Analysis of Lithium-Ion Battery Failure and PyBaMM's Viability in Simulating Them

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***Abstract*—As renewable energy sources become more popular, methods of energy storage, especially lithium-ion batteries, have become essential in making renewable energy practical. Lithium-ion batteries have seen widespread use in everyday machines such as smartphones and electric vehicles, mainly due to their power density and price. Despite their merits, lithium-ion batteries also have significant safety concerns, demonstrated by the several instances of these batteries catching fire or exploding. To ensure future battery safety, it is imperative to develop accurate testing procedures and determine the factors leading to catastrophic failure. The Oxford Mathematical Modelling Battery Group's Python Battery Mathematical Model (PyBaMM) was used to simulate these batteries in action along with experimental data from Dr. Thomas Hodson's lab at Columbia University [1]. By comparing these different types of data and exploring each individually, it was determined that discharge rate and repeated cycling are the leading causes of thermal runaway in lithium-ion batteries. It was also determined that PyBaMM, despite showing general trends of different factors that led to combustion, was unviable in the simulation of battery explosions due to its failure to recognize explosive battery temperatures and inability to simulate both realistic thermal behavior and heat exchange between cells and the surrounding environment.**

I. Introduction

Today, large scale energy storage is becoming more important than ever as renewable energies grow in popularity. Since most renewable energy sources experience significant variation in power output due to the unpredictability of the Earth's weather, energy storage is currently one of the best ways to make renewable energy practical [2].

Energy storage devices have the ability to store energy (charging) and release it later (discharging). There is a correlation between high energy storage and low charge/discharge speeds and vice versa, making balancing them a concern during energy storage device design. Furthermore, since energy transfer always causes losses, round trip efficiency is critical to ensure that the amount of energy put in is as close to the amount of energy taken out as possible [3].

Over the past few decades, the battery has emerged as one of the world's most popular forms of energy storage. Batteries convert chemical energy into electrical charge through chemical reactions causing electron flow. As batteries utilize chemical energy storage, they have a large energy density as well as a relatively high power density. Batteries also have a high round trip efficiency, allowing for the production of electric vehicles which are 2.5-6.5 times more efficient than their internal combustion engine counterparts [4].

Recently, lithium-ion batteries have emerged as the prominent rechargeable battery technology. They output power at a higher voltage than the average AA battery or NiCd/NiMH (3.7V vs. 1.5/1.4V) and also have higher energy and power densities. Additionally, lithium-ion batteries have significantly lower self-discharge rates than NiMH batteries, allowing them to store energy for long periods of time. Lithium-ion batteries are considered "secondary batteries", meaning that they are rechargeable (up to 3000+ full cycles in the Lithium-ion battery's case), whereas alkaline batteries are single-use. They are also incredibly modular and can be used in a plethora of electronic devices, from tiny wearables to megawatt-scale power stations. As a result of the increased worldwide manufacturing capacity and demand for lithium-ion batteries, prices have dropped significantly, and continue to fall [5]. Despite their benefits, lithium-ion batteries also suffer from one fatal flaw—the danger of fires and explosions [5]. Newsworthy

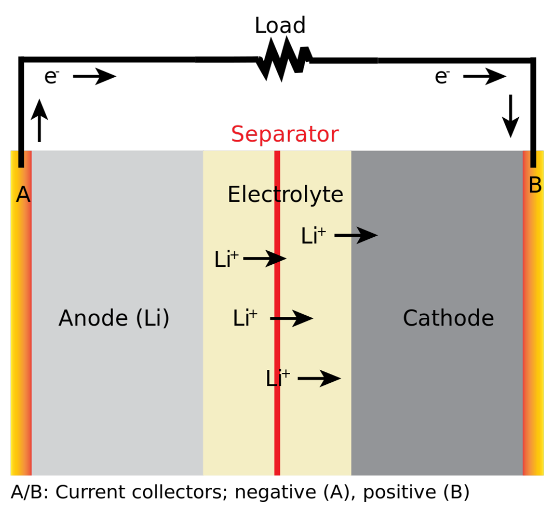

Fig. 1. The basic layout and components of a lithium-ion battery Source: [10]

examples include the Samsung Galaxy Note 7 explosions, electric vehicle explosions, and Boeing 787 battery fires [5-7]. Lithium-ion batteries are also hermetically sealed to prevent foreign liquids and gases from getting in, but this comes with the caveat that heat and gases generated from within the battery cannot escape easily either. This can become a problem, especially when batteries reach high temperatures. During regular use, Joule heating occurs within a battery, which usually does not lead to any kind of failure. However, short circuiting caused by abuse or other factors can cause a high current, resulting in dangerously high battery temperatures. As the battery heats up, it begins to degrade, eventually reaching a thermal runaway. Upon reaching high enough temperatures, the electrolyte vaporizes, causing hydrogen gas and oxygen gas to accumulate at the anode and cathode respectively. When enough of the gases are exposed to heat, a combustion reaction can spontaneously occur [8].

This study aims to develop a better understanding of lithium-ion battery explosions and how to prevent them. Both experimental data collected by Dr. Thomas Hodson at his lab at Columbia University and simulation data from PyBaMM, a Python-based battery simulation software developed by the Oxford Mathematical Modelling Battery Group, were utilized to build an understanding of how lithium-ion batteries react to varying conditions. As such, this study also examines PyBaMM's viability in simulating battery explosions. PyBaMM allows for the modification of several parameters that would normally be present during a battery experiment, such as charge and discharge current, cutoff voltages, battery chemistry, and ambient temperature. PyBaMM experiments were conducted on a remote server via Jupyter Notebook.

II. Experimental Procedure

A. PyBaMM Data Collection

PyBaMM battery tests were run to gather data about battery behavior under various conditions. For all voltage simulations, the Chen2020 battery model included with PyBaMM was used. A Python script was written to simulate a lithium-ion battery discharging to 3.3v and executing the following cycle:

1) Charge to 4.2 V at constant current
2) Rest for 30 minutes
3) Discharge to 2.7 V at constant current

This script was run under ambient temperatures of 5°C, 10°C, 20°C, and 50°C, at rates of C/10, C/2, 1C, and 2C. Temperature over time and voltage over time were recorded.

B. Experimental Data Collection

During experimental testing, a Neware BTS 3000 battery tester was utilized to accurately control the voltage and current of a battery and log data for further analysis. It has 0.1% full-scale accuracy and a 1Hz data logging rate. Shown in Fig. 2, the batteries tested were housed within a modified minifridge, which utilizes Peltier coolers to establish precise control of ambient temperature. The cells used were lithium-ion polymer battery cells from AA Portable Power Corp. They measure 29mm x 16.5 mm x 6.5 mm, have a nominal capacity of 210 mAh, and have a rating of at least 300 cycles. All cells tested were brand-new and ordered from the same batch.

Fig. 2. An image of the miniature refrigerator used to house the batteries during tests

The cells were tested under the same conditions and experimental procedures as the PyBaMM simulations. They were charged to 4.2 V, rested for 30 minutes, and discharged to 2.7 V under ambient temperatures of 5°C, 10°C, 20°C, and 50°C at rates of C/10, C/2, 1C, and 2C. During testing, data was collected for the cell current [A], voltage [V], charged capacity [mAh], and discharged capacity [mAh]. Experimental data was graphed for analysis using Pyplot.

C. Thermal Simulation

To test how PyBaMM simulates battery failure, an experiment was written to generate explosive battery temperatures. This was accomplished by establishing a temperature-intensive charge-discharge cycle, and running it one hundred times.

This code was then modified for another test to determine how changing certain parameters would impact the number of cycles needed to reach a temperature high enough to cause a catastrophic failure, around 140 degrees Celsius [9].

For these tests, the Marquis2019 parameter set was used, allowing for parameters such as ambient temperature, cell cooling surface area, charge-discharge rates, and electrolyte concentration to be modified. Starting at the default values of these parameters given in the Marquis 2019 set, each parameter was gradually increased and its impact on temperature was observed. The test was run nine times on ambient temperature, with each test increasing ambient temperature by ten degrees Celsius [°C]. The test on cell cooling surface area was run five times, with each test increasing cell cooling surface area by .001 meters squared [m^2]. The test on electrolyte concentration was run six times, with each test increasing electrolyte concentration by 100 mol per cubic meter [$mol \cdot m^{-3}$].

III. Results

A. PyBaMM voltage data compared with experimental data

Data gathered from PyBaMM simulations and experimental data were compared for analysis. An example comparison between the experimental results and PyBaMM simulations is shown below in Fig. 3. In this graph, voltage is plotted against time for both the experiment and simulation for one cycle. For the experimental data and the simulation, the protocol for this cycle was a 1C rate charge to 4.2 V, followed by a 30 minute rest, followed by a 1C rate discharge to 2.7v.

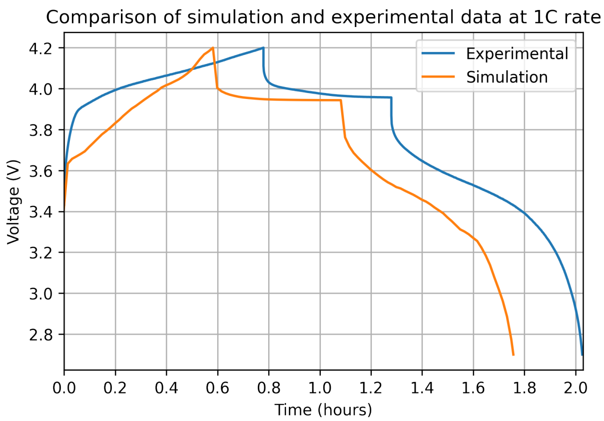

Fig. 3. Comparison of simulated and experimental voltage at a 1C rate

Comparing the experimental and simulation data from Fig. 3, there are a few key differences. First, the experimental cycle took 14% longer than the simulation, meaning that charging and discharging took longer experimentally. Possible reasons for this discrepancy include slight differences between the chemistry battery being tested and the battery being simulated. Additionally, the voltage versus time graph shape is similar, mainly during discharge. However, during charging, the experimental voltage appears to increase logarithmically while the simulated voltage increases linearly.

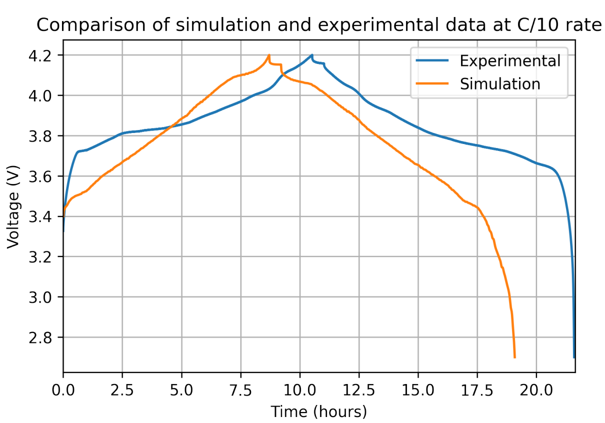

Fig. 4. Comparison of simulated and experimental voltage at a C/10 rate

Comparing data from a significantly lower rate in Fig. 4, similar observations can be made. In this test, the simulation completed 12% faster than the experiment, compared with 14% at 1C. Additionally, the difference in graph shape is also similar, with the simulated voltage following a more linear path, while the experimental data follows a curve.

B. Battery Explosion simulation results

After running a script that repeatedly cycled the battery, the PyBaMM battery delivered extremely high temperature values as shown in Fig. 5 that appeared to grow continuously.

C. Li-ion battery explosion factor simulations

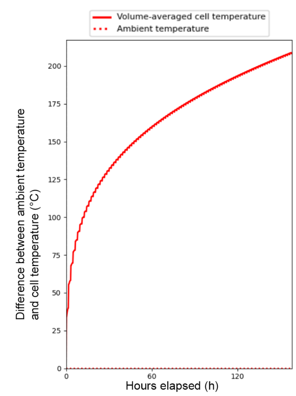

Fig. 5. Graph of the PyBaMM battery's Volume-averaged cell temperature relative to the ambient temperature, which was set to room temperature (25°C)

In the PyBaMM simulation data, it was discovered that the ambient temperature played absolutely no role in the temperature of the PyBaMM-simulated battery. Every single test had the battery explode after twenty-four cycles, regardless of temperature. Such was also the case for the cell cooling surface area. Again, every test exploded after twenty-four cycles, regardless of the surface area given to the program. The concentration of electrolyte does not play a role in battery temperature as well. Every test exploded after twenty-four cycles. The results from the ambient temperature, cell cooling surface area, and electrolyte concentration tests had identical results, regardless of what the values of these parameters were. However, the value of the discharge current plays a role in PyBaMM; by comparing the temperature increase of the simulated cell under different charge/discharge rates, insight can be gained about how discharge rate contributes to battery failure.

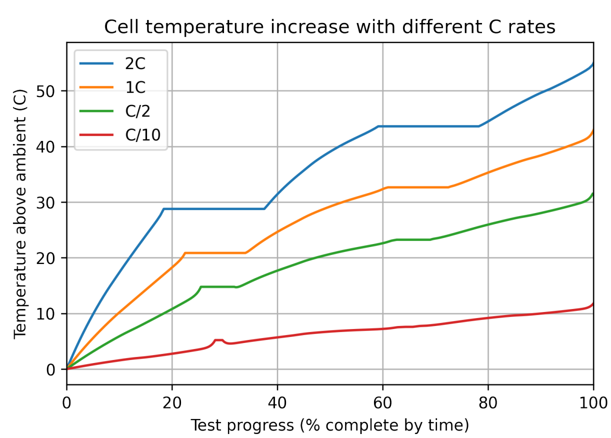

Fig. 6. Comparison between different discharge rates and their impact on the battery's change in temperature

Fig. 6 shows cell temperature plotted over total test progress and shows that a 2C discharge rate increases the cell's temperature over ambient temperature by more than 5 times as much as a C/10 discharge rate. Additionally, the 2C test cycle took less than one twentieth of the time of the C/10 test cycle, meaning that the temperature increased much more rapidly. This is because a higher current running through a battery leads to a higher amount of Joule heating, significantly increasing the cell's overall temperature above ambient. Extrapolating from this data, a short circuit, causing tens of amps to flow through a battery, definitely has the potential to heat the battery enough to cause vaporization of electrolyte and ultimately explode.

IV. Discussion

Based on the data collected, it can be determined that despite its advanced battery models, PyBaMM does not accurately simulate battery explosions and temperature. The first shortcoming that makes PyBaMM inaccurate is the software's inability to track heat loss from the battery or heat gain from external sources. This is best shown by the battery's constant temperature, even during rests, and the nonexistent effect of ambient temperature on the battery's internal temperature. This is inaccurate because although most lithium-ion batteries are hermetically sealed, heat is still transferred in and out through conduction, and during rest periods, heat should move in the direction of equilibrium with the ambient temperature.

Another limitation lies in PyBaMM's inability to simulate battery failure and general battery deterioration. The simulations do not take these behaviors into consideration whatsoever. In the test in which the battery was cycled one hundred times, there were no notifications or warnings when the battery approached over 200 degrees Celsius [°C] above room temperature, which is significantly more than enough to cause any lithium-ion battery to explode.

Despite PyBaMM's failure to properly simulate battery fatigue and thermal behavior, it did closely match the voltage over time results that were obtained from experimental testing. This makes PyBaMM a useful source of information for the electrical behavior of lithium-ion batteries, but gives it limited usefulness when attempting to understand and test the thermal properties of batteries. As such, the data gathered from the PyBaMM simulations should only be used to make general conclusions, like how a battery tends to act under certain conditions. More specific predictions of battery behavior should be based on data collected from physical batteries instead.

Potential sources of error in the experimental data may lie in the regulation of ambient temperature. The fridge used for temperature regulation maintains its temperature by heating and cooling consecutively, putting the temperature of the air inside the fridge in minute, but constant fluctuation. This means that the ambient temperature surrounding the battery will also fluctuate constantly. Furthermore, the temperature of the fridge is only measured at one location, so the temperature measurements made by the instrument may not reflect the effective temperature of the air around the battery. Another potential source of error is that despite being from the same batch, the batteries used for testing may not be completely identical due to tiny manufacturing variances.

V. Conclusions

While PyBaMM allowed for the execution of battery tests at a much higher rate than in a physical lab and the observation of basic trends in critical battery data, it is clear that despite its usefulness in simulating lithium-ion batteries, the PyBaMM modeling software is greatly flawed in that it fails to simulate the effects of factors leading to catastrophic battery failure, the basic thermodynamics of a battery such as heat leakage, and the catastrophic failure itself. Although these results exemplify the limitations of simulations and simulation-based research, it also provides an opportunity for the improvement of the PyBaMM package through a patch that allows for the simulation of how certain parameters impact catastrophic failure, accurate battery thermodynamics, and robust safety precautions to prevent the simulation of dangerous batteries.

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