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Thermal Behavior Simulation of Cylindrical Battery

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Abstract: Batteries are a collection of one or more cells whose chemical reactions create a flow of electrons in a circuit. Lithium ion battery (LIB) is said to has high energy density level, has a long life cycle and has zero memory effect. However, the temperature, on the other hand, has a significant impact on LIB performance such as potential thermal stability difficulties. For cylindrical geometry, the study determines the thermal behavior of LIB in term of surface temperature and maximum temperature of active battery material using different material for positive electrode and charge/discharge current. From the study, LIB with lithium manganese oxide (LMO) always show a good thermal behavior in term of surface temperature and maximum temperature of active battery material. The less charge/discharge current applied, the less temperature for surface and active battery material. The study of thermal behavior in cylindrical battery will give a better understanding and a better design of cylindrical battery with larger capacity can be produced. Thus, the design also can be added with cooling method such as air cooling, liquid cooling, heat pipe and phase change materials.

Keywords: Thermal Behaviors, Charge/Discharge Effect, Lithium Ion Battery, Positive Electrode

1. Introduction

Batteries are a collection of one or more cells whose chemical reactions create a flow of electrons in a circuit. All batteries are made up of three basic components: an anode (the '-' side), a cathode (the '+' side), and some kind of electrolyte (a substance that chemically reacts with the anode and cathode). The term "battery" was originally used to indicate a "grouping of similar objects organized together to accomplish a purpose," such as a battery of guns. Benjamin Franklin coined the word in 1749 to describe a series of capacitors he had connected for his electricity experiments. A battery, in general, is made up

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**Corresponding author: rosmila@uthm.edu.my* of five major components. Anode, cathode, current collectors on which they may be placed, electrolyte, and separator.

A lot of studies about Lithium Ion Battery (LIB) has been done. It has high energy density level, has a long life cycle and has zero memory effect [1]. Because of that factor, LIB often used as power source for the electric vehicles (EV). However, the temperature, on the other hand, has a significant impact on LIB performance such as potential thermal stability difficulties, such as capacity deterioration, thermal runaway, and even fire explosion, induced by overheating of the battery and/or thermal non-uniformity in the battery pack, preclude the commercial deployment of EV [2]. When the temperature of the LIB rises too high, the electrodes decompose and side reactions occur, reducing the battery's life [3].

Now, to keep the temperature of LIB exceed overheating, many proper strategies has been introduced such as air cooling, liquid cooling and heat pipe. Air cooling has the simplest and cheapest strategies [4]. Liquid cooling is particularly effective and has advantages such as compact structure and ease of setup, owing to the high heat conductivity and heat capacity of the liquid coolant. In simple way, all these strategies have their pros and cons in helping to reduce the temperature of LIB. In order to get a better understanding how temperature can affected the batteries condition, this study was proposed.

The main objective of this research is to design LIB with different material as positive electrodes by using COMSOL Multiphysics 5.5 Software. For this geometry, the study determines the thermal behavior of LIB in term of surface temperature and maximum temperature of active battery material using different material for positive electrode and charge/discharge current. From the result, the best LIB from different electrode material is proposed.

2. Materials and Methods

This part discusses and explains in detail about setting up and designing the model of cylindrical lithium ion battery with charge/discharge current and different positive electrodes. For this study, there were two results that was observed which are the surface temperature of batteries and temperature of active battery material which called maximum temperature. For the purpose of the LIB thermal management, the thermal behavior of the LIB was investigated.

The design of the LIB for this study was adapted from Wang and team [1]. In this design a cylindrical battery using finite element modelling to observe the temperature distribution for a better understanding of thermal analysis. Then, design was set up by using COMSOL Multiphysics Software but different electrodes and electrolyte was used. This study had some conditions that need to be followed which are the discharging/charging current and two different positive electrodes. The idea of this study also adapted from [1] but using different charge/discharge current and material of electrolyte. Battery casing also was added to observe the surface temperature. The result that had been obtained was not exactly accurate as the research because of the different type of battery and different current that has been used.

The design began by setting up seven cylinders for battery casing, positive electrode, negative electrode, two current collectors, separator and battery tabs as shown in Figure 1. Based on Table 1, each cylinder had different radius while the height of the cylinders is same except for the battery casing and battery tab. The battery also was set to 298.15 K as initial temperature.

Table 1: Parameter of LIB

Parameter	Height	Radius
Positive Electrode, mm	140.8	15.0
Negative Electrode, mm	140.8	18.0

Table 1: Continued

Separator, mm	140.8	17.0
Positive Current Collector, mm	140.8	16.0
Negative Current Collector, mm	140.8	19.0
Casing, mm	141.0	20.0

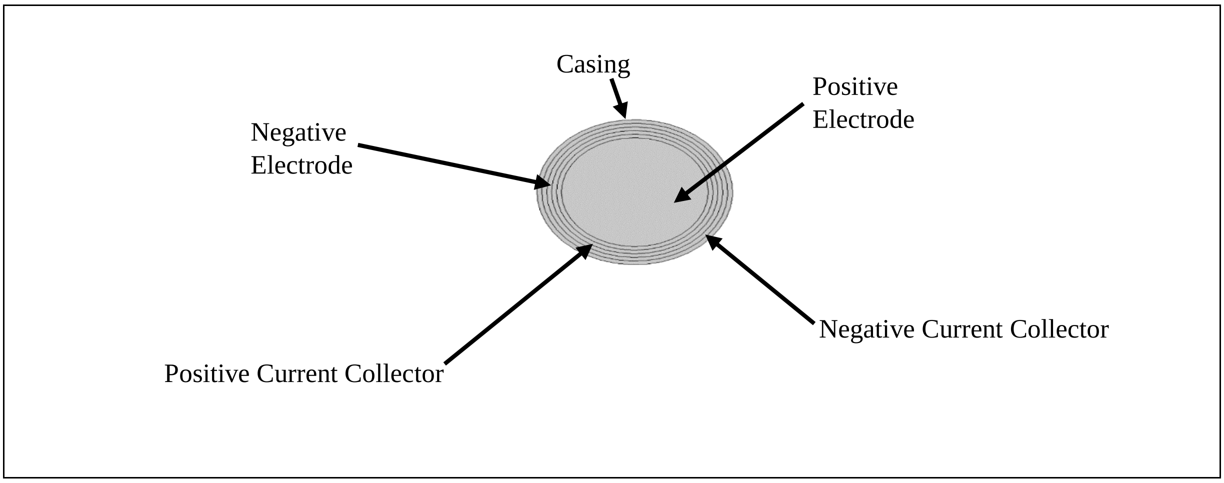


Figure 1: Component of the LIB from the upper view

2.1 Materials

The global parameter also need to be set to get the best result for this study. For this study, the size of the battery was not the variable. The material and properties for the component of the battery was shown in Table 2 and their thermo physical properties was shown in Table 3 while components of the battery is in Figure 1.

Table 2: Parameter of LIB

Component	Material
Positive Electrode	LMO and LCO
Negative Electrode	Graphite
Electrolyte	LiPF6 in 3:7 EC:EMC
Positive Current Collector	Aluminium
Negative Current Collector	Copper
Casing	Steel AISI 4340

Table 3: Properties of LIB materials

	Electrical conductivity, S/m	Thermal Conductivity, k (W/m•k)	Diffusion coefficient, m^2/s
LMO	3.50	-	1.00×10^{-14}
LCO	1.13	-	5.00×10^{-13}
Graphite	100.00	881.00	1.45×10^{-13}
Aluminum	3.77×10^{7}	238.00	-
Copper	5.99×10^{7}	400.00	-
Steel AISI 4340	4.03×10^{6}	4.55	-

For prolonged cycle life test assessments, LIB current collectors need to have strong electrochemical performance and cyclability, which was proven by electrochemical characterizations and cycle life testing. Apart of having a good electrical conductivity, aluminum (Al) has an ability to form a passive film [5]. This can make the electrolyte interface more stable. It also has a light weight and low cost to produce. Current collector need to have some characteristics which are high conductivity and high chemical and thermal stability [6]. Copper (Cu) as negative current collector will provide a good conductivity, more stable chemical properties, better flexibility, easy to process, and less expensive price.

2.3 Equations

For this study, heat from the active battery material assumed as heat source. *Eq. 1* is the equation for heat source. Q_o as the heat per unit volume, or as a heat rate. Heat generation occurs during the discharge cycle, which is driven by current (I) passing through the cell. The initial temperature of the LIB will be inserted in initial value. *Eq. 2* is heat generation of LIB during charge/discharge [3]. Q_{ir} is the irreversible heat; Q_{re} represents the reversible heat; *I* is the current; U_{ca} and U_{an} are the open circuit potential (OCP) of cathode and anode electrode, respectively; *U* is the terminal voltage; *T* denotes the temperature of LIB; *dU/dT*, the derivative of the OCP with respect to the temperature. In the right-hand side of *Eq. 2*, it takes the positive sign for discharge operations and the negative sign for charge operations. *Eq. 3* shows the boundary of heat flux , where n is the boundary normal pointing out of the domain.

$$Q_{gen} = Q_0 \qquad Eq.1$$

$$Q_{gen} = Q_{ir} + Q_{re} = \pm[I(U_{ca} - U_{an} - U) - IT\frac{d(U_{ca} - U_{an})}{dt} \qquad Eq.2$$

$$q_0 = h.(T_{ext} - T) \qquad Eq.\ 3$$

3. Results and Discussion

This part discusses and analyzes the thermal behavior of LIB model in term of surface temperature and maximum temperature of active battery material in LIB in different charge/discharge current for the LIB model. Temperature surface are used to show the temperature of the LIB after a cycle time of 600 s followed by a relaxing period after 1500 s. By using different materials for positive electrode, the difference of the temperature for the LIB can be studied. The results of the surface temperature were shown in Table 4 while the maximum temperature were shown in Table 5, Table 6 and Table 7 in YZ-plane.

3.1 Results

The temperature surface resulted from the LIB based on LCO and LMO as materials of positive electrode and 5C, 10C and 12C charge/discharge current in 1500s, where relaxing period start to happen showed by Table 1 while the maximum temperature of active material in LIB with LCO and LMO as positive electrodes was shown in Table 5, Table 6 and Table 7 at 0s, 1500s and 2100s.

Table 4: Surface Temperature of LIB

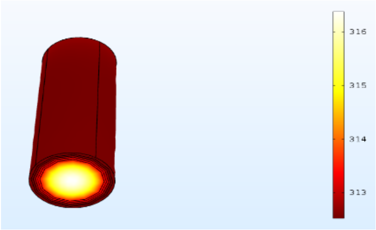
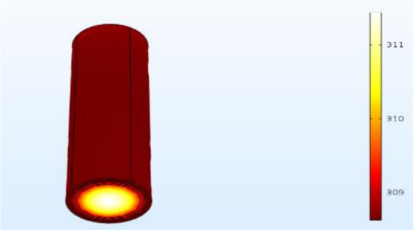
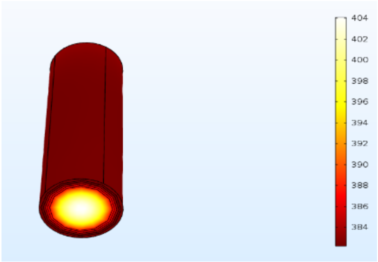
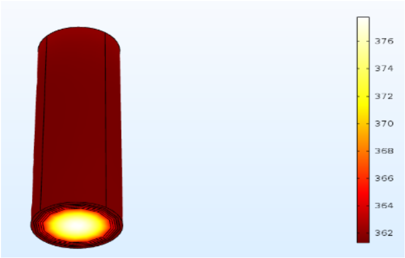
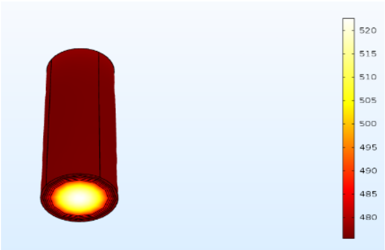
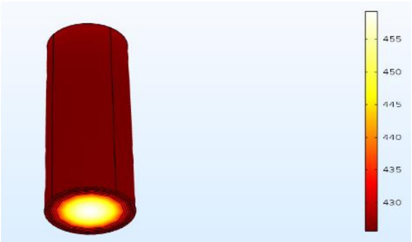
	LCO	LMO
5C		
10C		
12C		

Table 5: YZ-plane of LIB at 5C charge/discharge current

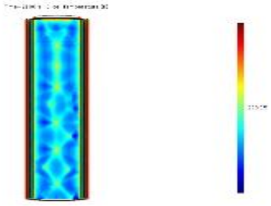
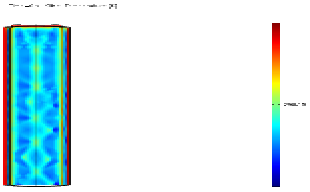
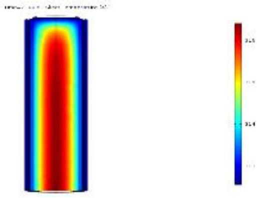
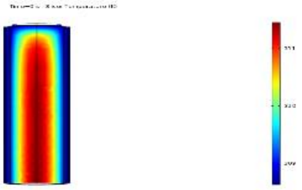
Time (s)	LCO	LMO
0		
1500		

Table 5: Continued

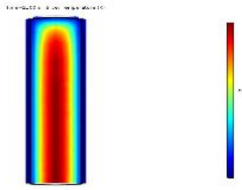
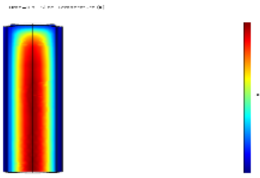
2100		

Table 6: YZ-plane of LIB at 10C charge/discharge current

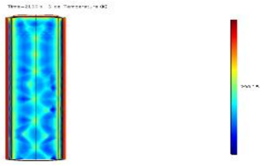
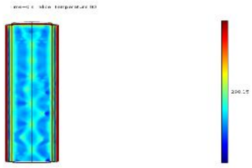
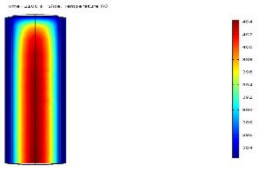
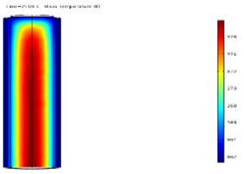
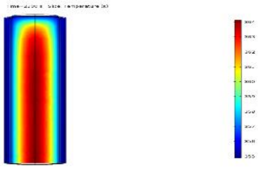
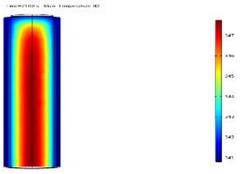
Time (s)	LCO	LMO
0		
1500		
2100		

Table 7: YZ-plane of LIB at 12C charge/discharge current

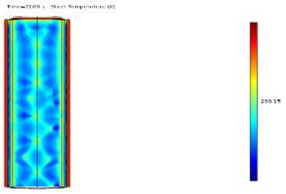
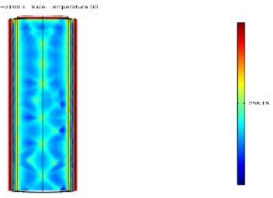
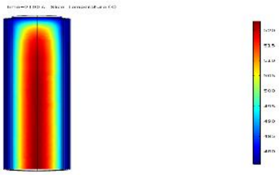
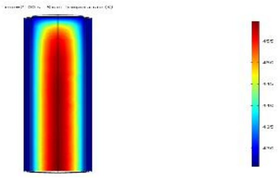
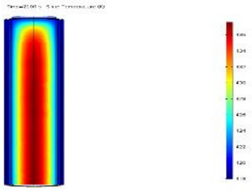
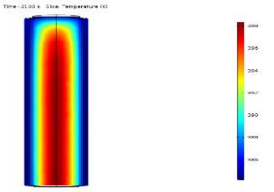
Time (s)	LCO	LMO
0		

Table 7: Continued

1500		
2100		

3.2 Discussions

The temperature need to be observed for thermal behavior of this battery has been studied. Table 4 shows the result of the surface temperature with different positives electrodes and different charge/discharge current. From the surface temperature, the source of the heating of LIB is the active material of the battery which is the electrodes and electrolyte. Then, the heat was transferred to the other material of the battery which is the battery casing and the separator [3]. From the table, the temperature of LIB with LMO as material has low surface temperature than LIB with LCO.

At 1500s, for 5C, the LIB with LCO reached until 313K while LIB with LMO only reached 309K. For other charge/discharge current, LIB with LCO always show a big difference of temperature. The temperature of LIB with LCO is 384K compared with LIB with LMO which is only 362K. For 12C charge/discharge current, both LIB show a big difference in term of surface temperature than other charge/discharge current. LIB with LCO is 480K while LIB with LMO is 430K. Among these two, the LIB with LMO as positive electrodes shows that it has lower surface temperature based on different charge/discharge current. Based on the Table 1 also, the heat from the active battery material also can be observed. For 5C of charge/discharge, the temperature is 316K for LIB with LCO and 313K LIB with LMO. For 10C, LIB with LCO reached 404K while LIB with LMO only reach 376K. For 12C, LIB with LCO has 520K of the active battery temperature while LIB with LMO has 455K temperature of active battery material.

Maximum temperature of the active material in LIB with LMO and always low than maximum temperature of the active material in LIB with LCO. At time 0s, the maximum temperature for both of the battery was 298.15K. As the LIB start to have charge/discharge process, the temperature casually increased. This is because of the ion exchange that happen in the electrodes and electrolyte.

3.3 Tables of Maximum Temperature of Active Battery Material

The result of maximum temperature of LIB with LCO and LMO at different charge/discharge current from 0s to 2100s was recorded and expressed in Table 8 until Table 10:

Table 8: Max Temperature of LIB at 5C charge/discharge current

Time (s)	Max Temperature (K) LCO	Max Temperature (K) LMO
0	1.72×10^{-8}	-1.27×10^{-9}
300	6.16	4.46
600	10.34	7.51
900	13.61	9.90
1200	16.20	11.80
1500	18.27	13.31
2100	11.56	8.43

Table 9: Max Temperature of LIB at 10C charge/discharge current

Time (s)	Max Temperature (K) LCO	Max Temperature (K) LMO
0	1.72×10^{-8}	-1.27×10^{-9}
300	41.61	30.54
600	66.04	48.93
900	83.42	62.27
1200	96.52	72.34
1500	106.20	79.82
2100	66.01	49.62

Table 10: Max Temperature of LIB at 12C charge/discharge current

Time (s)	Max Temperature (K) LCO	Max Temperature (K) LMO
0	1.72×10^{-8}	-1.27×10^{-9}
300	86.64	64.43
600	132.82	99.207
900	170.24	124.31
1200	200.66	144.89
1500	225.04	161.54
2100	139.47	100.20

3.4 Graph of Maximum Temperature of Active Battery Material

Graph of maximum temperature was plotted in Figure 2, Figure 3 and Figure 4 to show a better comparison between the maximum temperature from the active battery material in the LIB.

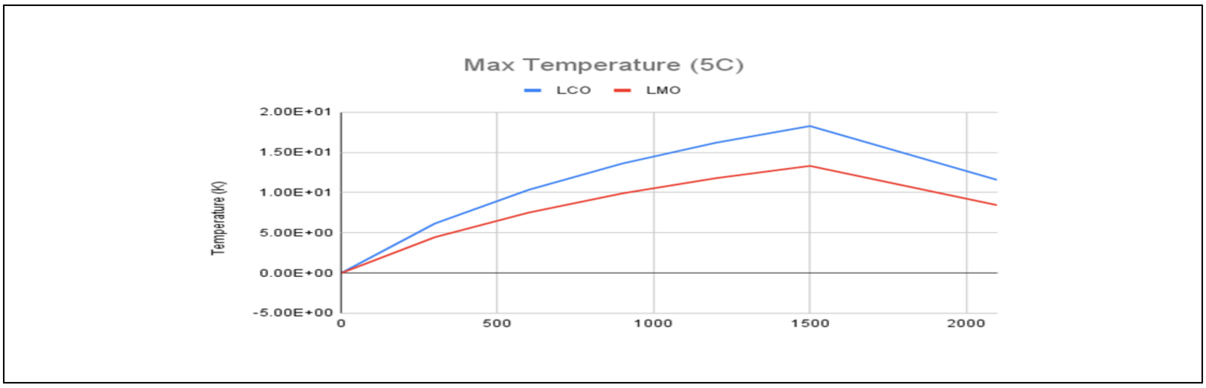


Figure 2: Max Temperature of LIB at 5C charge/discharge current

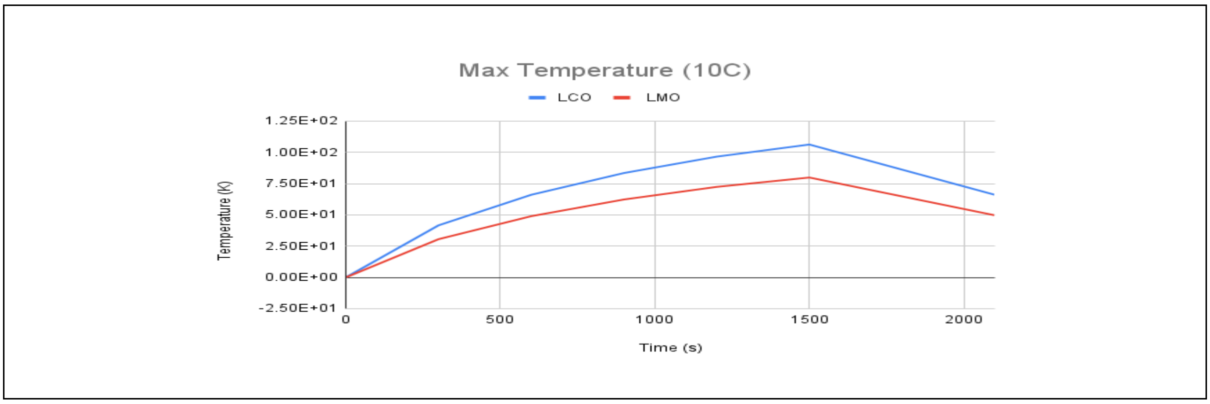


Figure 3: Max Temperature of LIB at 10C charge/discharge current

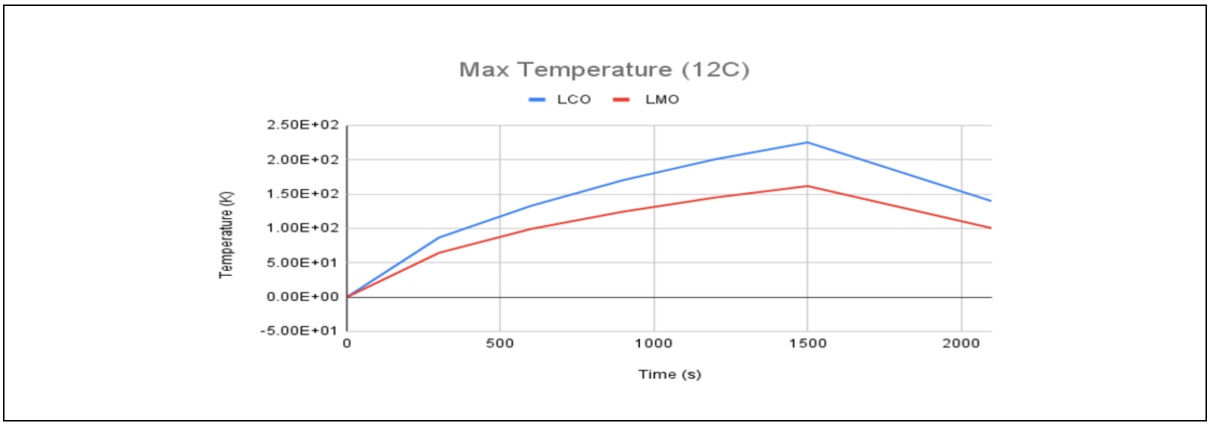


Figure 4: Max Temperature of LIB at 12C charge/discharge current

Figure 2 shows the maximum temperature of LIB with LCO and LMO. From the Figure 2, the max temperature for both of LIB start to decrease at 1500s as relaxing period start to happen. LIB with LCO can reach until 18.27K while LIB with LMO can reach until 13.32K at 1500s in 5C charge/discharge current. At 2100s, the temperature of the two LIB is 11.56K and 8.43K. From this comparison, LIB with LMO always show a low max temperature.

Figure 3 shows the max temperature of LIB with LCO and LMO at 10C charge/discharge current. From the Figure 3, the max temperature for both of LIB also start to decrease at 1500s as relaxing period start to happen, same as Figure 2. LIB with LCO can reach until 106.20K while LIB with LMO can reach until 79.82K at 1500s in 10C charge/discharge current. At 2100s, the temperature of the two LIB is 66.01K and 49.62K for LCO and LMO. From this comparison, LIB with LCO always show a low max temperature. The max temperature of the LIB at 10C has a big difference compared to LIB at 5C. This is because of total of charge/discharging current was used.

Figure 4 shows the maximum temperature of LIB with LCO and LMO at 10C charge/discharge current. The maximum temperature also starts to decrease by time because of the resting period at 1500s. LIB with LCO can reach until 225.04K while LIB with LMO can reach until 161.55K at 1500s in 12C charge/discharge current. At 2100s, the temperature of the two LIB is 139.47K and 100.20K for LCO and LMO. From this comparison, LIB with LMO always show the lowest maximum temperature. The maximum temperature of the LIB at 10C has a big difference compared to LIB at 5C. This is because of bigger charge/discharging current was used. From the comparison, it shows that LIB with LMO always have a promising max temperature at 5C, 10C and 12C charge/discharging current compared to LIB with LCO.

4. Conclusion

The model of the LIB has been successfully constructed by using COMSOL Multiphysics 5.5 Software. The surface temperature and maximum temperature of active battery material has been analyzed for LIB with LCO and LMO as negative electrodes. The charge/discharge current used for the study is 5C, 10C and 10C. From the study, it shows that LIB with LMO always show a good thermal behavior in term of surface temperature and maximum temperature of active battery material. The less charge/discharge current applied, the less temperature for surface and active battery material. In order to decrease the surface temperature and maximum temperature in the future work, air cooling, liquid cooling, heat pipe and phase change materials can be added in the LIB.

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