Part 02

Developing Battery Simulation Technologies

Safety Simulations for Lithium ion Batteries

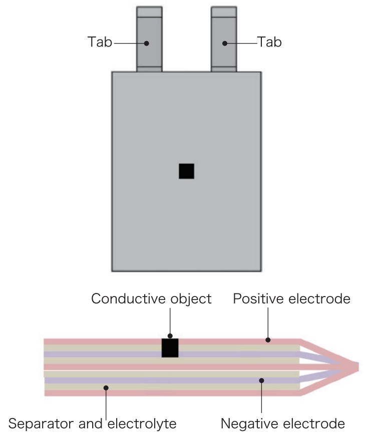
While lithium ion batteries are attractive for their high energy density, unsuitable design or improper usage can lead to a hazardous outcome. Therefore, safety tests, such as a forced internal short-circuit test or a heating test, are used to validate a design to verify the safety of a battery and battery system. However, given the difficulty of using tests or experimentation to comprehensively verify an enormous number of different cases, the use of computational simulation is expected to accelerate product development.
GS Yuasa has created an extensive library of battery simulation techniques through our approach of developing these techniques concurrently with our development of batteries and battery systems. Most recently, GS Yuasa used simulation to successfully create a visual representation of gas generation in a lithium ion battery, which may be brought about by an internal short-circuit or exothermic reactions. This article will introduce our model for simulating the behavior of a lithium ion battery that has an internal short circuit, and the technical concepts we use when simulating gas generation in a battery cell and the impact on immediate environment.

1. Simulating an Internal Short Circuit

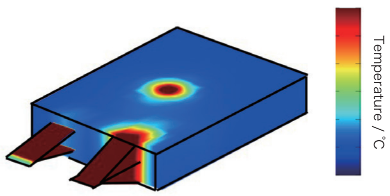
An internal short circuit occurs when an electrical connection is created between the positive electrode and negative electrode inside the case of a battery cell. In a (stacked-electrode) battery cell, where multiple positive electrode sheets and negative electrode sheets are layered alternately via a separator, a short circuit may occur when a conductive foreign object, e.g., a piece of metal, creates an electrical connection between a positive electrode sheet and a negative electrode sheet (●Fig. 1). When there is an internal short-circuit the short circuit current flows toward and concentrates at the short. The short circuit current generates heat which causes a localized increase in the temperature of the battery. The temperature increase results in exothermic reactions such as decomposition and oxidation. Here, a visual representation created using simulation may be effective in order to intuitively understand the behavior of current or heat when these internal short-circuits occur.

In the stacked-electrode cell, the multiple positive electrode sheets and multiple negative electrode sheets are connected in parallel via respective tabs; when an internal short-circuit occurs, current flows toward these tabs. Therefore, it is possible to simulate the behavior when the internal short-circuit occurs by calculating the short circuit current which is the current flowing toward the short from the tabs[1].
It is also possible to more precisely calculate the current or state of charge (SOC), or the heat generated in the cell by coupling an electrochemical model and a heat generation model along three dimensions. ●Fig. 2 illustrates a temperature distribution at a set time after an internal short-circuit occurred. We can see that the current concentrates at the short and the tabs, greatly increasing the heat value in the stacked-electrode cell; this suggests that exothermic reactions may originate at these locations. Simulation allows us to change, for instance, the location or resistance value of the short in a cell, thus enabling rapid and comprehensive verification of the behavior of a cell.

●Fig. 1 Internal short circuit in a stacked-electrode cell



●Fig. 2 Temperature distribution during an internal short-circuit



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In the case of a wound cell (i.e., a cell where a positive electrode sheet, separator, and negative electrode sheet are overlapped and wound), the short circuit current is calculated with the wound electrode sheets in a virtually unwound form[1]. Current flows in the wound cell along the circumference of the electrode sheet winding direction and does not concentrate at any portion as much as the current would at the tabs of a stacked-electrode cell. This may also be visualized via simulation[2].

2. Simulating Gas Generation

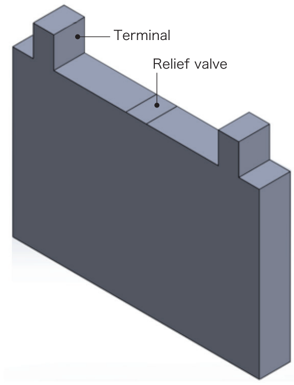
Once there is excessive localized overheating in the lithium ion battery due to an internal short-circuit, this causes multiple chemical reactions that accompany the decomposition and combustion of material. Heat generation and gas generation are brought about when there are a lot of these reactions. Gas generation and thermal expansion due to temperature rise increase the internal pressure. The increase in internal pressure in turn causes the relief valve (●Fig. 3) in the battery case to open, exhausting the gas to outside the cell. This high-temperature gas escapes at high speed; and therefore, it is important to understand the impact of the gas on the battery cell and its immediate environment (the battery system).

As previously mentioned, GS Yuasa has been successful at using simulation to create visualizations of the gas generation brought about by material decomposition in a lithium ion battery. ●Fig. 4 depicts a visual representation created via simulation of a battery assembly where another battery cell is positioned above the relief valve of a given battery cell. At first the gas generated stays inside the case; however, the relief valve opens when the internal pressure surpasses the release pressure and exhausts high-temperature gas to outside the case, heating the battery cell positioned above the relief valve. After a prescribed time passes, the upper battery cell also exhausts gas. We are also able to compute a gas generation rate and heat generation rate on the basis of the reaction speed for a material decomposition reaction. Here, the gas generation rate can be calculated as proportional to the reaction rate of a material decomposition reaction[1].

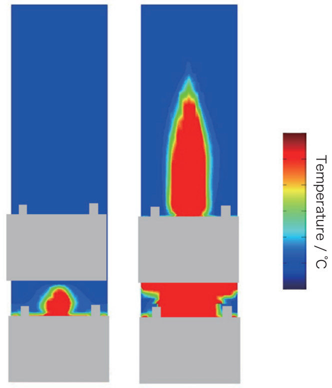
This kind of simulation may be used to predict whether or not gassing will occur under certain conditions, the temperature of the gas generated, and the impact of the gas on adjacent battery cells without actually performing a thermal runaway test. Thus, it is possible to drastically reduce the engineering time required to verify the safety of a battery or battery system.

This article introduced techniques for simulating the behavior of battery cells and the effect on the immediate environment when a lithium ion battery experiences an internal short-circuit or gas generation. GS Yuasa will continue to build its extensive library of battery simulation techniques to advance the development of safer, higher performance batteries and battery systems.

●Fig. 3 Battery cell (Simplified)



●Fig. 4 Propagation of generated gas



1. Japanese Patent No. 6699795 (Filed in 2019)
2. GS Yuasa Technical Report Volume 16, No. 2, published 2019

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