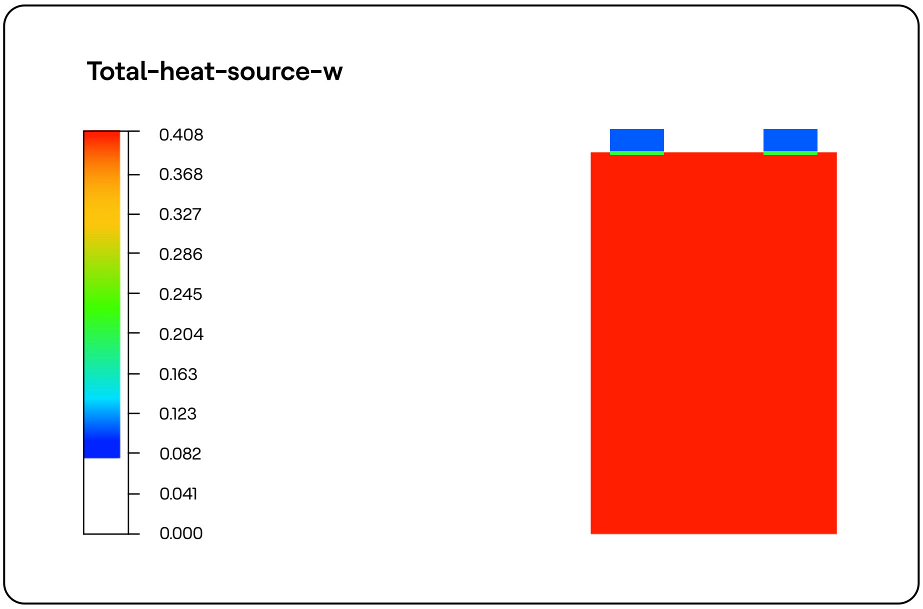


Figure 5: Total heat generation rate contour

Influence of ambient temperature

Figure 6 shows the graph of total heat transfer rate at different C-rates and different ambient temperatures of 5°C, 25°C and 45°C at constant SoC of 100%. In the graph, it is obvious that the total heat generation rate increases greatly with increase in discharge rate (1C – 3C discharge) at each ambient temperature condition (5°C, 25°C and 45°C) since the joule heat is dependent on current and reaction rate is proportionally dependent. There is an increase of approximately 400% from 1C to 3C discharge rate at 25°C ambient temperature. As seen in the figure, the total heat generation rate decreases with increase in the ambient temperature at each C-rate condition. It is observed that the joule heating in the total heat generation rate is in the range of 10%-14% for all the different ambient temperature cases.

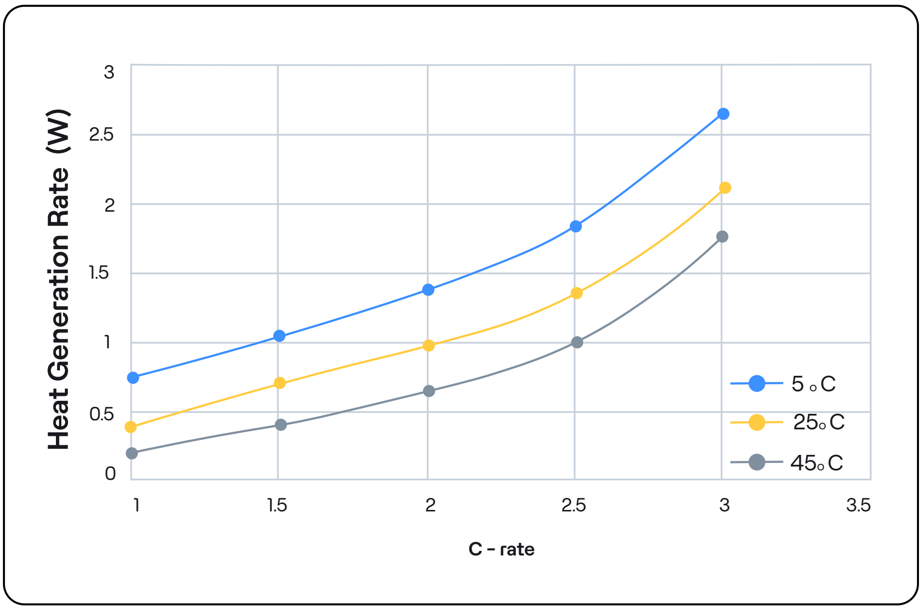


Figure 6: Heat Generation Rate vs C-rate Graph.

Fig 7 shows the graph of the percentage of joule heating in the total heat generation rate.

Influence of C-rate

Figure 7 estimates the influence of C-rate on heat generation rate at different SoC conditions. The higher the C-rate, the higher will be the heat generation due to the higher irreversible heat generation. Irreversible heat generation is shown in equation 1 and equation 2 as a function of current squared, whereas reversible heat generation is a linear function of current; therefore, increasing the discharge current causes a corresponding change in the proportion of the irreversible heat generation in the total heat generation of the battery. As seen from the figure, at 0% SoC condition the heat source is maximum at all C-rates and gradually decreasing as SoC increases and becomes almost stable after 0.4 SoC conditions. There is an enormous difference in the value of heat source from 0 SoC to 0.2 SoC condition at 3C rate and the difference is minimal at lower C rates.

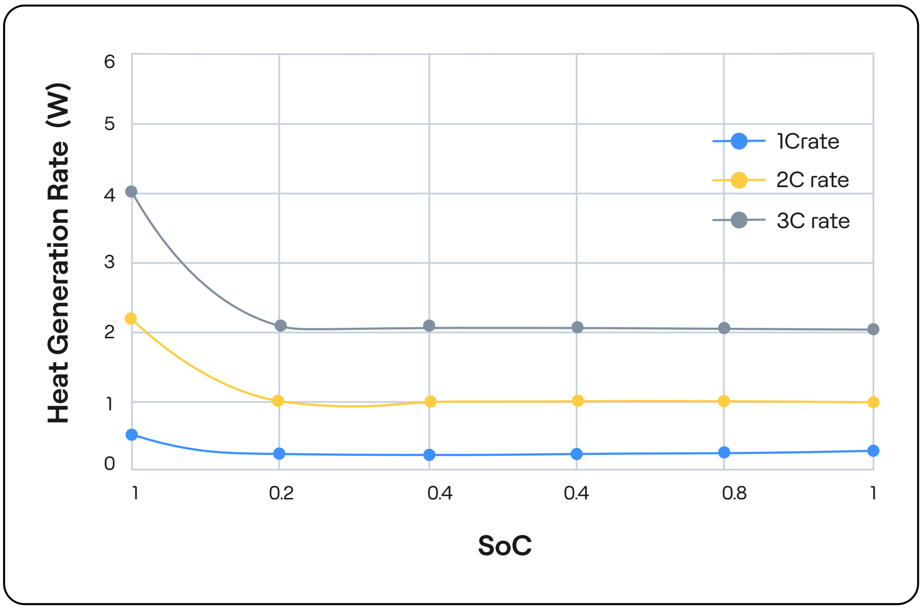


Figure 7: Heat Generation Rate vs SoC Graph

Conclusion

This paper simulates a rectangular Li-Ion battery cell using the ECM method to determine total heat generation. The calculated heat generation rate is then applied in system-level thermal simulations of the electronic devices where the battery is a key component requiring thermal monitoring. The thermal behavior of the battery is a crucial factor influencing its health and safe operation. To predict this behavior, the ECM model within Ansys Fluent is used for Li-Ion battery simulations. A series of numerical simulations were performed to calculate the heat generation rate under varying ambient conditions (5°C, 25°C and 45°C) and different C-rates (1C-3C). The study found that both discharge current (C-rate) and ambient temperature significantly affect the battery's thermal behavior and SoC conditions. Notably, the heat generation rate is highly sensitive to ambient temperature and discharge rates. With the increase in C-rate from 1C to 3C, at 0% SoC condition, the total heat generation rate is increased by 800%. When the ambient temperature is increased from room temperature, the battery generates less heat due to increase in the internal resistance. It is important to keep the battery ambient temperature to the moderate value based on applications to get the maximum efficiency of the battery.

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Kranthi has been with HCLTech since 2021. He has close to four years of experience in the CFD Domain. He has a master's degree in mechanical engineering from Germany, specialization in CAD and FEA. He has experties in handling wide range of CFD tools like Ansys Fluent, Spaceclaim, Simcenter FloEFD and Flotherm XT. He has solid command of technologies, tools and best hands-on experience in CFD/thermal models for predicting thermal response of electronic components.

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Chinnababu has been working with HCLTech since 2020. He has close to 17 years of industry experience in the CFD domain. He has a master's in mechanical engineering from IIT Madras, Chennai with Thermal Engineering Specialization. He has experience in Numerical Simulation and Thermal Analysis in a wide variety of industrial domains including Turbomachinery, IC engines, Aerospace, etc. At HCLTech, he is a part of MCOE CFD and Thermal team working on Consumer Electronics Cooling vertical with significant contributions to the development and thermal analysis of consumer electronic products.

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