Lithium-ion Battery Mathematical Modelling Using Python and IoT

Lincy Joy
Manipal Academy of Higher Education
Dubai, UAE
lincy.joy@dxb.manipal.edu

Ganesan Subramanian
School of Engineering and IT
Manipal Academy of Higher Education
Dubai, UAE
ganesan.subramanian@manipaldubai.com

Asha Sunilkumar
School of Engineering and IT
Manipal Academy of Higher Education
Dubai, UAE
asha.sunilkumar@manipaldubai.com

Shri Krishna Pandey
School of Engineering and IT
Manipal Academy of Higher Education
Dubai, UAE
skpandy@manipaldubai.com

2023 International Conference on Computational Intelligence and Knowledge Economy (ICCIKE) | 979-8-3503-3826-3/23/$31.00 ©2023 IEEE | DOI: 10.1109/ICCIKE58312.2023.10131736

***Abstract*— Optimizing the utilization of lithium battery packs has become essential due to the increased demand for lithium-ion batteries. Because battery deterioration is unavoidable, some recent research has focused on maximizing the usage of lithium-ion battery cells in the pack. Reconfigurable battery packs and cell replacement are two viable ideas for limiting the harmful impact of early-degraded cells on the overall pack. This paper includes designing and developing a battery monitoring system for individual cells in a pack that is integrated with the Internet of Things (IoT), as well as validating simulation results produced with PyBaMM, the Python Battery Mathematical Model. While charging individual cells, the cell balancing factor is primarily considered, and temperature is maintained during both charging and discharging stages. The cell replacement method was developed to increase the overall number of cycles a battery pack has gone through, therefore increasing its life. This procedure is also likely to be more cost-effective than the current basic pack replacement method. Individual cell monitoring and easy access to cells during the failure stage are two design criteria that must be addressed for the cell replacement concept to be successful. Comprehensive testing guarantees that changes aren't impacted, making model expansions easy to adopt.**

Keywords—Lithium-ion, batteries, internet of things, IoT, pybamm, python, battery monitoring systems, BMS.

I. INTRODUCTION

For battery-powered technologies ranging from portable electronic gadgets to electric vehicles (EVs), lithium-ion batteries are the most often used energy storage solutions for their high efficiency and energy density [1]. During the forecast period (2022-2027), the major factors driving the market are the development via electric vehicle and energy storage systems (ESS) in fields such as commercial and residential applications, reduction in prices of the batteries and steady increase in sale of consumer electronics [2].

The necessity of highlighting the significance of battery management system (BMS) for rechargeable batteries applications is important to assure the safety, dependability, and optimal functioning. Earlier the purpose of BMS was limited to monitoring and detecting the status of the battery and informing the user through a battery indicator within the car. Because of advancements in notification system design, internet of things (IoT) technology may be utilized to alert the manufacturer and users about the battery state. Other functions of BMS involve computing the battery capacity, charging/discharging battery deterioration, optimization for longer usage and communicates this information to users in real-time, thus reducing the occurrence of possible malfunction with regular battery assessments [3]. Empirical electrical equivalent circuit models (ECMs) are often used in conventional BMSs and are made up of a supply voltage, capacitors, and resistors in a network with the aim of simulating the current-voltage response of a battery cell. The parameters collected from the ECMs can change based on the state-of-charge (SOC), temperature, state-of-health (SOH), and current [4].

Each cell analysis being adopted can identify any damage and relevant warnings issued against the consumer-specified values and preventive measures can be implemented, protecting other cells from similar damage, thereby prolonging battery life [5]. There is continuous innovation drive to enhance clean energy research and EV being one of the successful in its mission to promote carbon reduction. It is challenging for even a manufacturer to produce comprehensive relevant data that covers all failure situations and mechanisms at the battery pack level. Additionally, data on actual EV usage, erratic driving patterns, dynamic charging procedures, and unpredictable noises are particularly crucial in revealing the underlying condition of the automobile battery [6]. The impact of BMS approaches on the predictive modeling of automobile batteries based on practical applications, however, has only been the subject of a very small number of research.

IoT has become the centre of interest for battery control and monitoring in recent years. A continuous data logging facility for monitoring essential battery operations is one of the main features of an IoT-based battery management system. The user and the manufacturer could be notified of the battery's state and condition via IoT. IoT goes beyond traditional applications by allowing a wide range of gadgets and devices to connect to the internet, putting the whole world at the user's fingertips [7].

In this paper, motivated by the stated problems, the design and development of a battery monitoring system with the involvement of IoT technology is carried out. The results obtained compared with the simulation results acquired using a python battery mathematical modeling (PyBaMM) that is an open-source tool available for quick and flexible simulations of battery models.

979-8-3503-3826-3/23/$31.00 ©2023 IEEE

II. BACKGROUND THEORY

A. Lithium-ion Battery

During discharge and subsequent recharge of a lithium-ion battery, lithium ions move through an electrolyte from the negative electrode to the positive electrode. While the negative electrode is often made of graphite, a lithium-ion cell's positive electrode is made of an intercalated lithium compound. High energy density, less self-discharge rate, and minimal memory effect are all characteristics of lithium-ion batteries. In the design of cells, energy or power density may be prioritized. Lithium-ion batteries do, however, contain volatile electrolytes that, if mishandled or charged poorly, can cause explosions and flames, which can be a safety concern.

Anode, cathode, separator, electrolyte, and two current collectors are the constituents of a rechargeable battery. The lithium is kept on the anode and cathode. The electrolytes transfer lithium ions that are positively charged from the anode to the cathode and vice versa through the separators. Lithium-ion migration results in the formation of charged particles in the anode, which generates a charge at the positive current collector. The electrical current then travels through a powered device from the positive current collector to the negative current collector. The barrier inhibits electrons from moving freely within the cell. As the battery discharges and delivers an electric current, the anode transfers lithium ions to the cathode, causing a flow of electrons from one side to the other. Lithium ions are released by the cathode when the device is plugged in, and the anode subsequently absorbs them.

The two most common notions relating to cells are those of energy density and power density. Watt-hours per kilogram (Wh/kg) are used to measure how much energy a battery can hold in total. Watts per kilogram (W/kg) is a unit of measurement used to express how much energy a battery can provide in relation to its mass. The internal structure of charging and discharging a lithium-ion battery is depicted in Fig.1 below.

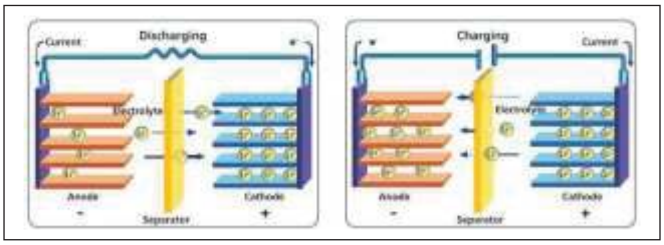

Fig.1: Charging and discharging of lithium-ion battery [8]

B. Battery Management System

An operating system called a battery management system (BMS) keeps track of a battery pack, which is a collection of battery cells electronically arranged in a row-by-column matrix to supply a specific range of voltage and current for a predetermined amount of time in response to expected load scenarios. The highest energy density is provided by lithium-ion rechargeable cells, which are utilized for a variety of consumer goods, including computers and electric vehicles. BMS has a challenging task, and its overall complexity and oversight scope may involve electrical, digital, control, thermal, and hydraulic disciplines. Fig.2 shown below depicts the lithium-ion battery recycling.

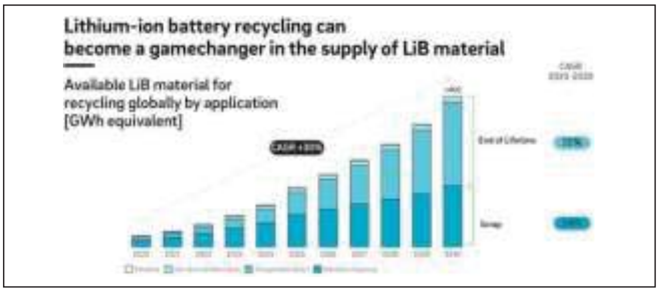

Fig. 2: Lithium battery recycling graph for 2020-2030 [9]

Lithium-ion batteries have differing charging and discharging current limits, and both processes are capable of withstanding higher peak currents—though only for brief intervals. The maximum continuous charging and discharging current constraints and the maximal charging and discharging current limits are often set by lithium battery manufacturers. Almost certainly, a current-protecting BMS will use a maximum continuous current. However, this might be added to allow for a sudden change in load conditions, such the acceleration of an electric car. Peak current tracking may be implemented in a BMS by integrating the current and, after delta period, choosing whether to lower the obtainable current or stop the pack current entirely. This allows the BMS to be sensitive to severe current peaks almost instantly, such as a short-circuit situation that has escaped the notice of any resident fuses, while also being forgiving of high peak requirements if they are not excessive for an extended period of time. Fig.3 shown below depicts the electrical management protection by BMS for current.

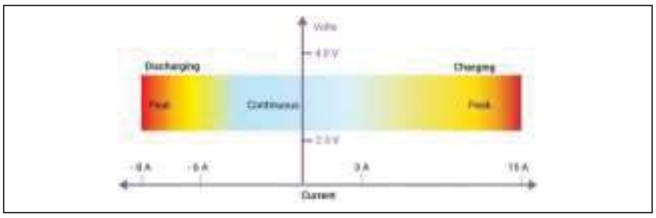

Fig.3: Optimal current ratings for battery [10]

Lithium-ion cells appear to have a wide temperature working range at first glance, but their total capacity decreases at low temperatures when chemical reaction rates reduce dramatically. They operate far better than lead-acid batteries in terms of low-temperature capabilities; yet temperature control is cautious because charging below 0 °C (32 °F) is physically difficult. During sub-freezing charging, a process known as metallic lithium plating can occur on the anode. This is irreversible damage that not only reduces capacity but also makes cells more sensitive to failure when exposed to vibration or other stressful situations. The temperature of the battery pack may be controlled by a BMS using heating and cooling. Fig.4 shown below depicts thermal management protection of BMS for temperature.

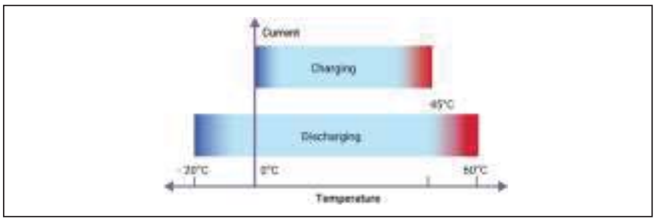

Fig.4: Optimal temperature for battery [10]

C. Simulation using Python

As the battery modeling community expands, software that employs advanced software engineering methodologies to promote cross-institutional coordination and empower research progress is becoming increasingly important. Using both numerical techniques and asymptotic analysis, the Python Battery Mathematical Modelling (PyBAMM) project creates open-source models of batteries. It allows for the modification of several parameters making it more flexible for various battery experiment, such as charge and discharge current, cut-off voltages, battery chemistry, and ambient temperature. PyBaMM is free and open source, and it can be found on GitHub [11].

The battery cell chemistry was determined using an LG M50 cylindrical cell in 21700 forms utilizing the Chen2020 [11] parameter set. To predict the electrochemistry and electrical behavior of lithium-ion battery cells, the Doyle Fuller Newman (DFN) model is utilized. This describes how ions travel across the cell and how charge is transferred. It combines an electrolyte model that accurately simulates both ion transport and electrical conduction with nonlinear diffusion models for lithium-ion transport inside electrode particle.

The model is made up of one-dimensional macroscopic equations that are posed over the cell's width L1 < x < L4 to capture the data. These explain the movement and conduction of lithium ions in the electrolyte that fills the pores of the electrode matrix, as well as the electrical conduction in the anode and cathode solid matrices. Equation (1) demonstrates how the electric potentials at the anode and cathode current collectors Va and Vc, respectively, may be calculated using the results of solving the entire cell DFN model and a given galvanostatic current I(t),

$$V_a(t) = \phi_a|_{x=L_1} \; ; \; V_c(t) = \phi_c|_{x=L_4} \qquad (1)$$

and hence the potential drop across the cell is given by equation (2),

$$V(t) = V_c(t) - V_a(t) - R_{cont}\, I(t) \qquad (2)$$

Where Rcont refers to the total contact resistance of the cell with I (t) for the current flow into the cell.

The DFN model may also be utilized in more advanced methods, such as simulating a wide range of cell chemistries, realistic driving cycles, or graded electrodes with varying particle sizes throughout the electrode.

D. PyBAMM Library

PyBaMM (Python Battery Mathematical Modelling) is a Python tool that allows you to simulate battery models rapidly and efficiently. It offers a modular framework in which existing or new tools may be combined to solve battery models, allowing for more collaboration and research relevance. PyBaMM does this by separating the models, discrete functions, and solver, allowing the end user more flexibility, and offering a common platform for adding new models, alternate variables in discrete form, and flexible time-stepping methods. The model's flexible "plug-and-play" submodel structure allows for the addition of additional physics to existing models. As a result, there's no need to restart again for each new effect, and it's simple to test a range of typical battery model expansions at the same time, such as linking together many degradation processes. A robust set of tests maintains the open-source framework's reliability, allowing new models and solvers to be added on a regular basis.

PyBaMM's design is based on two fundamental components, the first of which is an expression tree, that theoretically encodes mathematical equations. A variable, parameter, mathematical operation, matrix, or vector are all represented by a collection of symbols in an expression tree. Each battery model is defined in PyBaMM as a collection of symbolic expression trees. The expression trees for each model are stored in python dictionaries that also hold the model's governing equations, boundary equations, and initial conditions.

The pipeline process is the PyBaMM design's second most important feature. During the pipeline process, many modular components act on the model in turn. The pipeline is written in Python and uses PyBaMM classes to provide users full control over the process and the flexibility to alter or add new components at any moment.

III. Methodology

The system can be divided into software and hardware sections to give an overview of the complete system. Firstly, the software section includes the simulation conducted using the Python script and its library PyBAMM for research purposes in battery technology. PyBAMM adopts default state model and internal chemistry that applies according to the experiment considered. Secondly, the hardware involves different sensors like the current sensor, potential divider circuit, a temperature sensor for monitoring the individual Lithium-ion battery cells conditions when charging and discharging states. Arduino nano as a microcontroller controls the functions of each component and transmits the data to NodeMCU with inbuilt Wi-Fi module helps to upload the obtained data to a front-end local server build using XAMPP Package. The charging and discharging of li-ion batteries is observed and data plotted to give an overview of the battery condition at complete cycles.

A. Hardware Design

Fig.5 depicts the hardware part of the project with integration of IoT devices for a complete battery monitoring system. The lithium-ion battery during charging/discharging state, the code set in Arduino nano microcontroller allows to initiate the voltage, current and temperature sensors to continuously collect data. This data is then collected and transferred to two pathways. Firstly, the voltage, current & temperature readings are displayed on the LCD screen connected to the microcontroller. Secondly, using the NodeMCU with in-built Wi-Fi builds a connection to send the data to a XAMPP local server. The front-end of the server built using HTML displays the state of each cell during the charging and discharging state.

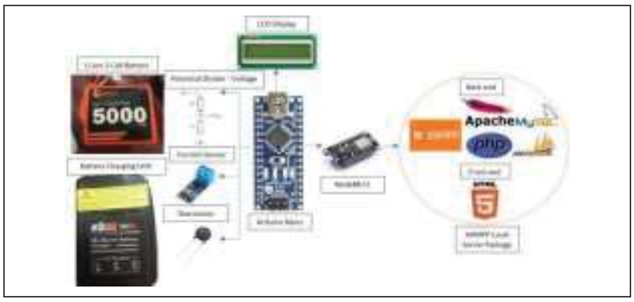

Fig. 5: IoT based Battery monitoring system.

The sensors and microcontroller are built on customized printed circuit board (PCB) for easy construction of the system as shown in Fig.6 below.

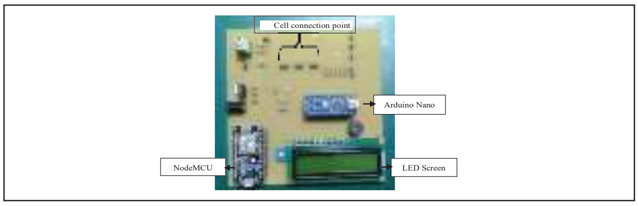

Fig. 6: Components placed on PCB

Lithium-ion three cell battery pack has a nominal voltage of 11.1 V and the 4 pin out from it is connected to current sensors (CS) and potential dividers to obtain the current and voltage respectively. A Thermistor is attached on the battery that allows to read the temperature of the battery during both charging and discharging states. This allows us to understand the battery when it starts to heat up and take preventive measures.

Current sensors are used to monitor the current through the cells and the potential divider can safely read voltage up to 15V is used to monitor the voltage in real-time. The current sensor can monitor the current of up to 30A. Each cell voltage is around 3.7V. The temperature sensor will monitor the temperature of the battery to determine its performance while at the charging and discharging stage. As the outputs of the current sensor, voltage sensor, and temperature sensor are analog in nature, using an inbuilt ADC of the microcontroller which is 10-bit and 6-channel ADC the obtained data is converted to digital format. The microcontroller used here is an Arduino Nano.

During charging state, the lithium-ion battery is connected to a balance charger in which each cell is charged evenly, with no voltage differences. Simultaneously, the code set in Arduino nano microcontroller allows to initiate the voltage, current and temperature sensors to continuously collect data. This data is then collected and transferred to two pathways. Firstly, the voltage, current & temperature readings are displayed on the LCD screen connected to the microcontroller.

Secondly, using the NodeMCU with in-built Wi-Fi builds a connection to send the data to a local server. This information is updated in real-time to a local server build using XAMPP package. The front-end of the server build using HTML script displays the state of each cell during the charging state.

Similarly, during discharging of the battery, a load of 12V 30RPM gear motor is attached to the circuit during the discharging condition, and the discharging current, voltage, and power ratings are recorded (Fig.18). The charging and discharging of lithium-ion batteries is observed and data plotted to give an overview of the battery condition at complete cycles. The discharging state is continuously recorded in the front-end server and recorded for plotting the graph.

B. *Software Design*

The python battery mathematical model (PyBAMM) is a tool for fast and flexible simulations of battery models. The python code is constructed on Google Colab, so that it is possible to run them on the cloud without having to install pybamm in the system.

Initially, pybamm library need to be imported into the notebook. Then to begin with, it is necessary to construct an experiment, which consists of a set of instructions on how to cycle the battery. A cycle is defined by a tuple of operating instructions. The instructions include a cycle of constant current C/10 or until 3.3V discharge, a one-hour rest, a constant current (1 A) constant voltage (4.1 V) and another one hour rest, all of it repeated three times, discharging the battery, resting for 1 hour, charging until it reaches 4.1V, holding for current to reach 50mA and battery put to rest for 1 hour before starting the new cycle. This instruction is considered for three continuous cycles.

The PyBaMM syntax is used to specify a battery model and geometry. The model is represented by a set of expression trees. The Doyle-Fuller-Newman (DFN) model is used, which successfully predicts the current/voltage response while representing solid-state and electrolyte diffusion dynamics. Then the simulation is created by passing the experiment using a keyword argument. The executed simulation is plotted with the commands sim.solve() and sim.plot() in which a slider with a set of graphs being displayed. The duration for three cycles to run is approximately 38.91 hours (140076 seconds). The parameter values considered to build the graphs are from the default model under the Chen2020 database in which the nominal cell capacity considered is 5Ah.

Finally, it is required to construct an experiment command that works with the default state parameters making the pybamm flexible for any analysis. For charging, the battery is intended to charge at constant current until 4.1V and simulated using DFN model and default experiment for three cycles. Like charging cycle, discharging cycle is built with constant current until 3.3V and run using the DFN model and default instructions.

IV. Results and Discussion

A. *Simulation*

When the code is run initiated, it is possible to observe the plot constructed for the Chen 2020 battery model using the Doyle Fuller Newman (DFN) model and cycle instruction. The cycle is run three times for about 38 hours. It is possible to slide back and forth to view the graphs change at each cycle (Figure 7).

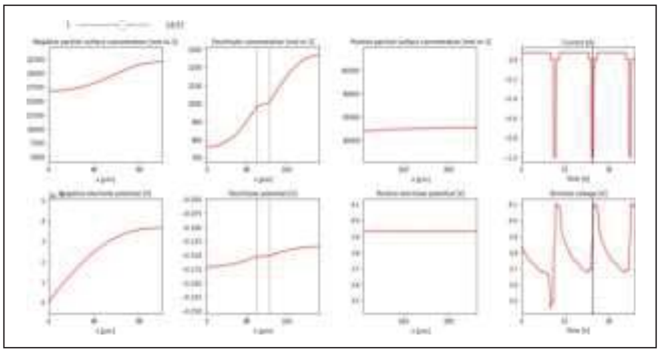

Fig.7: Simulation of default battery for three cycles The

code run for instruction with charging at 0.75A until the battery reaches 4.1V gives an output plot as shown in Fig.8 below.

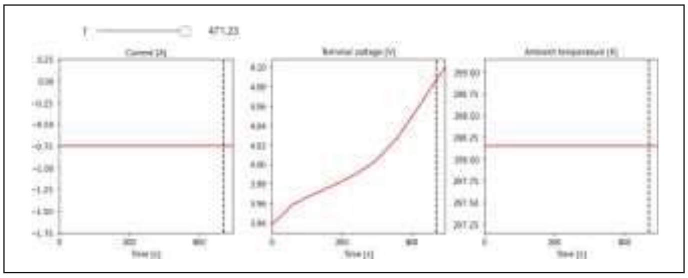

Fig. 8: Charging state plot for 471 seconds.

For discharge, simulation constructed based on discharge at 0.9A until the terminal voltage is 3.3V which gives an output plot as shown in Fig.9 below.

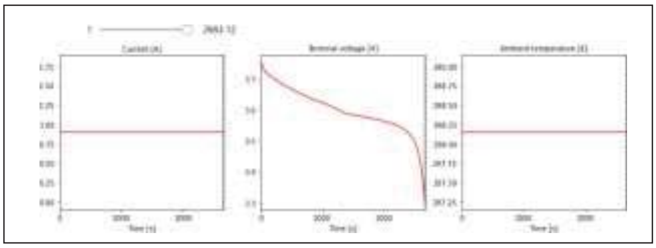

Fig. 9: Discharging plot for 2663 seconds.

B. *Calibration test*

The multimeter readings taken for each cell were recorded prior to connecting it to the circuit and documented in the following table 1.

Cell Number	Voltage (V)
Cell 1	3.76
Cell 2	3.77
Cell 3	3.76
Total Voltage obtained	11.32

Table 1: Multimeter test for each cell of battery pack

C. *Charging state of the battery*

The battery is kept for charging using the balance charger that helps to charge each cells equally. Due to the high sensitivity of battery cells, particularly lithium cells, to overcharging and over-discharging, the balancing concept is a crucial factor in battery management. The readings are continuously recorded in the backend of the server and current readings displayed in the front end before it refreshes (Fig.10).

Fig.10: Real-time of battery at charging state

The voltage and current plots are constructed for each cell and displayed below (Fig.11,12). It is observed that the average current rating remains within the range of 0.75 and the battery charged until the terminal voltage read until 4.1V.

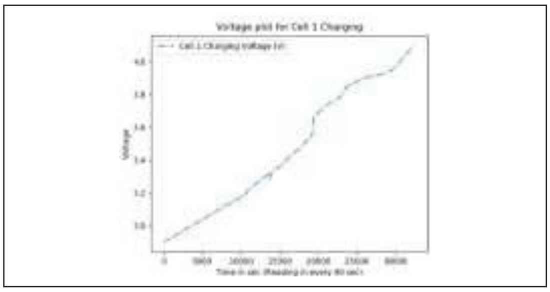

Fig.11: Voltage plot for Cell 1 during charging state

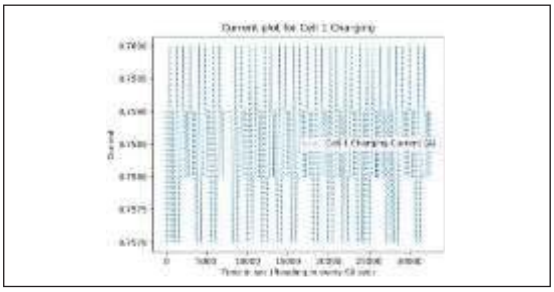

Fig.12: Current Plot for Cell 1 during charging state

Similar to cell 1 voltage and current plots, cell 2 and cell 3 are measured and plotted. Constant voltage mode takes over when the battery reaches its maximum charge cut-off voltage, and the charging current drops. When the battery's full charge voltage does not reach 100 percent, trickle charge mode kicks in, charging the remaining battery capacity while balancing the cells at the same time.

D. *Discharging state of the battery*

During the discharging state of the battery, a load of 12V 30RPM gear motor is connected to the circuit. The readings are continuously recorded in the backend of the server and current readings displayed in the front end which is updated continuously (Fig.13).

Fig.13: Real-time view at discharging state

The graph is plotted for the cell that is discharged from 11V to 9V (Fig.14) with average current rating remaining in 1.2A (Fig.15).

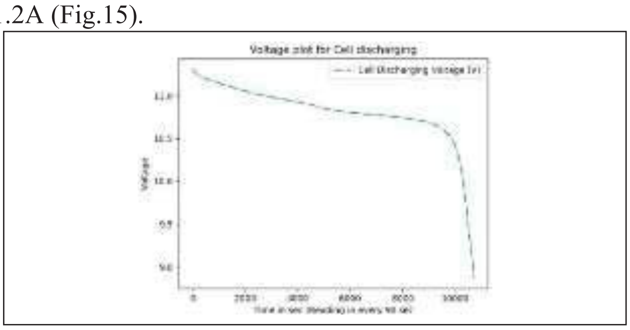

Fig.14: Voltage plot for cell during discharging

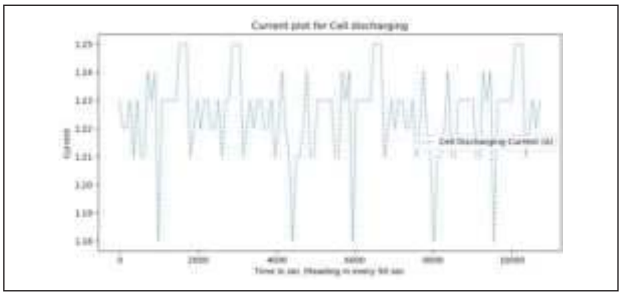

Fig.15: Current plot for cell during discharging Even

though the cell may be emptied entirely, it is vital to keep the cell discharge at 80-85 percent to avoid the cell being over-discharged, since the subsequent shortage might cause the cell to enter thermal runaway. Lithium-ion cells must not be charged or discharged at temperatures over 45°C or 60°C, since this may increase the internal resistance of the battery, resulting in a loss of power. High temperatures can increase a battery's aging process, resulting in fast degradation. If batteries are abused or manufactured incorrectly, it can lead to thermal runaway, which is one of the most serious safety concerns associated with lithium-ion batteries. Up to 40 degrees Celsius, the temperature in both the charging and discharging stages remained in the ideal range (Figure 16). Individual cell temperature reading is also visible on the LCD connected to the Arduino.

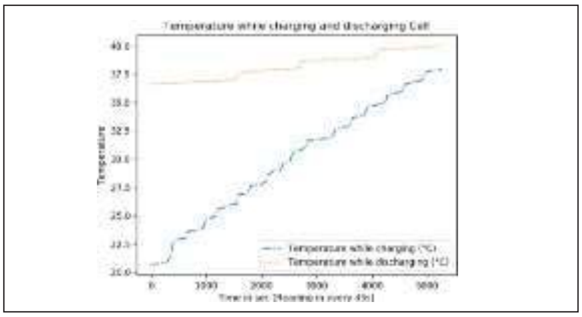

Fig.16: Temperature plot of the cell at two states

V. Conclusion and Future Scope

Lithium-ion batteries have piqued the interest of the EV sector due to its high energy density, longevity, nominal voltage, power density, and low cost. A sophisticated BMS is a key component in EVs; it not only precisely analyzes battery conditions, but also assures safe operation and extends battery life.

A BMS's functional safety is its top priority. During charging and discharging activities, it is essential to maintain any cell or module that is under supervisory control's voltage, current, and temperature within predetermined ranges. The second most important component of a BMS is the battery pack's performance, which involves both electrical and thermal management. To maximize the total battery capacity, electrical balancing must be performed on each cell in the pack. Lithium-ion batteries as an energy source were evaluated for use in IoT devices to EV's. The paper describes the design and development of an IoT-based battery monitoring system that ensures the battery performance degradation by monitoring it online. The objective is to identify individual cell's conditions more closely and monitor it to avoid any accidents. The outcomes of this study suggest that cell replacement is a realistic alternative to replacing the complete pack.

The future scope of this project can be developed involving the mobile based application and integrating artificial intelligence for vital analysis. Different assessment criteria need to be studied in the future to emphasize the benefits of the cell replacement idea, such as supply chain benefits, maintenance ease, waste reduction, and other chemistries of lithium-ion batteries, as well as the usage of superior battery models. For the battery and EV manufacturers, recycling and reusing lithium-ion batteries is becoming a necessity rather than a choice. Lithium-ion battery recycling businesses in the circular economy are working with battery producers to create easily disassembled product designs that enable the environmentally friendly recovery of all valuable battery components, which will aid in further streamlining and automating the recycling procedure.

Acknowledgment

I would like to take this opportunity to sincerely thank my guide, family and friends for all the support and guidance provided until the completion of the paper.

References

[1] Capata, R. (2018). Urban and Extra-Urban Hybrid Vehicles: A Technological Review. *Energies*, 11(11), p.2924. doi:10.3390/en11112924.

[2] Mordor Intelligence. (2021). *Lithium-ion Battery Market Size, Share, Report (2022 - 27)*. [online] Available at: https://www.mordorintelligence.com/industry-reports/lithium-ion-battery-market-industry2 [Accessed 21 May 2022].

[3] Helmy, M., et.al. (2018). *IoT-Based Battery Monitoring System for Electric Vehicle*. [online] ResearchGate. Available at: https://www.researchgate.net/publication/343786968_IoT-Based_Battery_Monitoring_System_for_Electric_Vehicle [Accessed 21 May 2022].

[4] M.-K. Tran et al., "A comprehensive equivalent circuit model for lithium-ion batteries, incorporating the effects of state of health, state of charge, and temperature on model parameters," *Journal of Energy Storage*, vol. 43, p. 103252, Nov. 2021, doi: 10.1016/j.est.2021.103252.

[5] Asaad, M., Ahmad, F., Alam, M.S. and Rafat, Y. (2017). IoT Enabled Monitoring of an Optimized Electric Vehicle's Battery System. *Mobile Networks and Applications*, 23(4), pp.994–1005. doi:10.1007/s11036-017-0957-z.

[6] Zhao, J., Ling, H., Wang, J., Burke, A.F. and Lian, Y. (2022). Data-driven prediction of battery failure for electric vehicles. *iScience*, 25(4), p.104172. doi:10.1016/j.isci.2022.104172.

[7] A. Gairola, "Cloud IoT Battery Management System in Electric Vehicles," Bacancy, Apr. 20, 2022. https://www.bacancytechnology.com/blog/iot-based-battery-management-system-in-electric-vehicles

[8] Sulzer, V., Marquis, S.G., Timms, R., Robinson, M. and Chapman, S.J., 2021. Python Battery Mathematical Modelling (PyBaMM). *Journal of Open Research Software*, 9(1), p.14. doi: http://doi.org/10.5334/jors.309

[9] IONOS Digitalguide. (2019). *XAMPP tutorial: installation and first steps*. [online] Available at: https://www.ionos.com/digitalguide/server/tools/xampp-tutorial-create-your-own-local-test-server/.

[10] Synopsys. (2021). *What is a Battery Management System (BMS)? – How it Works | Synopsys*. [online] Available at: https://www.synopsys.com/glossary/what-is-a-battery-management-system.html.

[11] V. Sulzer, S. G. Marquis, R. Timms, M. Robinson, and S. J. Chapman, "Python Battery Mathematical Modelling (PyBaMM)," *Journal of Open Research Software*, vol. 9, no. 1, p. 14, Jun. 2021, doi: 10.5334/jors.309.