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Thermal Modeling and Safety Assessment of Banana Peel Derived Carbon for Sustainable Lithium Ion Battery using 2D COMSOL Simulation

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Abstract

Lithium-ion batteries are sophisticated accessories in electrochemical industry. But in industry the process of their production techniques is hazardous for our environment. By searching for a good carbon carrier from agricultural waste, banana peel was found as a potential candidate. It is cost-effective and environmentally friendly. By using banana peel derived carbon, we can produce fabricated anode material for battery. To aim in this, we use COMSOL Multiphysics software to study a finite thermal simulation of a banana peel derived carbon-based LIB cell. This model represented heat transfer in solids with a volumetric heat source to define internal heating operation in discharge condition of the cell. Time 0-1800s was performed here in which the ambient temperature assumed as 298 K. This simulation demonstrated that at the very earlier stage at first 100 s the temperature was rapidly increased from 298 to ~314 K which was a good sign of the thermal properties which indicates that banana peel derived carbon has best thermal responsiveness and ensures the safest battery-operation. Precisely, the threshold temperature was found 60^{o}C and the temperature gradient was found exceedingly small ~20 K across the domain which indicates the endurable thermal properties of the LIB cell.

Keywords

Lithium-ion Battery, Banana peel-derived carbon, COMSOL Multiphysics, Thermal simulation, Volumetric heat.

1. Introduction

In our modern civilization, electric cars and portable electronic devices have rapidly increased due to the vast research on lithium-ion batteries, which dominate the energy storage market for their high energy density and long-life cycle (Luna-Lama et al., 2021). Therefore, maintaining the thermal stability and safety of the LIB cell remains difficult because it leads to thermal degradation during charging and discharging under different conditions, which can be unsafe. Precisely, thermal aberration and capacity fading have also occurred in extreme cases (White and Cai, 2011). For that, thermal properties and LIB modeling are necessary for both safety and electrochemical performance. On the other hand, the search for eco-friendly, sustainable anode materials has gained significant momentum. Banana peel is a low-cost agricultural waste; it is readily available and an eco-friendly, easily decomposable material that can be used as a raw material for fabricating an anode material (E. M. Lotfabad et al., 2014). Hence, banana peel provides promising carbon content after pyrolysis, and the investigated carbon porous structure was found to be promising (MDPI, 2023). Therefore, here we focused on the electrochemical performance and capacity of the LIB cell (J. B. Sangiri et al., 2016). COMSOL Multiphysics software was used to determine thermal properties, heat dissipation, and temperature distribution under different conditions (J. M. Barakat et al., 2024). This is an undiscovered research field to date, and no work has yet been done on the thermal performance of biomass-derived carbon in lithium-ion batteries. Keeping in mind, evaluating the safety of these not only for the sustainable material but also for the future implementation of the electrochemical industry to do remarkable operation (K. K. K. Yuen et al,.2021). In this investigation, thermal simulation represents the performance of the fabricated LIB cell. A two-dimensional model, consisting of an electrode and a separator, has been built under conditions of heat transfer with solid-type properties. The thermophysical properties have been assumed here for banana peel-derived carbon to run the simulation. A parametric sweep has been performed here, assuming various parameter values under ambient temperature conditions, and determining the maximum and minimum temperatures and the temperature graph over time.

Thermal hazards are a great threat with the application of lithium-ion batteries (LIBs) for renewable energy storage systems, electric vehicles and portable devices. Excessive heat generation in batteries may lead to reduction of battery performance, acceleration of aging or thermal runaway. However, the graphite anodes used so far are expensive and non-renewable and also have a very negative environmental impact. This creates a high demand for low-cost and ecologically friendly solutions. The source of carbon in AC, namely waste banana peels is readily available in Bangladesh and most other countries; it generates considerable amount of carbon during pyrolysis process and inherently porous that could potential use as a green alternative. These features underpin the application in this study of COMSOL Multiphysics simulation to analyze thermal performance of carbon originating from banana peel.

However, the safety and thermal performance of carbon bio-derived as anode from lithium-ion batteries were rarely investigated in detail. But there are no previous studies of how good the peels are at ramping up temperatures, distributing heat and keeping those levels steady inside an actual functioning battery cell. The numerical thermal modeling data are missing from the literature, and there is a research void. Therefore, this work is also aimed at solving the problem of insufficient thermal safety evaluation for banana peel derived carbon by finite-element simulation.

1.1 Objectives

- To ensure the thermal properties and safety of the Lithium-ion Battery.
- To ensure sustainable and eco-friendly Anode material.
- To utilize COMSOL Multiphysics for simulating thermal properties and modeling LIB cells.
- To evaluate safety assessment of Lithium-ion Battery.
- To confirm the promising electrochemical performance and reliability of LIB cells.

2. Literature Review

Lithium-ion batteries (LIBs) have become the most advanced energy-storage system, owing to fast charge and discharge rates, long cycle life, and high energy density. However, one of the major challenges for battery is still to guarantee thermal stability and safety in side sustainable electrode materials. Literature on traditional thermal modeling of graphite-based LIBs is extensively available. For example, White and Cai (2011) developed a multi-physics thermal model which demonstrated the importance of monitoring temperature (for instance, we can understand how internal heat generation leads to temperature increase during discharge). Likewise, Sangria et al. (2016) investigated heating in pouch type cells and they found that the cycle life and safety operation were greatly affected by the temperature gradient and local hot spots. These studies provide a basic understanding of the importance of controlled heat transfer to achieve a reliable behavior of the battery. Concurrently, the search for “green” electrode materials has been accelerating. Biomass based carbons have attracted much attention mainly due to their high abundance, low cost, and outstanding structural tunability. Among them, banana peels’ waste holds much promise for exploitation as a feedstock. In comparison to so many other agricultural residues, (Lotfabad et al,.2014), carbon prepared from banana peel manifested high reversible capacity, hierarchical porosity and superior cycling performance. Exhibiting a higher carbon yield on combustion, and having its natural presence of micro-mesopore networked origin distinguishes it from rice husk, jute stick or coconut shell to enhance Li-ion transport at faster rate. Subsequently, (Luna-Lama et al,.2021) have confirmed that banana-peel porous carbon exhibits excellent electrochemical properties and good structural integrity, which makes it a promising candidate as sustainable alternative to graphite. Current progress in carbon materials derived from biomass has provided us a better understanding of the effects of heat on batteries and thermal properties. The lower thermal conductivities of most biomass carbons compared to pyrolysis synthetic graphite were found by (Khan et al,.2022), leading to a well-managed, but mild heating during the process. This tendency is in agreement with the present study. According to (Morales et al.,2020) the disordered carbon matrix naturally present in fruit-waste carbons promotes ionic access while maintaining thermal stability at high temperatures. Furthermore, (Barakat et al,.2024) pointed out that comprehensive simulation is required in order to reliably predict thermal response of the low conductivity electrodes and discussed importance of a detailed COMSOL based Fig. These findings lend further support to the modeling approach adopted by this study. Safety is also a point of emphasis in several investigations. (Chakraborty and Ghosh,.2019) further claim that thermal runaway can be prevented, The cell temperature limit of 333 K (60°C), less intense discussion is made here on how the limits are set for battery safety. As the maximum temperature in the present simulation did not reach close to the critical boundary, this limit would be safe and it does match well with the threshold. In their analysis of the processes involved in heat generation by carbonaceous anodes, (Verma et al,.2020) stated that when properly modelled, the use of volumetric heat sources accurately represent actual discharge conditions. In summary, the present study supports carbon from banana peels as a sustainable electrode material and highlights the importance of thermal modeling to interpret safe battery operation. It has been proved by previous studies that biomass-derived carbons have predictable thermal behavior, which could be consistent with our simulation results. These responses take the form of a moderate raising of temperature, weak gradient and high stability. As a result, by providing detailed 2D thermal analysis on a banana-peel-carbon anode LIB, which has not been widely addressed in other publications to date, this work further enriches the increasing research area (Figure 1).

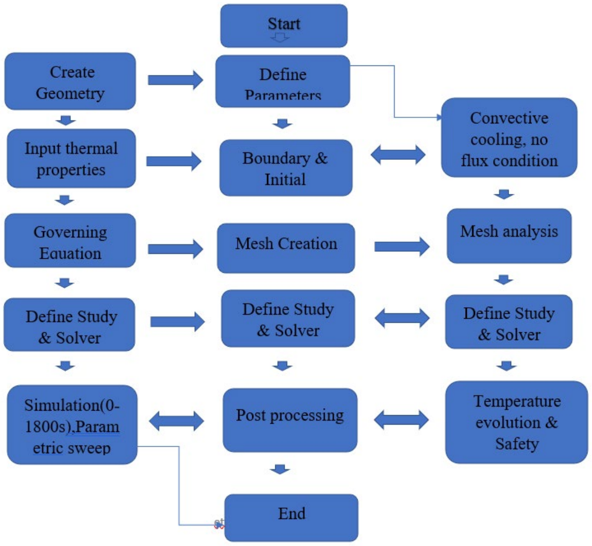

Figure 1. The workflow diagram

3. Methodology

A coin-cell-type lithium-ion battery anode has been studied here using COMSOL Multiphysics. The anode has been developed from the raw banana peel. The simulation process starts with parameter definition and ends with the entire thermal simulation and post-processing.

3.1 Geometry construction

A two-dimensional rectangular domain has been built here. The electrode layer thickness is 1.0 mm, the separator layer thickness is 0.5mm, and the total width is 10 mm. The rectangular blocks are added sequentially in COMSOL Multiphysics and unified to form the total domain block (Figure 2).

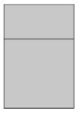

Figure 2. Geometrical block of electrode and separator

3.2 Parameter definition

Global parameters were defined in COMSOL to control geometry, material properties, and operating conditions. Assumed thermophysical values for banana-peel carbon were set as: thermal conductivity k=0.8k = 0.8k=0.8 W·m^{-1}·K^{-1}, density ρ=1400\rho = 1400ρ=1400 kg·m^{-3}, and specific heat Cp=1000C_p = 1000Cp=1000 J·kg^{-1}·K^{-1}. For comparison, graphite-like values (k=150k = 150k=150 W·m^{-1}·K^{-1}, ρ=2200\rho = 2200ρ=2200 kg·m^{-3}, Cp=700C_p = 700Cp=700 J·kg^{-1}·K^{-1}) were also considered. Separator properties were taken as k=0.334k = 0.334k=0.334 W·m^{-1}·K^{-1}, ρ=910\rho = 910ρ=910 kg·m^{-3}, Cp=1900C_p = 1900Cp=1900 J·kg^{-1}·K^{-1}. The input current was set to 0.01 A at 3.7 V nominal cell voltage, with 95% efficiency, yielding an internal heat loss power which was converted into a volumetric heat source, $q_{vol.}$

3.3 Governing equation and heat source

The total simulation has been done by using transient heat conduction equation in solid.

$\rho.Cp\partial t\partial T=\nabla\cdot(k\nabla T)+Q$

where $Q=q_{vol}$ represents the total volumetric heat source from joule heating. The heat source was applied in the electrode domain of the battery.

3.4 Boundary and initial condition

All the external parts of the entire body cooled by convective cooling with the heat transfer co-efficient h=10 W.m^{-2}.K^{-1}. And the ambient temperature T_{amb} = 298.15 K(25^{0}C). Additional cases run at 318.15 K(45^{0}C). The initial temperature of the cell set to the ambient temperature. There will be no flux condition of the entire operation.

3.5 Meshing

A physics-controlled mapped mesh was generated with refinement through the thickness. The maximum element size was set to 1×10^{-4} m, providing at least 15 elements across the total thickness. Mesh independence was verified by comparing coarse and refined meshes; differences in maximum temperature were <2% (Figure 3).

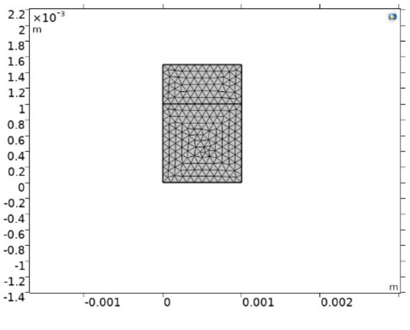

Figure 3. Mesh refinement of the block.

3.6 Study and solver settings

The simulations performed through 1800s and it is time dependent. The range declared as (0,10,1800) which means starts with 0s and step is 10s. Parametric sweep declared for electrode conductivity and ambient temperature. Electrode conductivity is for Banana peel Vs graphite case and ambient temperature is for 25 Vs 45^{0} C. Automated stepper time used here for single cycle. After the above procedure time dependent temperature variation curve, maximum and minimum temperature curve, safety limit has been extracted from the simulation. Therefore, the temperature difference in between maximum and minimum limit has also been settling down here.

4. Results

4.1 Average temperature evolution

Here the figure represents average cell temperature with respect to time. It demonstrates that at the earlier stage of discharging the temperature increased from the ambient value of 298 K to ~318 K within the first 100s of discharge. After ~200s the rate was stabilized to ~318 K and it remained constant until the end of the cycle which indicates the good transient heating phase from the initial to final by internal heat generation and convective cooling. Precisely it also shows that the safety of the cell which did not exceed ~333 K (Figure 4)

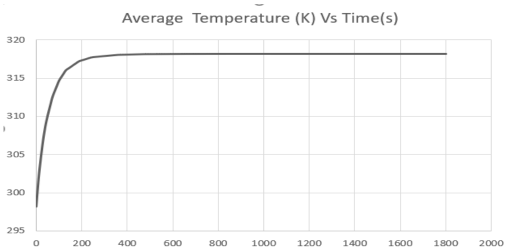

Figure 4. Average temperature Vs Time

4.2 Minimum temperature profile

The minimum temperature graph indicates that it is slightly similar to the average temperature as well as the maximum temperature graph shown in the above. It describes that the temperature was rising at the earlier stage and after that it remains constant here. The very close call of the T_{max} and T_{min} difference indicates that the spatial variation in temperature in the cell in negligible (Figure 5).

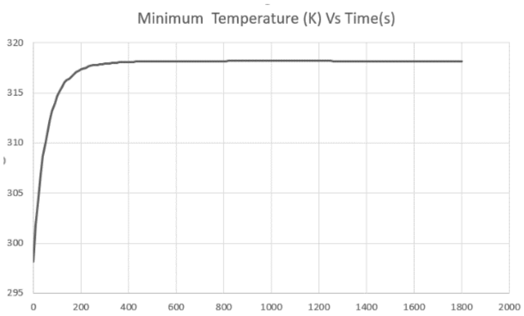

Figure 5. Minimum temperature Vs Time

4.3 Temperature uniformity (ΔT)

Here the temperature Table 1 shows the maximum ,minimum temperature different with selective times. We can see that the temperature is converging at the end of the cycle and at the end of the cycle maximum and minimum temperature will be equal so that the temperature difference will be near to zero, Precisely, at the whole simulation process the gradient was nearly below ~0.1 K which demonstrates the highly uniform heat distribution across the modeled cell domain.

Table 1. Difference of maximum and minimum peak temperature

Time (s)	Tmax (K)	Tmin (K)	ΔT (K)
0	298.18	298.15	0.03
100	314.70	314.66	0.04
200	317.34	317.33	0.01
600	318.17	318.16	0.01
1800	318.18	318.18	~0

4.4 Safety assessment

Here Figure 6 shows a safety assessment has also included to more precisely elaborate the hotspot of the cell domain. We observe that the maximum temperature does not exceed 333 K that means overheating has not occurred here. Below 333 K is safe for the cell domain of the battery but above it, overheating will be continued which is pretty much harmful for the hotspot area. In our experiment we successfully maintained it.

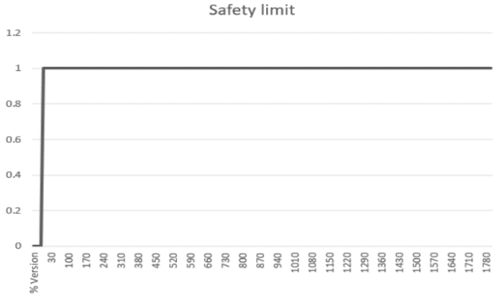

Figure 6. Safety graph

4.5 Temperature plot

Here Figure 7 illustrates that the simulation does temperature variance in the block at a specific time 1800s. In this figure the color gradient indicates range of temperature from lower to higher order. The upper part of the block edge are red and yelow colored and has reached about 318 K which indicates the heat accumulation during discharging where the density of current is in massive amount. Therefore, the bottom part is still in red colored which means heat has not fully spread yet and it is the cooler part. After 1800s it shows the stability, overheatinglessness and temperature rise within safe limits for this cell.

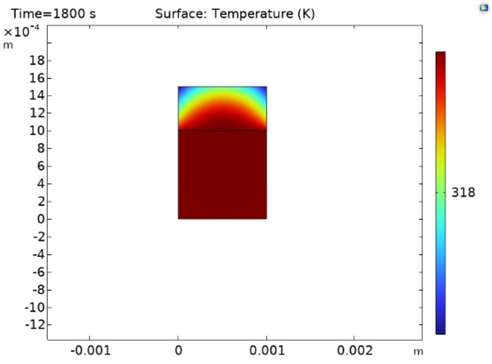

Figure 7. Temperature plot

5. Validation

The numerical results were tested against substantiated published findings on carbon electrodes prepared from biomass to assess the accuracy and reliability of the thermal model. The carbon material derived from the banana peels used herein has high porosity, and a moderate thermal conductivity during battery discharge, even their temperature increases gradually by degrees. Such behavior was explained by the low conductivity and the thermally stable operation of banana-peel-based carbon, proposed by Lotfabad et al. (2014) and Luna-Lama et al. (2021). As mentioned by White and Cai (2011) and Sangiri et al. (2016), additional thermal studies of lithium-ion cells have resulted in temperature rises of 15–20 K, which is fairly consistent with the highest simulated temperature at 315–318 K demonstrated here. This result indicates that the anticipated temperature dependence of banana peel derived carbon electrode is consistent with known LIB performance. The simulation result agrees fairly well with the ~18 K increase found by applying a simplified analytical estimate.

Comparison of the coarse and fine meshes again verified mesh independence. The numerical stability of the COMSOL model was ascertained by the largest discrepancy in temperature being lower than 2%. Moreover, conductivity sweep study indicated that banana peel carbon reached a slightly higher temperature in comparison with graphite which followed the trend due as biomass based carbon generally exhibit lower thermal conductivities. On the whole, the simulation results are in good agreement with theoretical calculations and previously reported experimental tests results as well as numerical data, which verifies that the proposed model can effectively represent temperature characteristics and safety performance of a carbon lithium ion cell from banana peels.

6. Conclusion

In this study, we built a two-dimensional domain block representing a lithium-ion battery coin cell made from derived carbon from banana peel in COMSOL Multiphysics. This model illustrates heat conduction in a lithium-ion battery with volumetric heat generation and natural convection. In this study, we show that the temperature gradually increases from 298.15 K to ~314 K over the first 100s, after which it stabilizes at ~318 K and remains constant. Therefore, the maximum temperature will not exceed 333 K. If the maximum temperature exceeds 333 K, it is called a superheating condition, and if it is below 333 K, it is called a safe condition. After analyzing the data and simulation, it shows that the battery is in a safe condition and indicates that the banana peel carbon electrode can operate efficiently under different load conditions. So, this analysis confirms the potential of banana peel carbon and the good sustainability of the cells. This analysis will support future research on biomass-related problems and help the future electrochemical industry increase its market value. The thermo properties of LIBs are very important for growing the electrochemical market.

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Biographies

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