

T.R.
GEBZE TECHNICAL UNIVERSITY
GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES

**ANALYSIS OF PARAMETERS ON HEAT GENERATION OF A
LITHIUM-ION BATTERY**

YİĞİTALP GÖKMEN
A THESIS SUBMITTED FOR THE DEGREE OF
MASTER OF SCIENCE
MECHANICAL ENGINEERING DEPARTMENT

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THESIS SUPERVISOR
ASSOC. PROF. DR. GAMZE GEDİZ İLİŞ

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YÜKSEK LİSANS JÜRİ ONAY FORMU

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İMZA/MÜHÜR

SUMMARY

Nowadays, the demand for lithium-ion batteries is increasing rapidly due to their large range of usage. This thesis aims to investigate multiple parameters (porosity of electrodes, maximum lithium concentration of electrodes, salt concentration of electrolyte, and thickness of electrodes) which are affecting the cell voltage and thus thermal behavior of the battery cell. The change of the parameters that directly affect thermal heat generation is parametrically discussed in this thesis. To understand the change of these parameters on heat generation a 3D electrochemical-thermal model is developed. Lithium Iron Phosphate (LFP), graphite, and LiPF₆ (in 1:1 EC:DEC) have been selected for cathode, anode, and electrolyte as a battery materials, respectively.

Key Words: Lithium-Ion Battery, Pouch Cell, Lithium Iron Phosphate (LFP), 3D Model, Heat Generation, Temperature Distribution

ÖZET

Günümüzde, geniş kullanım alanları nedeniyle lityum iyon pillere olan talep hızla artmaktadır. Bu tez, hücre voltajını ve dolayısıyla pil hücresinin termal davranışını etkileyen parametreleri (elektrotların gözenekliliği, elektrotların maksimum lityum konsantrasyonu, elektrolitin tuz konsantrasyonu ve elektrotların kalınlığı) araştırmayı amaçlamaktadır. Bu tezde termal ısı üretimini doğrudan etkileyen parametrelerin değişimi parametrik olarak ele alınmıştır. Bu parametrelerin ısı üretimi üzerindeki değişimini anlamak için bir 3 boyutlu elektrokimyasal-termal model geliştirilmiştir. Pil malzemesi olarak sırasıyla katot, anot ve elektrolit için Lityum Demir Fosfat (LFP), grafit ve LiPF₆ (1:1 EC:DEC) seçilmiştir.

Anahtar Kelimeler: Lityum-İyon Batarya, Kesecik Hücre, Lityum Demir Fosfat (LFP), 3B Model, Isı Üretimi, Sıcaklık Dağılımı

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LIST OF ABBREVIATIONS AND ACRONYMS

<u>Abbreviations</u>	<u>Explanations</u>
<u>and Acronyms</u>	
1D	: One-Dimensional
3D	: Three-Dimensional
amb	: Ambient
cc	: Current Collector
ncc	: Negative Current Collector
pcc	: Positive Current Collector
eff	: Effective Value
el	: Electrolyte
ne	: Negative Electrode
pe	: Positive Electrode
ref	: Reference Value
sp	: Separator
surf	: Surface of Active Material Particles
mix	: Mixture
eq	: Equilibrium
therm	: Thermal
Ah	: Ampere-Hour
JH	: Joule Heating
SOC	: State of Charge

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1. INTRODUCTION

Nowadays, the demand for lithium-ion batteries is increasing rapidly due to their large range of usage. These rechargeable power storage components can be used in electronic devices, electrical vehicles, or in plants for energy sustainability. Lithium-ion batteries offer high specific energy and power (Figure 1.1 [1]), low heat dissipation, high cycle life, fast recharge, and better safety conditions when compared with other battery types [1]. For that reason, mathematical modeling and experimental studies of lithium-ion batteries, development and optimization of the battery management system, and thermal management system are important.

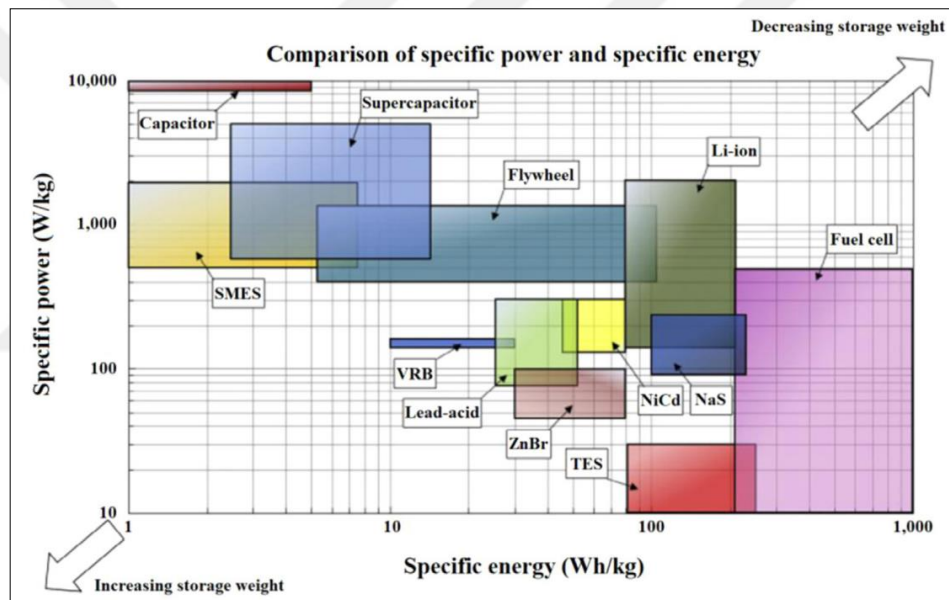


Figure 1.1: Comparison of specific energy and power for different battery types.

Lithium-ion batteries working principle and components are similar to the other battery types. As shown in Figure 1.2 [2], a simple battery cell has electrodes (anode and cathode), a separator, an electrolyte, and current collectors. The anode and cathode store the lithium. While charging the cell, positively charged lithium ions move from the cathode to the anode through the separator. Also, due to the blockage of electrons by the separator, free electrons from lithium ions move from the positive current collector to the negative current collector through the circuit and are stored in the anode. For the discharge, the process is vice versa.

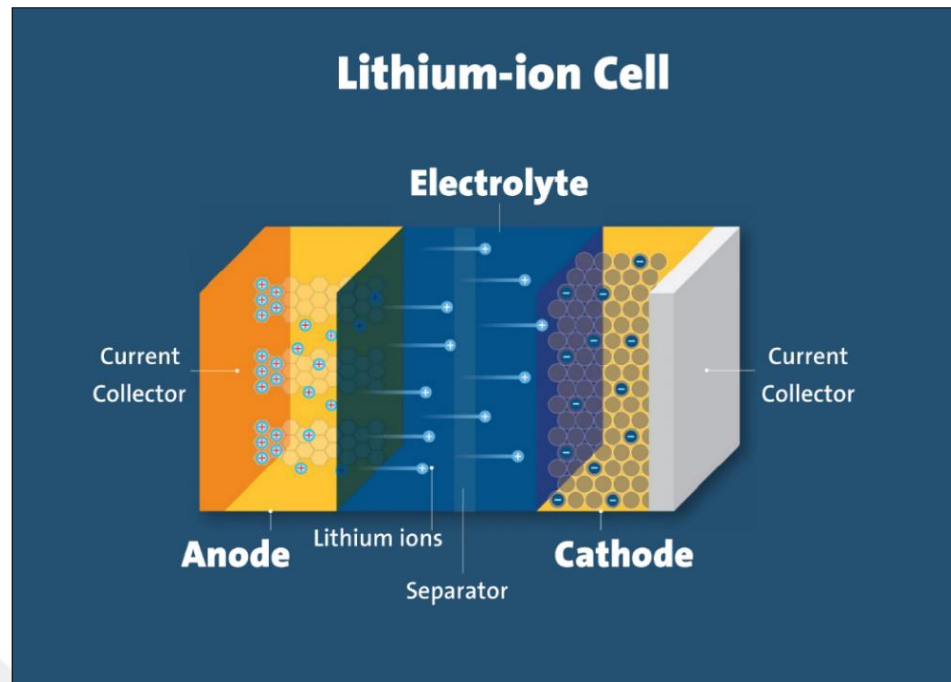


Figure 1.2: Basic lithium-ion cell diagram.

There are many commercial materials available for lithium-ion batteries in the industry which are listed below in Table 1.1 [3].

Table 1.1: Common materials for different components in lithium-ion battery.

Anode	Electrolyte	Cathode
Graphite	LiPF6 in 1:1 EC:DEC	LFP (LiFePO ₄)
Hard Carbon	LiPF6 in 3:7 EC:EMC	NCA (LiNi _{0.8} Co _{0.15} Al _{0.05} O ₂)
Silicon/Carbon	LiPF6 in 1:2 EC:DMC	NMC (LiNi _{1/3} Mn _{1/3} Co _{1/3} O ₂)
Tin/Cobalt Alloy	LiPF6 in 2:1 EC:DMC	LMO (LiMn ₂ O ₄)
LTO (Li ₄ Ti ₅ O ₁₂)	LiPF6 in 0.1:0.27:0.63 PC:EC:EMC	LCO (LiCoO ₂)

There are several important properties such as; affordability, energy, power, safety, performance, durability, and maturity for material selection in making lithium-ion batteries. For instance, the cathode material comparison chart can be seen in Figure 1.2 [1]. LFP meets requirements greatly such as power, performance, durability, and safety when compared to other materials. On the other hand, LFP has low specific

energy and low affordability which causes bigger application areas like electrical vehicles instead of smaller devices.

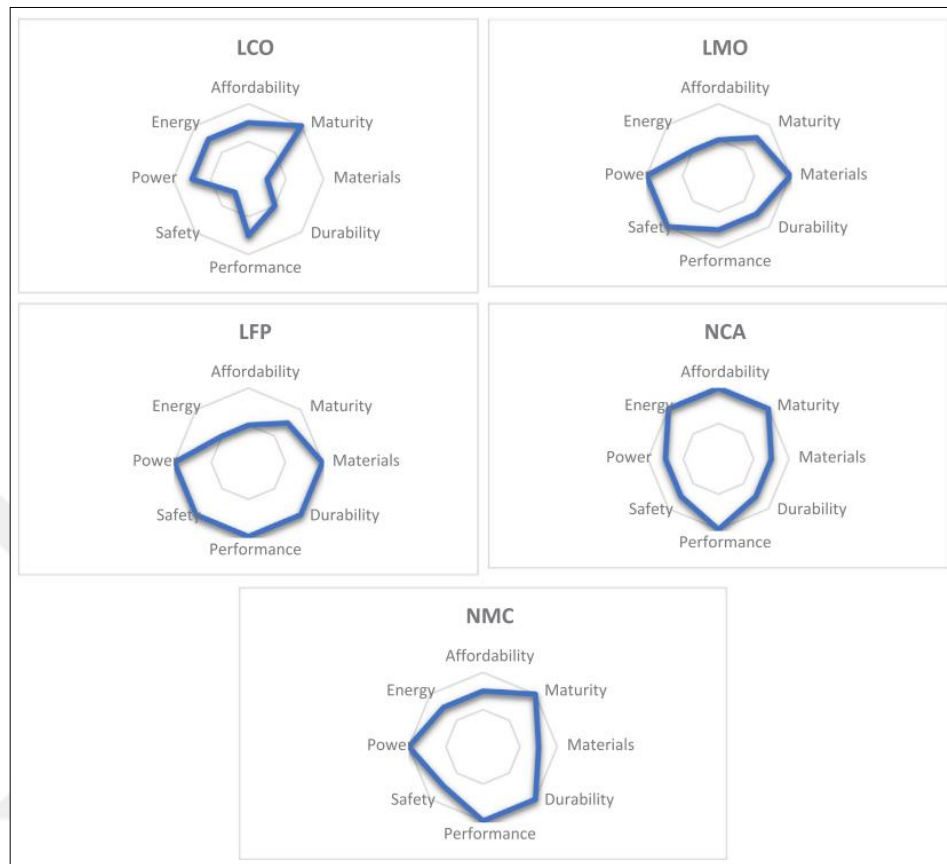


Figure 1.3: Cathode material comparison chart.

Lithium-ion battery literature can be thematically categorized into electrochemical modeling and thermal modeling of a lithium-ion battery:

About the electrochemical modeling, Pal et al. [4] created a 1D electrochemical model of a lithium-ion single cell at 10, 30, and 45°C environmental temperatures for 1C charge/discharge ranges using COMSOL Multiphysics 5.0 Software and optimized parameters for better battery performance. Dees et. al. [5] modeled a 2D electrochemical model under the complex cycling protocols for lithium polymer cells to identify and optimize the processes that limit the cell performance. Dees et. al. [6] modeled an electrochemical alternating current impedance model to examine aging effects in the positive electrode. Dangwal et. al. [7] suggest new approaches to improve common methods of parameter calibration for modeling. Samadani et. al. [8] created

an empirical model of lithium-ion batteries with electrochemical impedance spectroscopy tests.

In the studies on thermal modeling, Zhang et al. [9] created an electrochemical-electrical-thermal coupled model for pouch-type cells for optimizing the temperature distribution. Alipour et al. [10] analyzed the multilayer modeling approach to investigate its effect on the thermal behavior of the pouch-type battery. Xu et al. [11] created an electrochemical-thermal model of a prismatic battery to investigate tab placement effects on thermal behavior. Gökmen et al. [12] compared 1D and 3D electrochemical-thermal models in single and multilayered cells in terms of computation time. Zhao et al. [13] investigated the effects of the thickness of electrodes with the 1D electrochemical and 3D thermal models.

This thesis aims to investigate multiple parameters (porosity of electrodes, lithium concentration of electrodes, the salt concentration of electrolyte, and thickness of electrodes) which are affecting the cell voltage and thus thermal behavior of the battery cell. The change of the parameters that directly affect thermal heat generation is parametrically discussed in this thesis. The change of these parameters on heat generation and thus the effect on temperature distribution of the battery cell is analyzed. To understand the change of these parameters on heat generation a 3D electrochemical-thermal model is developed by using Comsol Software. The model is also validated with the experimental data shared by [10]. Lithium Iron Phosphate (LFP), graphite, and LiPF₆ in 1:1 EC:DEC have been selected for cathode, anode, and electrolyte in this thesis as a battery material, respectively. In addition, aluminum and copper, the most common materials, also have been selected for current collector plates.

During cycles, a high amount of heat is generated in lithium-ion batteries which causes a temperature rise in the cells. This heat is generated by electrochemical reactions and internal resistances. The thesis aims to determine the major parameters that affect heat generation in lithium-ion batteries. Later on, parameters are selected and analyzed under specified conditions.

In Chapter 2, the electrochemical and thermal models which are used for the analysis of the battery heat generation are summarized. The governing equations are also explained in this chapter. The model that is used to analyze the heat generation of the battery taken into account in this thesis is validated and the validation results are

summarized in Chapter 3. The results of the thesis on the influence of the parameters on heat generation are presented in Chapter 4. Chapter 5 includes the conclusion of this thesis.



2. COUPLED ELECTROCHEMICAL-THERMAL MODEL

2.1. Computational Domain and Model Assumptions

A 3D coupled electrochemical-thermal model which is studied in this thesis was developed with COMSOL Multiphysics 6.0 software for a single pouch cell whose dimensions are shown in Figure 2.1.

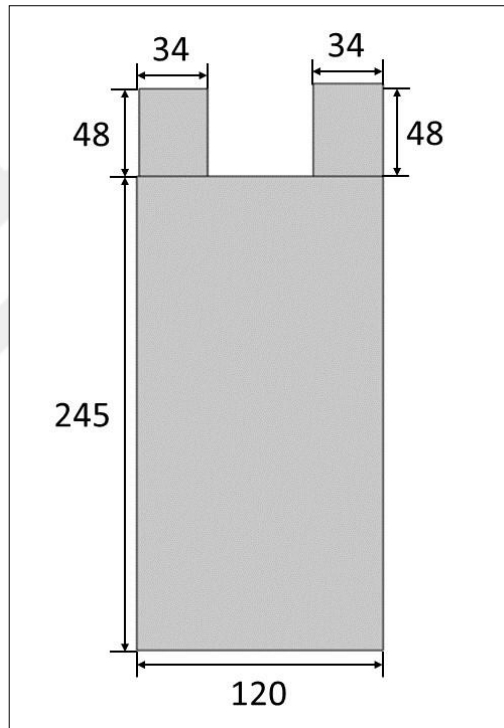


Figure 2.1: Dimensions of the single pouch cell in millimeters.

The properties which are necessary for the electrochemical and thermal modeling of the pouch battery taken into consideration in this thesis are taken from Alipour et al. [10] to validate the electrochemical-thermal model properly. This pouch battery is 20 Ah LFP/graphite with 20 cells inside. The nominal voltage and capacity for one cell are 4.0 V and 1 Ah, respectively. To simulate a single pouch cell; principles of mass, energy, charge conservations, and electrochemical kinetics were used.

3D pouch cell model has the positive current collector (positive cc), the positive electrode (pe), the separator (sp), the negative electrode (ne), and the negative current collector (negative cc) which are shown in Figure 2.2.

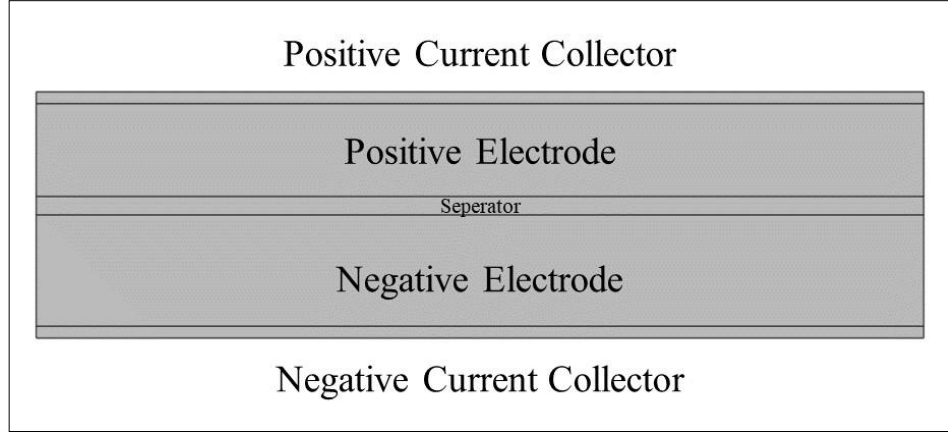
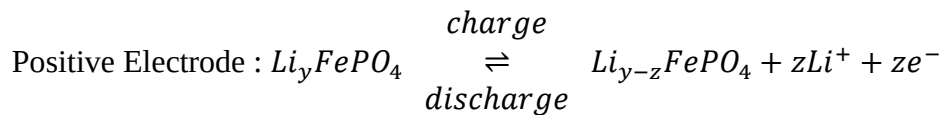
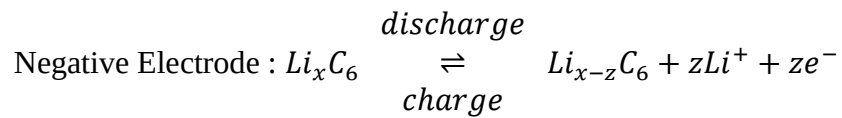


Figure 2.2: Cross-sectional view of single pouch cell.

Positive and negative current collectors are copper and aluminum foil with 16 μm thickness each, respectively. Their main purpose is to distribute and collect the current for cell components. The electrodes are a porous solid matrix that contains spherical active material particles such as LFP and graphite. The separator is a membrane made of porous polymer that prevents electrons from passing through. Both electrodes and separator are filled up with non-aqueous electrolyte LiPF₆ which is dissolved in 1:1 EC (ethylene carbonate):DEC (dimethyl carbonate). During the charge/discharge process, electrochemical reactions occur between the electrodes and electrolyte. These reactions are:



where Li^+ is the lithium-ion, x and y are the number of moles of lithium present in the graphite and iron phosphate structures, respectively, and z is the number of moles of lithium-ions.

In the COMSOL software, the 3D Lithium-Ion Battery Module and 3D Heat Transfer in Solids Module were coupled with a multiphysics module called Electrochemical Heating.

2.2. Electrochemical Kinetics

The lithium insertion equation in Eq. 1 below, determines the local current density:

$$i_{loc} = i_0 \left\{ \exp\left(\frac{\alpha_a F \eta}{RT}\right) - \exp\left(-\frac{\alpha_c F \eta}{RT}\right) \right\} \quad (1)$$

where the local surface overpotential is η , the Faraday constant is F , the anodic and cathodic charge transfer coefficients are α_a and α_c , and the exchange current density i_0 which is shown below in Eq. 2:

$$i_0 = i_{0,ref} \left(\frac{2c_{s,surf}}{c_{s,max}} \right)^{\alpha_c} \left(\frac{2(c_{s,max} - c_{s,surf})}{c_{s,max}} \right)^{\alpha_a} \left(\frac{c_l}{c_{l,ref}} \right)^{\alpha_a} \quad (2)$$

where $c_{s,surf}$ is the lithium concentration on the surface of active particles, $c_{s,max}$ is the maximum concentration of lithium in the active electrodes, $c_{l,ref}$ is the reference salt concentration in the electrolyte, and $i_{0,ref}$ is the reference exchange current density value.

η local surface overpotential equation in Eq. 3 is given below:

$$\eta = \phi_s - \phi_l - U_{eq} \quad (3)$$

where ϕ_s is the solid phase potential, ϕ_l is the electrolyte phase potential, and U_{eq} is the open-circuit potential of the electrode.

2.3. Charge Conservation

The following are equations for charge conservation for electrodes:

$$Q_l + Q_s = 0 \quad (4)$$

$$Q_l = \nabla \cdot i_l = S_a i_{loc} \quad (5)$$

$$Q_s = \nabla \cdot i_s = -S_a i_{loc} \quad (6)$$

where Q_l and Q_s are the electrical charge in electrolyte and electrode respectively, i_l is the ionic current density in the electrolyte phase, i_s is the electrical current density in the solid phase, and S_a is the specific surface area.

Ohm's law is applied for the transport of electrons in the solid phase and is given below in Eq. 7:

$$i_s = -\sigma_{s,eff} \nabla \phi_s \quad (7)$$

where $\sigma_{s,eff}$ refers to the effective electrical conductivity of the solid phase.

The following Eq. 8 gives the transport of lithium ions in the electrolyte:

$$i_l = -\sigma_{l,eff} \nabla \phi_l + \left(\frac{2\sigma_{l,eff}RT}{F} \right) \left(1 + \frac{\partial \ln f_{\pm}}{\partial \ln c_l} \right) (1 - t_+) \nabla c_l \quad (8)$$

where $\sigma_{l,eff}$ is the effective ionic conductivity of the electrolyte phase, R is the universal gas constant, T is the temperature of the electrolyte, $f_{\pm}$ is the average molar activity coefficient, and t_+ is the transferring number of lithium ions in the electrolyte phase.

2.4. Mass Conservation

The mass conservation of lithium in the spherical active material particle is given below in Eq. 9:

$$\frac{\partial c_s}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} \left(-r^2 D_s \frac{\partial c_s}{\partial r} \right) = 0 \quad (9)$$

where c_s is the concentration of lithium in the active material particles of the electrode, t is time, D_s is the diffusion coefficient of lithium in the solid phase, and r is the radial coordinate inside a spherical particle.

The mass conservation of lithium ions in the electrolyte is given below in Eq. 10:

$$\varepsilon_l \frac{\partial c_s}{\partial t} + \nabla \cdot J_l = \frac{S_a J_n}{F} \quad (10)$$

$$J_l = -D_{l,eff} \nabla c_l + \frac{i_l \cdot t_+}{F} \quad (11)$$

where J_l is the molar flux of lithium ions, $D_{l,eff}$ is the diffusion coefficient of lithium ions in the electrolyte, ε_l is the volume fraction of the electrolyte phase, and subscript n is the direction.

2.5. Energy Balance

There are three types of heat generation in the battery: reversible entropic heat, irreversible electrochemical reaction heat, and ohmic heat. The energy balance equation (Eq. 12) and their equations (Eq. 13-15) are given below respectively:

$$\rho c_p \frac{\partial T}{\partial t} - \lambda \nabla^2 T = q_{rea} + q_{act} + q_{ohm} \quad (12)$$

$$q_{rea} = S_a i_{loc} T \frac{\partial U_{eq}}{\partial T} \quad (13)$$

$$q_{act} = S_a i_{loc} \eta \quad (14)$$

$$q_{ohm} = -i_s \cdot \nabla \phi_s - i_l \cdot \nabla \phi_l \quad (15)$$

Furthermore, all of the equations related to the energy balance Eq. 12 are inserted in Eq. 16:

$$\rho c_p \frac{\partial T}{\partial t} - \lambda \nabla^2 T = S_a i_{loc} \left(T \frac{\partial U_{eq}}{\partial T} + \eta \right) - i_s \cdot \nabla \phi_s - i_l \cdot \nabla \phi_l \quad (16)$$

2.6. Parameters That Depend on Temperature and Concentration

The temperature and state of charge-dependent open circuit potential equation are given below in Eq. 16. In addition, the concentration-dependent state of charge formula for each electrode is given below in Eq. 17:

$$U_{eq} = U_{eq,ref}(SOC, T_{ref}) + \frac{\Delta S(SOC)}{F} (T - T_{ref}) \quad (17)$$

$$SOC = \frac{c_s}{c_{s,max}} \quad (18)$$

where $U_{eq,ref}(SOC, T_{ref})$ is the open circuit potential under the state of charge and reference temperature, T_{ref} is the reference temperature, and $\Delta S(SOC)$ is the state of charge-dependent entropy change.

Empirical calculation of electrolyte's temperature and concentration-dependent ionic conductivity is given below in Eq. 19 [11]:

$$\begin{aligned}
\sigma_l(c_l, T) = & 10^{-4}c_l \times 1.2544 \times (-8.2488 + 0.053248T \\
& - 0.00002987T^2 + 0.26235 \times 0.001c_l \\
& - 0.0093063 \times 0.001c_lT + 0.000008069 \times 0.001c_lT^2 \\
& + 0.22002 \times 10^{-6}c_l^2 - 0.0001765 \times 10^{-6}c_l^2T)^2
\end{aligned} \tag{19}$$

Temperature and concentration-dependent empirical diffusion coefficient in the electrolyte are given in Eq. 20 [11]:

$$D_l(c_l, T) = 10^{\left(-4.43 - \left(\frac{54}{T-229-5 \times 0.001c_l}\right) - 0.22 \times 0.001c_l\right) - 4} \tag{20}$$

Temperature-dependent diffusion coefficients in each electrode are given below [11, 14]:

$$D_{s,pe} = 1.25 \times 10^{-15} \exp\left(\frac{E_{ad}}{R} \left(\frac{1}{T_{ref}} - \frac{1}{T}\right)\right) \tag{21}$$

$$D_{s,ne} = 1.4523 \times 10^{-13} \exp\left(\frac{E_{ad}}{R} \left(\frac{1}{T_{ref}} - \frac{1}{T}\right)\right) \tag{22}$$

where E_{ad} is the diffusion activation energy of positive and negative electrodes.

2.7. Boundary and Initial Conditions

Boundary and initial conditions are given for each interface below. Electrode-separator interface conditions are:

$$\begin{aligned}
n \cdot i_s &= 0, & n \cdot i_l|_{pe} &= n \cdot i_l|_{ne}, \\
n \cdot J_l|_{pe} &= n \cdot J_l|_{ne}, & n \cdot q|_{pe} &= n \cdot q|_{ne}
\end{aligned} \tag{23}$$

Electrode-current collector interface conditions are:

$$n \cdot i_l = 0, \quad n \cdot i_s \big|_{pe} = n \cdot i_s \big|_{ne}, \quad (24)$$

$$n \cdot J_l = 0, \quad n \cdot q \big|_{pe} = n \cdot q \big|_{ne}$$

The positive current collector tab boundary is the input of applied current and its condition is:

$$n \cdot i_s = i_{app} \quad (25)$$

The negative current collector tab boundary is grounded and its condition is:

$$\phi_s \big|_{ncc,tab} = 0 \quad (26)$$

The working voltage of the cell is given below in Eq. 27:

$$E_{cell} = \phi_s \big|_{pcc,tab} - \phi_s \big|_{ncc,tab} \quad (27)$$

The cell's outer surface is insulated and no convective heat flux is applied:

$$n = x: -\lambda_{\perp} \frac{\partial T}{\partial n} = 0 \quad (28)$$

$$n = y, z: -\lambda_{\perp} \frac{\partial T}{\partial n} = 0 \quad (29)$$

where $\lambda_{\perp}$ is the cross-plane thermal conductivity along the thickness direction, $\lambda_{\perp}$ is the plane thermal conductivity along the length-width direction.

The initial conditions of single cell model are:

$$c_s = c_{s,0}, \quad c_l = c_{l,0}, \quad T = T_{ref} \quad (30)$$

Below, 20 Ah LFP battery base model parameters are shown in Table 2.1 [10,11,15-17]:

Table 2.1: 20 Ah LFP battery base model parameters for charge.

Parameter	Unit	Positive CC	Cathode	Separator	Anode	Negative CC	Ref.
δ_i	μm	16	125	25	150	16	[10, 11]
r_0	μm	-	1.15	-	14.75	-	[10, 11]
$c_{s,0}$	$\text{mol}\cdot\text{m}^{-3}$	-	22107	-	1064	-	initial
$c_{s,max}$	$\text{mol}\cdot\text{m}^{-3}$	-	26390	-	31540	-	[10, 11]
$c_{l,0}$	$\text{mol}\cdot\text{m}^{-3}$	-	-	1000	-	-	[15]
ε_s		-	0.435	-	0.56	-	[10, 11]
$i_{0,ref}$	$\text{A}\cdot\text{m}^{-2}$	-	0.7	-	0.96	-	[16,17]
ε_l		-	0.28	0.4	0.3	-	[10, 11]
α_a		-	0.5	-	0.5	-	[10, 11]
α_c		-	0.5	-	0.5	-	[10, 11]
D_s	$\text{m}^2\cdot\text{s}^{-1}$	-	Eq. 21	-	Eq. 22	-	[11, 14]
D_l	$\text{m}^2\cdot\text{s}^{-1}$	-	-	Eq. 20	-	-	[10, 11]
E_{aD}	$\text{kJ}\cdot\text{mol}^{-1}$	-	20	-	68	-	[10, 11]
σ_s	$\text{S}\cdot\text{m}^{-1}$	3.774×10^7	11.8	0	100	5.998×10^7	[10]
σ_l	$\text{S}\cdot\text{m}^{-1}$	-	-	Eq. 19	-	-	[10, 11]
t_+		-	-	0.363	-	-	[10, 11]
$\lambda_{\perp}$	$\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	238	1.79	0.334	1.06	400	[10]
$\lambda_{\parallel}$	$\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	238	23	0.334	31	400	[10]
ρ	$\text{kg}\cdot\text{m}^{-3}$	2700	1500	1009	2660	8900	[10, 11]
c_p	$\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$	903	1260.2	1978	1437.4	385	[10]
T_{ref}	K	-	-	303.15	-	-	[10]
F	$\text{C}\cdot\text{mol}^{-1}$	-	-	96478	-	-	-
R	$\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$	-	-	8.3145	-	-	-

2.8. Selection of Parameters

Our paper's subject is to investigate the most effective parameters for heat generation. The parameters affecting heat generation are categorized into two: Chemical parameters and geometric parameters.

Chemical parameters are the porosity of electrodes (ε_s , ε_{pe} , $\varepsilon_{s,ne}$), lithium concentration of electrodes ($c_{s,max,pe}$, $c_{s,max,ne}$), and salt concentration of electrolyte ($c_{l,0}$), whereas geometric parameters are the thickness of electrodes (δ_{pe} , δ_{ne}). Since the sum of the porosities equals 0.995, positive electrode porosity changed with the negative electrode porosity range.

Seven parameters in total are changed in the range of $\pm 20\%$. The parametric switch ranges can be seen in Table 2.2. A total of 75 simulations were done when 1, 2, and 4C current rates were included.

Table 2.2: Parametric switch ranges.

		Switch Ranges				
		-20%	-10%	0	+10%	+20%
Chemical Parameters	$\varepsilon_{s,pe}$	0.323	0.379	0.435	0.491	0.547
	$\varepsilon_{s,ne}$	0.448	0.504	0.560	0.616	0.672
	$C_{s,max,pe}$	21112	23751	26390	29029	31668
	$C_{s,max,ne}$	25232	28386	31540	34694	37848
	$C_{l,0}$	800	900	1000	1100	1200
Geometric Parameters	δ_{pe}	100	112.5	125	137.5	150
	δ_{ne}	120	135	150	165	180

3. VALIDATION OF THE MODEL

COMSOL Multiphysics 6.0 finite element software was used to simulate a 3D coupled electrochemical-thermal model. All of the numerical simulations are performed on a computer that has a six-core processor with a 3.3 GHz base clock and 16 GB RAM (random access memory). Mesh properties of the 1 Ah LFP single cell model for validation are 5700 vertices, 4720 hexahedra, 3090 quads, 566 edge elements, 36 vertex elements, 0.9183 average volume ratio, and 0.1635 element volume ratio. Mesh is created with the mapped surface at the negative current collector, then swept method is applied. This method has a much higher mesh calculation speed than automatic mesh by the program. The mesh view of the single cell is shown in Figure 3.1 below:

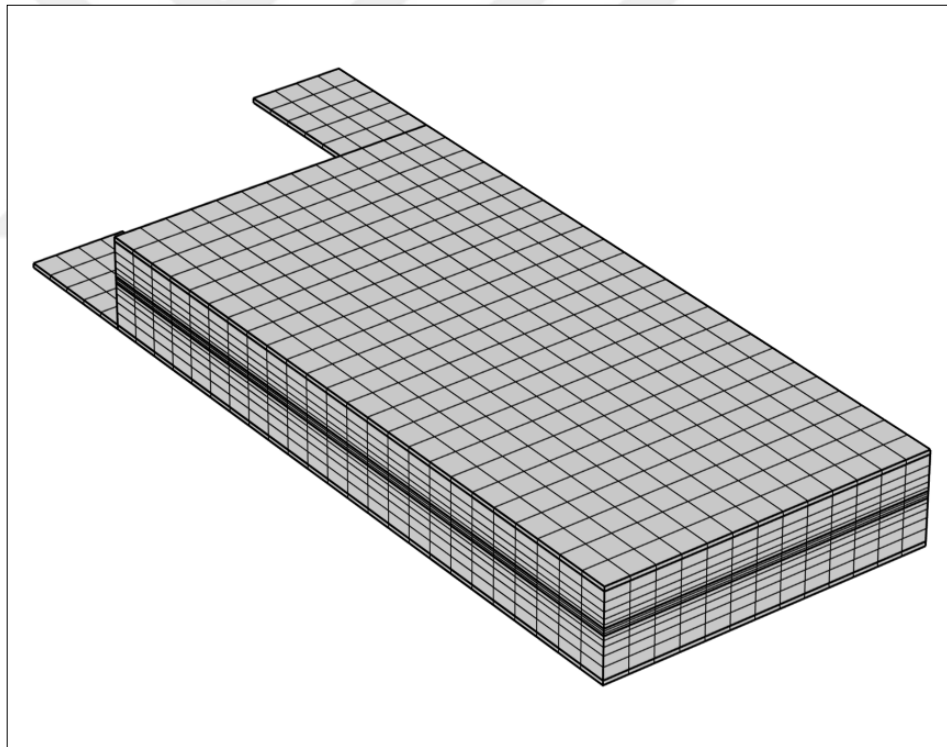


Figure 3.1: Mesh view of the single cell.

Charge simulation started with 7% SOC and ran 3312 seconds with 1 Ampere constant current to 99% SOC was completed in 34 minutes 51 seconds in real-time. Using the initial cell charge distribution module on COMSOL was useful to define initial SOC instead of manually inputting the initial concentration of each electrode.

In addition to that, initial cell voltage and current distribution on the cell are also automatically calculated by COMSOL's current distribution initialization study option. Single-cell modeled in one component which has a lithium-ion battery design module, heat transfer in solids module, and electrochemical heating module which couples two modules together. The lithium-ion battery design module is generating cell voltage and volumetric heat generation data in 3D, and heat transfer in the solids module uses these heat data via an electrochemical heating module to generate temperature distribution on a 3D cell.

Electrochemical and thermal validation was studied by Alipour et al. [10] for 1C charge and 303.15 K ambient temperature both experimentally and numerically. The model that is developed in this thesis is validated by the results of Alipour et al. [10]. The voltage results of the thesis are compared with the model [10] and the comparison is given in Figure 3.2. As seen in the graph, initial and nominal voltages are the same but charge durations are slightly different. Our simulation and experimental durations are 3312 and 3640 seconds, respectively. Despite the different durations, peak values of voltages are 3.65 and 3.85 V which are similar.

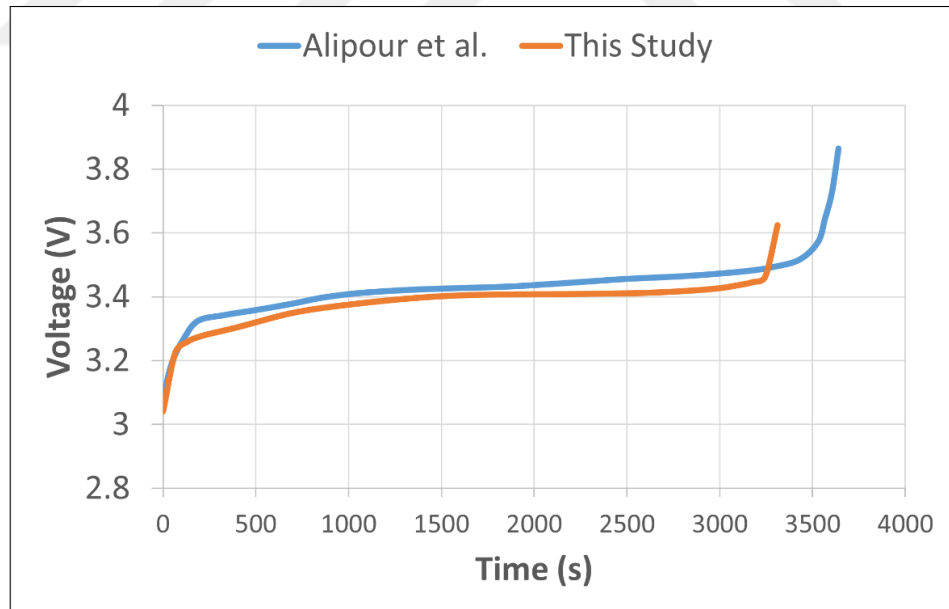


Figure 3.2: Single cell voltage comparison graph at 1C charge for validation.

Due to a single cell layer model, convective heat flux condition is assumed as negligible and not applied to the exterior boundaries. It should be the multi-layered battery model to define the boundaries of the outer cell for proper convection.

Therefore, the temperature of the battery cell rising under the same conditions is found as different when compared to Ref [10]. However, the temperature distributions are seen as consistent. The temperature distribution of the base model can be seen in Figure 3.3. The initial cell temperature is taken as 303.15 K. After the 1C charge process, the average temperature rises from the initial value of 303.15 K to 316.8 K. The negative tab is at 316.9 K whereas the positive tab is at 317.15 K. The positive tab is the hottest part of the cell due to the applied charge current. The maximum and minimum temperature differences on the cell are low as 0.48 K because of the low current charge rate.

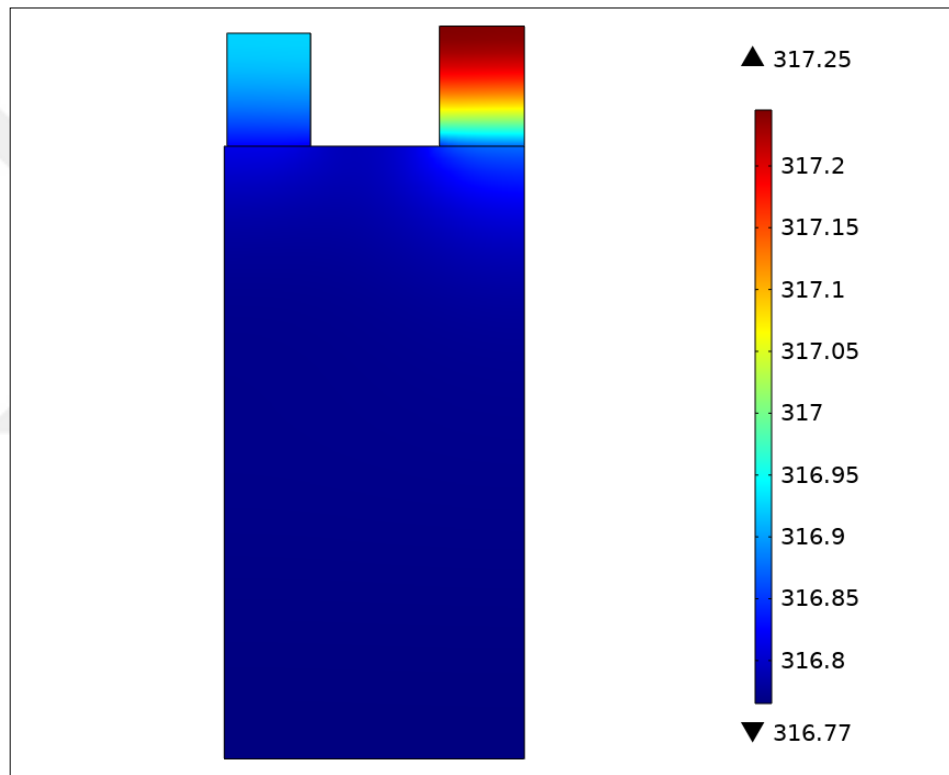


Figure 3.3: Single cell temperature distribution at 1C charge for validation.

Furthermore, a multicell model which has 20 cells with convective heat flux over the surfaces was simulated for a more detailed distribution of temperature elevation. It was assumed that every layer is equivalent without randomness at open-circuit voltages and heat generations. The 20-layered cell model includes two COMSOL multiphysics components: The first component has the same modules and mesh properties as the single-cell module, and the other one has the multicell geometry and heat transfer in the solids module. The second component takes volumetric heat

generation data from the first component and generates temperature distribution of the whole battery which has 20 cells. In this case, 1C, and 2C discharge currents were applied and convective heat flux which is $8 \text{ W}\cdot\text{m}^{-2}\cdot\text{K}^{-1}$ is assigned to the exterior boundaries of the battery.

Voltage values of multicell are validated with Ref [10]. The compared voltage changes during discharge for 1C, and 2C between Ref [10] and our study is shown in Figure 3.4. Voltage drops do not start at similar times due to slightly different experiment durations but both voltages stop at similar values. Considering discharge capacity when plotting the data, both 1 and 2C rate voltages have similar characteristics in that starting voltage is 3.3 V whereas the cut-off voltage is 1.8 V.

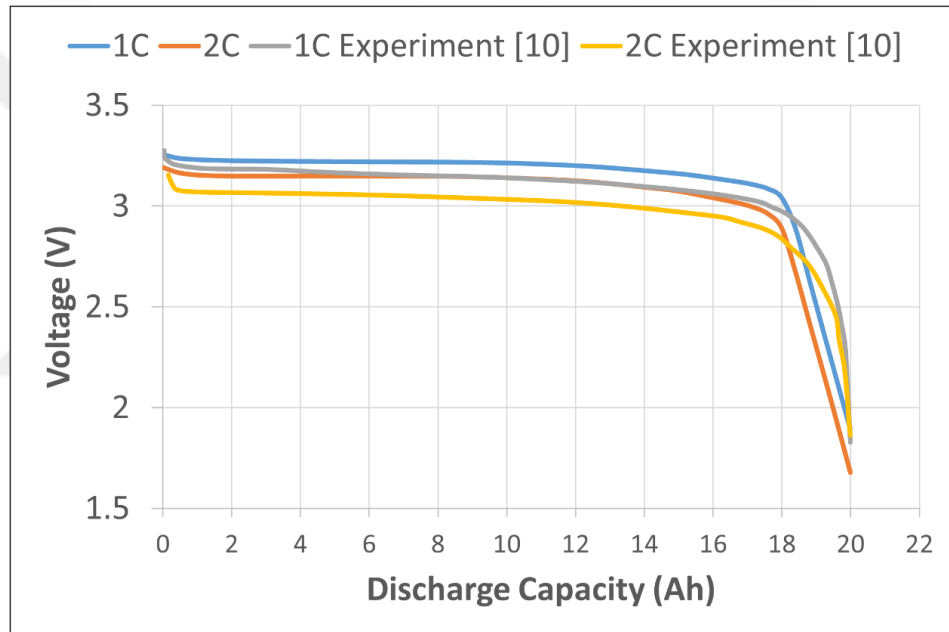


Figure 3.4: Multicell voltage graph at 1-2C discharge for validation.

The thickness of the cell was scaled by 10 times after the completed simulation for visual purposes only at the camera properties and the 3D temperature distribution at 2C discharge is given in Figure 3.5. Tabs are ignored since the multicell simulation is only for temperature elevation validation purposes. The average battery temperature is 315.25 K where the maximum value is 315.38 K and the minimum value is 315.05 K.

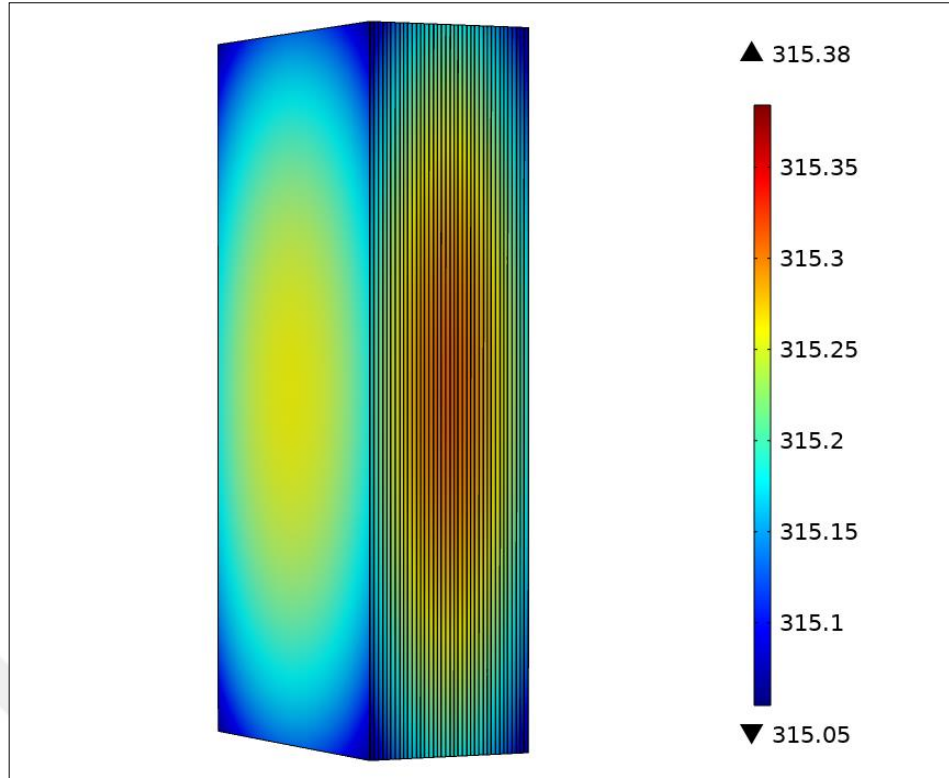


Figure 3.5: Multicell temperature distribution at 2C discharge with convective heat flux for validation.

Figure 3.6 [10] illustrates the Temperature elevation comparison graph. Final temperature differences at 1 and 2C are increasing with the discharge current which is 0.01 and 0.64 K, respectively.

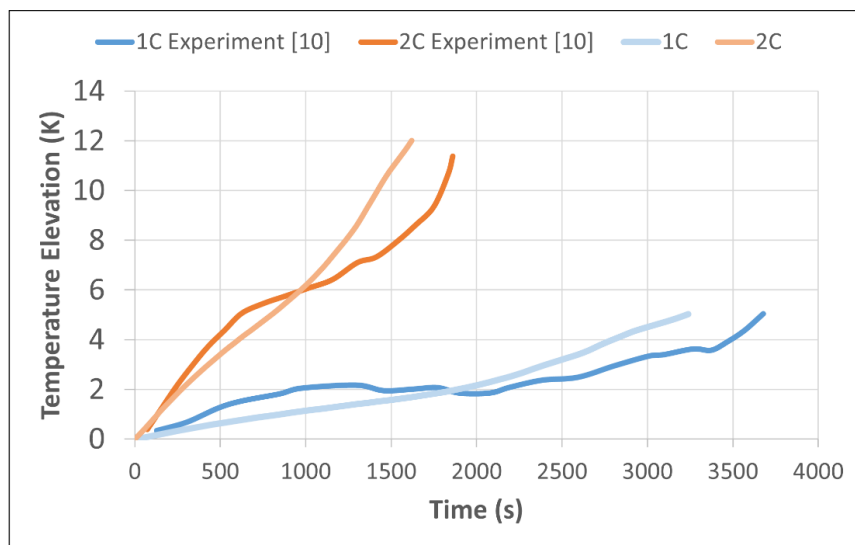


Figure 3.6: Multicell temperature elevation comparison graph at discharge for validation.

4. RESULTS AND DISCUSSION

4.1. Comparison of 3D and 1D Electrochemical Models

Firstly, it is important to take into account the comparison of 1D and 3D electrochemical models. Most of the researchers created the electrochemical model in 1D in their studies. In our recent conference paper [12], differences between 1D and 3D electrochemical models are investigated. In this paper, two separate models under the same conditions are modeled. In Figure 4.1, 1D (a) and 3D (b) schematic geometries are represented. In 1D, thickness and numerical overall area are assigned to the model whereas in 3D, thickness and 3D geometry are assigned to the model.

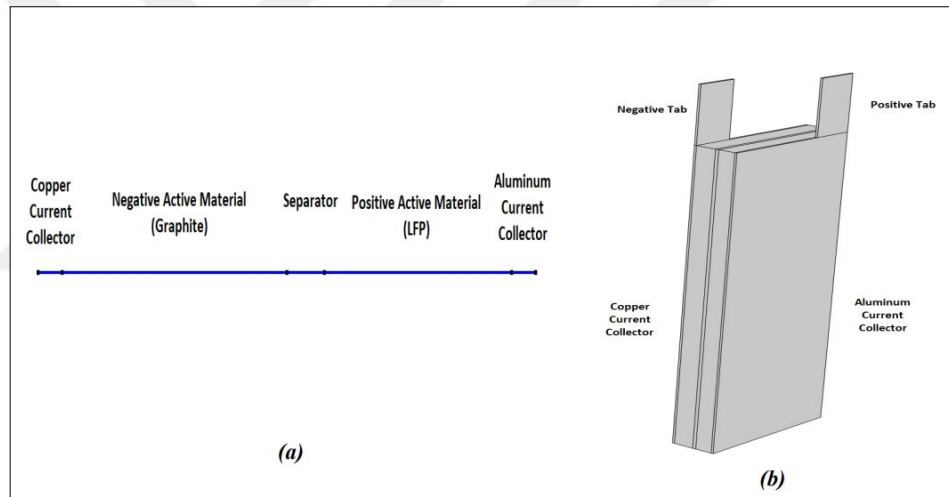


Figure 4.1: Schematic of 1D (a) and 3D (b) lithium-ion cell geometry.

Both 1D and 3D electrochemical models generate heat data and insert their data into a 3D thermal model to calculate temperature distribution, as seen in Figure 4.2.

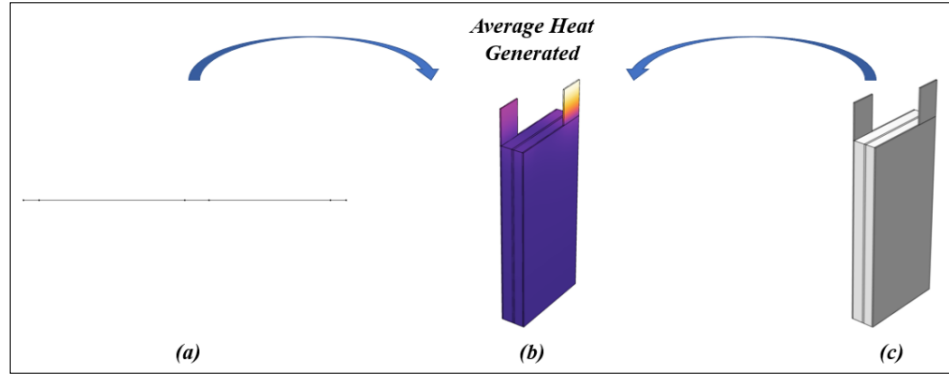


Figure 4.2: Schematic representation of the 1D electrochemical model (a), 3D electrochemical model (c), and 3D thermal model as a coupled model (b).

The voltage change of the models under the same conditions for each 1D and 3D model shows the same voltage change, as seen in Figure 4.3.

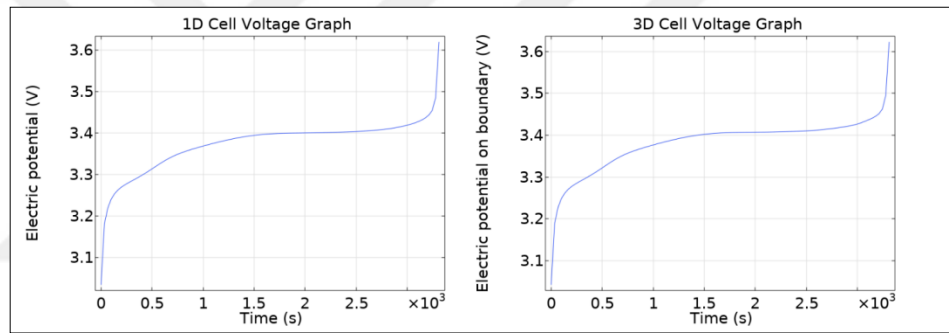


Figure 4.3: 1D and 3D single cell voltage change at 1C charge.

As seen in Figure 4.4 [12], the single-cell temperature distributions for 1D and 3D electrochemical models are shown. Temperature distributions are 316 and 316.8 K for 1D and 3D models, respectively. Due to the modeling of the tabs and current collectors in the 1D model, inserting heat generation data from the 1D lithium-ion battery model to heat transfer in the solids module causes isothermal temperature distribution, as can be seen in Figure 4.4 (a). The tabs and current collectors can not be considered in 1D electrochemical modeling. As seen, the temperature distribution does not differ (around 1 K) if it is modeled in 1D or 3D form. In addition to that, this modeling technique greatly decreases the real-time computation time.

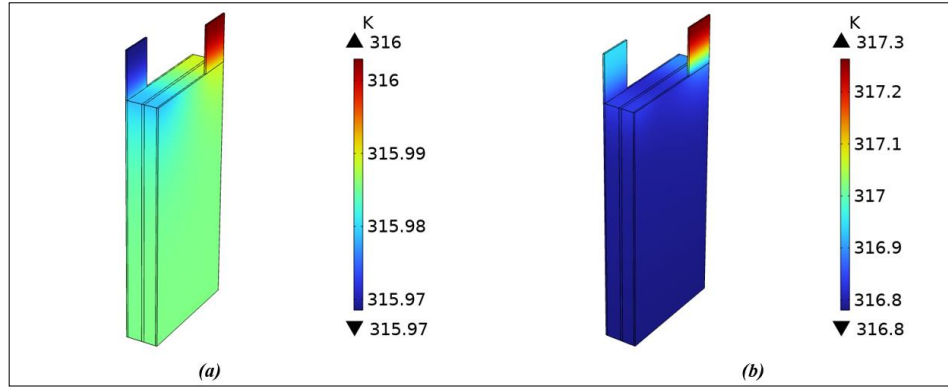


Figure 4.4: Single cell temperature distribution at 1C charge without convection, (a) 1D, (b) 3D.

Furthermore, 20 layered cells are compared, as seen in Figure 4.5 below. Unlike isothermal temperature distribution in the 1D single-cell model, temperature change in the 1D model has the same characteristics as the 3D model. On the other hand, a 1.15 K temperature difference occurs between 1D and 3D models.

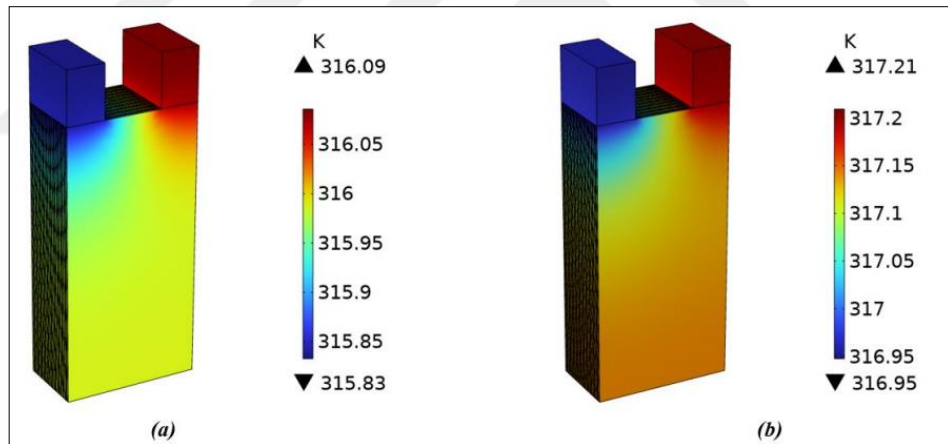


Figure 4.5: 20 layered cell temperature distribution at the end of 1C charge, (a) 1D, (b) 3D.

4.2. Analysis of Parameters

Parameters mentioned in section 2.8 are analyzed individually to investigate their effect on the heat generation of the battery cell. Model input parameters are mentioned in section 2.7 in detail. In addition to inputs, simulations were performed at 1, 2, and 4C current rates. Unlike the base model that is validated with Alipour et

al. [10] experimental results, ending SOC is set to 90% due to maintaining the same conditions for all simulations. The total charge simulation time decreased from 3312 to 2988 seconds in 1C. Besides, for 2C and 4C charge rates, the charge time is found as 1494 and 747 seconds for each simulation, respectively.

The final cell voltage, final volume-averaged temperature, and the final overall heat generation are considered the simulation outputs. Cell voltage is important because the change of the specified parameters affects the capacity of the cell thus the capacity of the cell changes. Keeping cell voltage inside the specified ranges is important for the temperature and heat generation values of the cell.

As shown in the previous chapter, parameters are considered in two groups; chemical and geometrical parameter sets.

As grouped in the chemical parameter set, the change of the porosity of electrodes ($\varepsilon_{s,pe}, \varepsilon_{s,ne}$), lithium concentration of electrodes ($C_{s,max,pe}, C_{s,max,ne}$), and salt concentration of electrolyte ($C_{l,0}$) on heat generation are analyzed and the results are given separately for each parameter are given below. Also, the change of the geometric parameters such as the thickness of electrodes (δ_{pe}, δ_{ne}) are analyzed and the results of the change of these parameters on heat generation are given in detail.

4.2.1. The Porosity of the Electrodes

Firstly, the results of the change of the porosity of electrodes ($\varepsilon_{s,pe}, \varepsilon_{s,ne}$) on heat generation are shown in Table 4.1. As given in Table 4.1, the gray cells represent base model outputs. The above rows over the gray row represent the decrease of the porosity of electrodes as down to -10% and -20% whereas the below rows over the gray row represent the increase of the porosity of electrodes as up to +10% and +20%. The change in the values of the cell voltage, volume averaged temperature, and overall heat generation of the battery cell are tabulated in Table 4.1 for 1C, 2C, and 4C charge rates. The right column of Table 4.1 represents the change of the heat generation of that row values from base gray row values. As seen, the change of the porosity of electrodes highly affects the heat generation up to more than 35%, 45%, and 88% for 1C, 2C, and 4C charge rates, respectively.

Table 4.1: Results of changing porosity of electrodes.

C rate	$\varepsilon_{s,ne}$	%	Cell Voltage (V)	Temperature (K)	Heat (W)	Change of Generated Heat from Base Model
1	0.448	-20%	3.49	322.3	0.225	36.1%
	0.504	-10%	3.47	318.5	0.185	11.7%
	0.560	0	3.43	314.7	0.166	
	0.616	+10%	3.41	311.2	0.134	-18.8%
	0.672	+20%	3.40	308.0	0.104	-37.3%
2	0.448	-20%	3.60	334.5	0.736	44.3%
	0.504	-10%	3.56	328.6	0.610	19.5%
	0.560	0	3.52	323.0	0.510	
	0.616	+10%	3.49	317.9	0.408	-20.1%
	0.672	+20%	3.46	313.3	0.307	-39.9%
4	0.448	-20%	3.91	356.4	3.031	87.9%
	0.504	-10%	3.74	345.2	2.043	26.7%
	0.560	0	3.68	336.4	1.613	
	0.616	+10%	3.63	328.6	1.282	-20.5%
	0.672	+20%	3.58	321.7	0.963	-40.3%

To understand the change in the temperature distribution and heat generation of the battery cell by changing the value of the porosity of electrodes, Figure 4.6 and Figure 4.7 are given. The overall heat generation on 1C, 2C, and 4C charge rates and the change of the temperature of the battery cell with the change of the porosity of electrodes are given in Figure 4.6 and Figure 4.7, respectively. On the other hand, the figures (Figure 4.6 and Figure 4.7) are useful to visualize both temperature and heat generation values. Linearity can be seen in both figures. Also, an exponential curve occurs on 4C heat generation values. Overall, decreasing the porosity of the positive electrode causes to preventing of lithium ions travel. But, if the nominal cell voltage is maintained at a certain level with other configurations, it could have a huge useful effect for decreasing cell temperature.

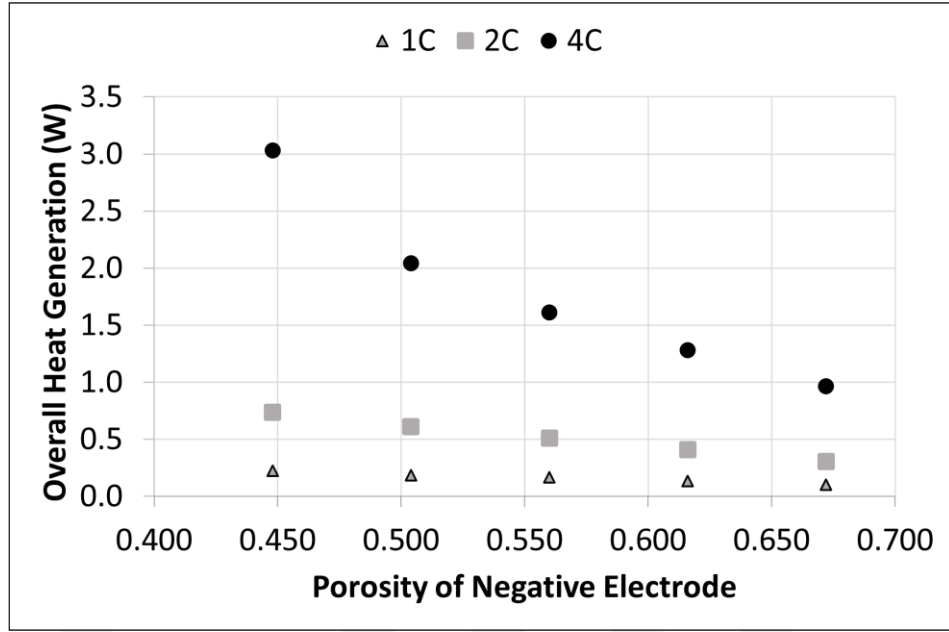


Figure 4.6: Overall heat generation graph at a porosity of electrodes.

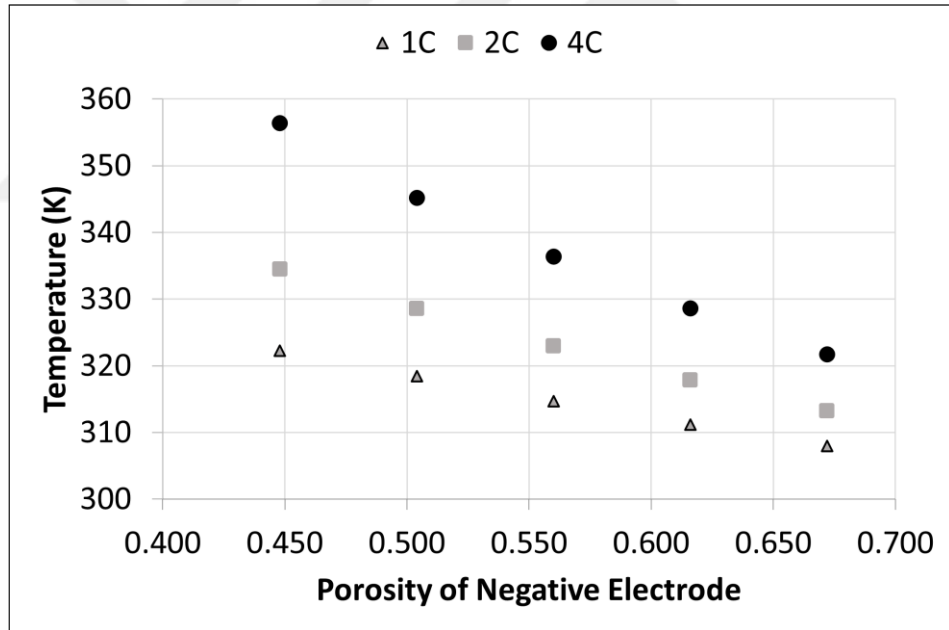


Figure 4.7: Average temperature graph at a porosity of electrodes.

4.2.2. The Concentration of the Positive Electrode

Secondly, the lithium-ion concentration of the positive electrode ($C_{s, max, pe}$) is the other chemical parameter to analyze. The same table and figure templates are also generated for this parameter and are shown in Table 4.2, Figure 4.8, and Figure 4.9.

The change in the concentration of the positive electrode is another parameter that highly affects heat generation. For 1C, 2C, and 4C charge rates, around 28%, 33%, and 41% increase in heat generation is found if a $\pm 20\%$ change occurs in the concentration of positive electrodes, respectively. Considering the 1C rate, increasing the concentration of the positive electrode (the concentration of the negative electrode remains the same), increases the overall heat generation as well. From 21112 to 31668 $\text{mol}\cdot\text{m}^{-3}$ concentration, generated heat almost doubled. And the effect of this parameter is nearly 1.5 times when considering changing ranges. This value can be seen clearly at higher current rates as well. As a result of the generated heat, the temperature differences are also quite large as 9.3 K at a 1C rate. Even if this parameter has a big impact on heat generation and temperature, final cell voltage differences are not changing significantly. On the other hand, cell capacity is affected by this parameter. Whether increasing or decreasing the value of the concentration of the positive electrode should be determined before the manufacturing process. Decreasing concentration helps to reduce heat generation whereas bigger cells or thicker layers of electrodes are required to achieve the same cell capacity.

Table 4.2: Results of changing lithium-ion concentration of positive electrode.

C rate	$C_{s, \max, pe}$	%	Cell Voltage (V)	Temperature (K)	Heat (W)	Change of Generated Heat from Base Model
1	21112	-20%	3.40	310.3	0.119	-28.1%
	23751	-10%	3.41	312.4	0.140	-15.3%
	26390	0	3.43	314.7	0.166	
	29029	+10%	3.44	317.1	0.191	15.3%
	31668	+20%	3.46	319.6	0.212	28.0%
2	21112	-20%	3.48	316.1	0.356	-30.1%
	23751	-10%	3.50	319.4	0.432	-15.4%
	26390	0	3.52	323.0	0.510	
	29029	+10%	3.54	326.8	0.593	16.1%
	31668	+20%	3.57	330.8	0.678	32.9%
4	21112	-20%	3.61	325.3	1.120	-30.5%
	23751	-10%	3.64	330.6	1.355	-16.0%
	26390	0	3.68	336.4	1.613	
	29029	+10%	3.72	342.7	1.908	18.3%
	31668	+20%	3.76	349.5	2.268	40.7%

The change of the temperature distribution and heat generation of the battery cell by changing the value of the concentration of the positive electrode is given in Figure 4.8 and Figure 4.9. The same linearity as seen from the change in the porosity of the electrodes can be seen in both figures.

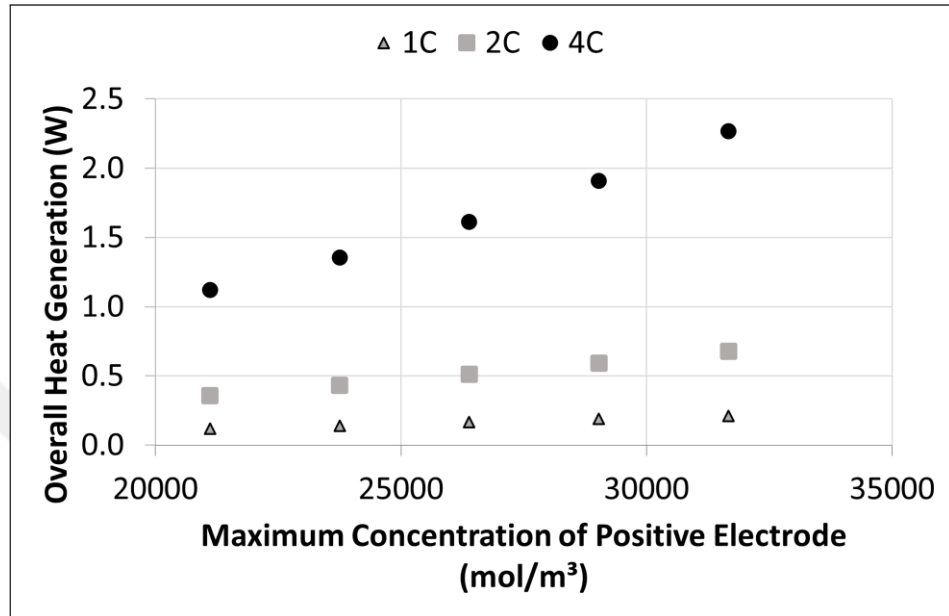


Figure 4.8: Overall heat generation graph at lithium-ion concentration of positive electrode.

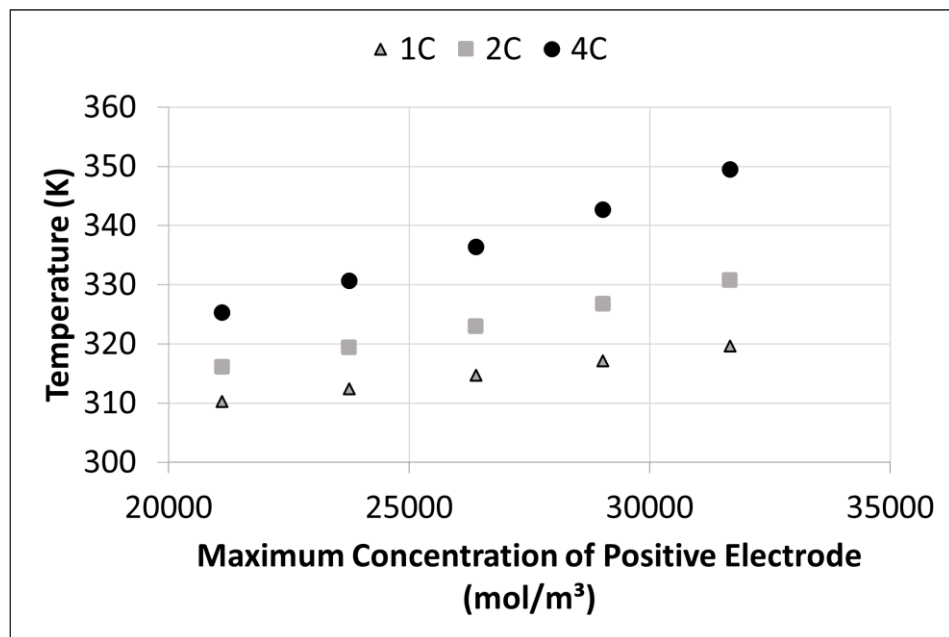


Figure 4.9: Average temperature graph at lithium-ion concentration of positive electrode.

4.2.3. The Concentration of the Negative Electrode

For the change of lithium-ion concentration of the negative electrode ($C_{s, max, ne}$), results are shown below in Table 4.3. The same table and figure configurations are applied to this parameter as well. If the first result at the 1C rate (20% decrease at 1C), is not considered, the rest of the results show that there is no significant change occurring in heat generation (around 0%, 4%, and 0.5% for each current rate). The positive electrode is the main source of the lithium material, whereas the negative electrode which is like the adsorbent material, absorbs the lithium-ions during the electrochemical reactions. Overall, there will be no significant change in heat generation if the concentration of the positive electrode changes.

Table 4.3: Results of changing lithium-ion concentration of negative electrode.

C rate	$C_{s, max, ne}$	%	Cell Voltage (V)	Temperature (K)	Heat (W)	Change of Generated Heat from Base Model
1	25232	-20%	3.45	315.3	0.148	-10.6%
	28386	-10%	3.44	315.0	0.163	-1.6%
	31540	0	3.43	314.7	0.166	
	34694	+10%	3.42	314.4	0.165	0.2%
	37848	+20%	3.42	314.0	0.166	0.0%
2	25232	-20%	3.54	323.5	0.491	-3.9%
	28386	-10%	3.53	323.3	0.504	-1.2%
	31540	0	3.52	323.0	0.510	
	34694	+10%	3.51	322.7	0.514	0.7%
	37848	+20%	3.51	322.3	0.514	0.7%
4	25232	-20%	3.69	337.0	1.620	-0.5%
	28386	-10%	3.68	336.7	1.612	-0.0%
	31540	0	3.68	336.4	1.613	
	34694	+10%	3.68	336.1	1.617	0.2%
	37848	+20%	3.67	335.8	1.615	0.2%

Also, Figure 4.10 and Figure 4.11 illustrate the lithium-ion concentration of the negative electrode. As seen in both figures, a straight line occurs despite the concentration change of the negative electrode for all C rates.

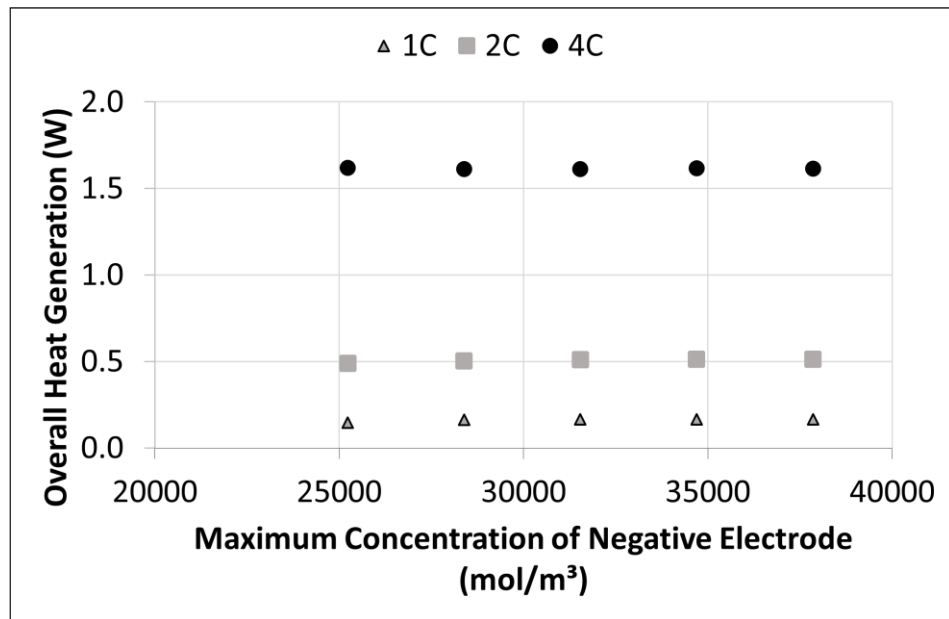


Figure 4.10: Overall heat generation graph at lithium-ion concentration of negative electrode.

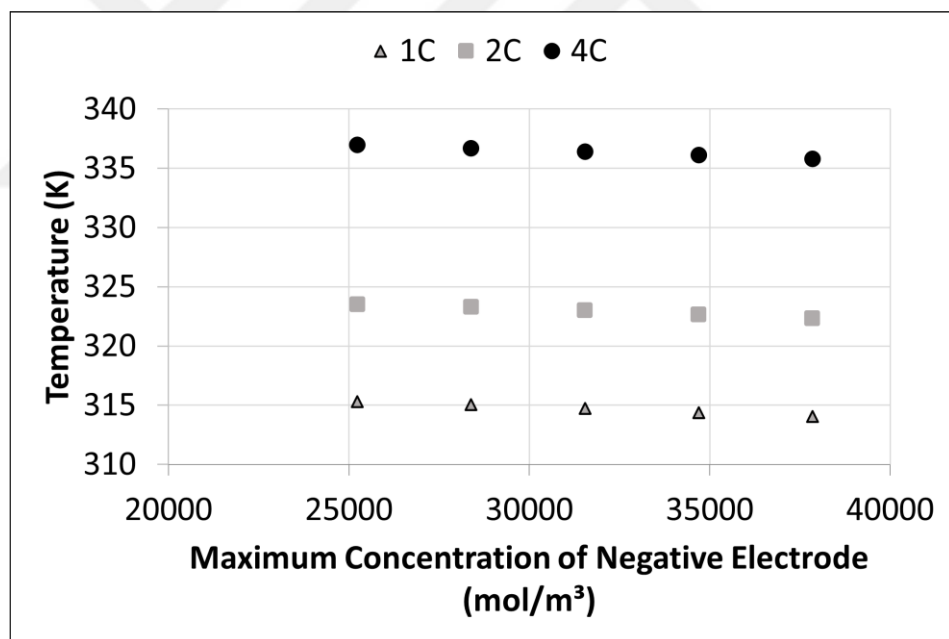


Figure 4.11: Average temperature graph at lithium-ion concentration of negative electrode.

4.2.4. Salt Concentration of Electrolyte

The next parameter to analyze is the change in salt concentration of electrolyte. Table 4.4, Figure 4.12, and Figure 4.13 show the results if the salt concentration of

electrolyte changes. As seen in Table 4.4, despite the 20% change in salt concentration, there is no significant change in heat generation as 1.4%, 1.9%, and 3.9% for each current rate, respectively. This leads to small temperature changes only in decimal. In addition, cell voltages are not affected at all. In general, it can be said that salt concentration is not an important parameter for the heat generation of the cell. But further investigations are needed to analyze its effect in cycle loads and aging experiments.

Table 4.4: Results of changing the salt concentration of electrolyte.

C rate	$c_{l,0}$	%	Cell Voltage (V)	Temperature (K)	Heat (W)	Change of Generated Heat from Base Model
1	800	-20%	3.43	314.9	0.168	1.4%
	900	-10%	3.43	314.8	0.167	0.6%
	1000	0	3.43	314.7	0.166	
	1100	+10%	3.43	314.7	0.165	-0.5%
	1200	+20%	3.42	314.7	0.164	-0.7%
2	800	-20%	3.53	323.4	0.520	1.9%
	900	-10%	3.52	323.2	0.514	0.8%
	1000	0	3.52	323.0	0.510	
	1100	+10%	3.52	322.9	0.508	-0.5%
	1200	+20%	3.52	322.8	0.505	-0.9%
4	800	-20%	3.70	337.6	1.676	3.9%
	900	-10%	3.69	336.9	1.639	1.7%
	1000	0	3.68	336.4	1.613	
	1100	+10%	3.67	336.0	1.592	-1.3%
	1200	+20%	3.67	335.7	1.577	-2.2%

Also, heat generation and temperature distribution results can be seen in Figure 4.12 and Figure 4.13 below. As seen in both figures, almost there is no change in heat generation at all.

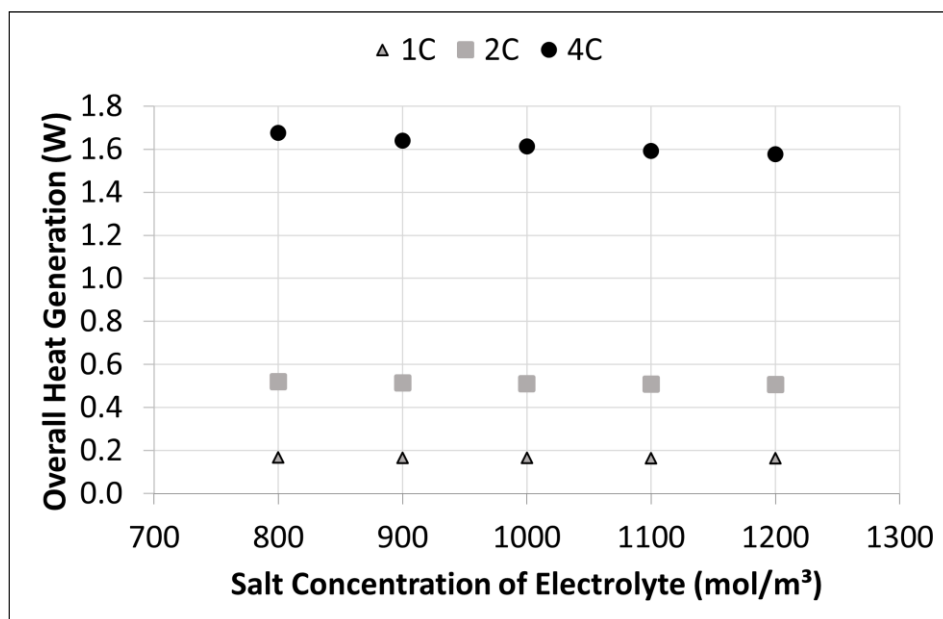


Figure 4.12: Overall heat generation graph at a salt concentration of electrolyte.

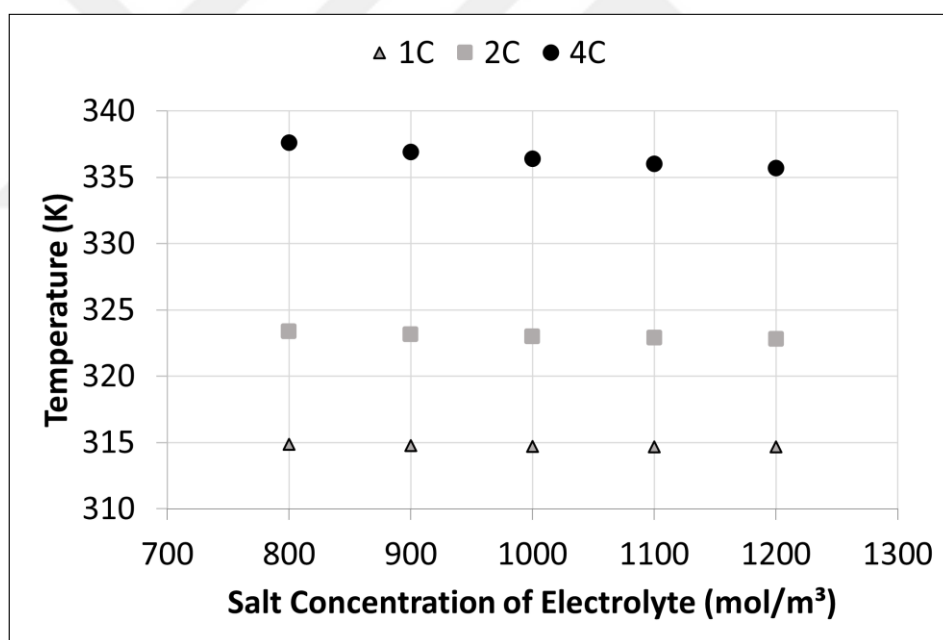


Figure 4.13: Average temperature graph at a salt concentration of electrolyte.

4.2.5. The Thickness of the Positive Electrode

The geometric parameters are another parameter that should be taken into account for the heat generation of the cell. Thus, the thickness of the positive electrode

is analyzed on heat generation. Results are shown below in Table 4.5, Figure 4.14, and Figure 4.15. The same table and figure templates with other parameters are applied to this parameter as well. Increasing the thickness by 20% affects the heat generation by 30%. Even if the cell capacity is changed by the same percentage as the change of the cell thickness, the cell voltage is not affected and stayed in small ranges. Compared with Table 4.2, the results are very similar to each other. Because both parameters affect directly the lithium amount in the positive electrode.

Table 4.5: Results of changing the thickness of the positive electrode.

C_{rate}	δ_{pe}	%	Cell Voltage (V)	Temperature (K)	Heat (W)	Change of Generated Heat from Base Model
1	100	-20%	3.40	310.5	0.120	-27.4%
	112.5	-10%	3.41	312.6	0.141	-14.8%
	125	0	3.43	314.7	0.166	
	137.5	+10%	3.45	316.9	0.190	15.0%
	150	+20%	3.47	319.2	0.213	28.8%
2	100	-20%	3.47	316.5	0.355	-30.4%
	112.5	-10%	3.49	319.7	0.430	-15.6%
	125	0	3.52	323.0	0.510	
	137.5	+10%	3.55	326.5	0.597	17.0%
	150	+20%	3.58	330.1	0.694	36.0%
4	100	-20%	3.60	326.0	1.095	-32.1%
	112.5	-10%	3.64	331.0	1.334	-17.3%
	125	0	3.68	336.4	1.613	
	137.5	+10%	3.73	342.4	1.960	21.5%
	150	+20%	3.81	349.4	2.486	54.2%

In both Figure 4.14 and Figure 4.15 below, the linearity of the rise of the heat generation with the temperature change can be seen. Also, these graphs are consistent with Figure 4.8 and Figure 4.9.

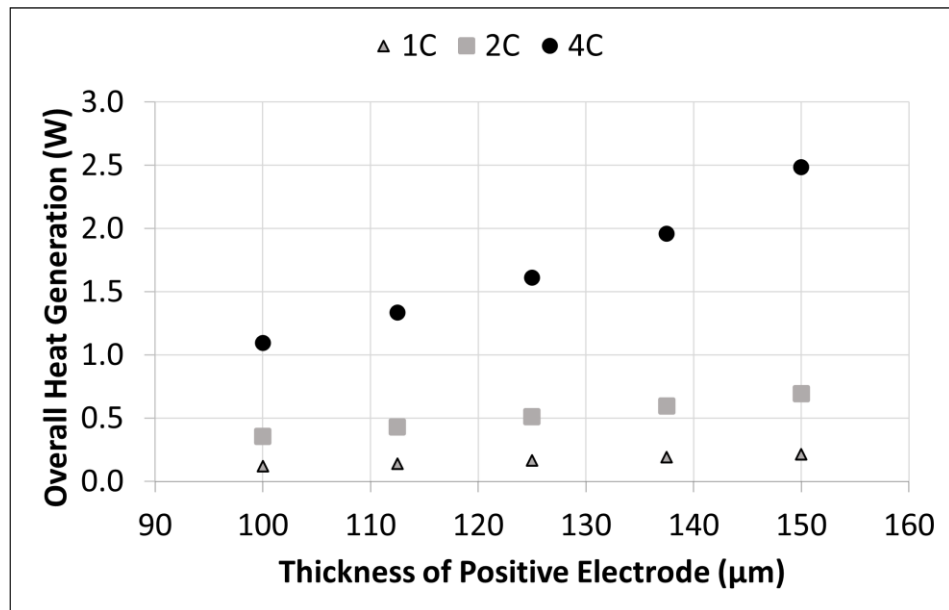


Figure 4.14: Overall heat generation graph at the thickness of the positive electrode.

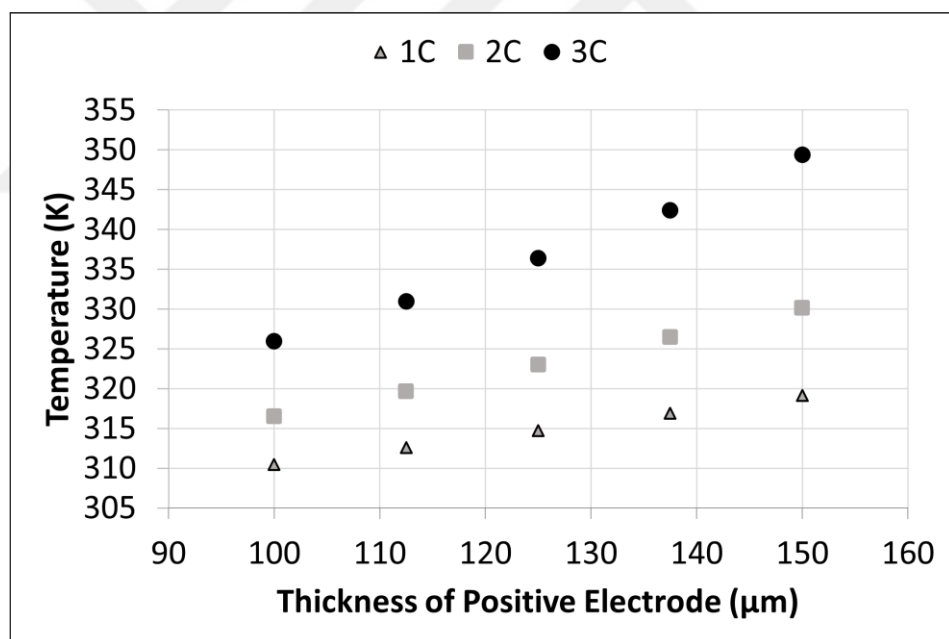


Figure 4.15: Average temperature graph at the thickness of the positive electrode.

4.2.6. The Thickness of the Negative Electrode

The last parameter is the thickness of the negative electrode. Results are shown below in Table 4.6. The same table and figure template is applied to this parameter. The results are similar to the concentration change of the negative electrode. There is no significant change in overall heat generation but cell temperature is affected more than generated heat. Since the measured temperature is volume-averaged, it is expected to see a decrease in temperature while increasing the thickness of the negative electrode. The heat dissipation in the increasing volume due to the increase in thickness causes the cell volume average temperature to decrease. This result can be useful for thermal management design but the geometry change could increase the cost the of cell. Furthermore, investigations are needed in cycle loads and aging experiments.

Table 4.6: Results of changing the thickness of the negative electrode.

<i>C rate</i>	δ_{ne}	%	Cell Voltage (V)	Temperature (K)	Heat (W)	Change of Generated Heat from Base Model
1	120	-20%	3.46	317.8	0.156	-5.6%
	135	-10%	3.44	316.2	0.168	1.2%
	150	0	3.43	314.7	0.166	
	165	+10%	3.42	313.5	0.162	-2.4%
	180	+20%	3.42	312.4	0.160	-3.3%
2	120	-20%	3.55	327.3	0.510	0.0%
	135	-10%	3.53	325.0	0.515	1.0%
	150	0	3.52	323.0	0.510	
	165	+10%	3.51	321.3	0.504	-1.2%
	180	+20%	3.50	319.8	0.497	-2.6%
4	120	-20%	3.71	346.5	1.670	3.5%
	135	-10%	3.69	339.3	1.637	1.5%
	150	0	3.68	336.4	1.613	
	165	+10%	3.67	333.9	1.590	-1.4%
	180	+20%	3.66	331.8	1.562	-3.2%

As seen in Figure 4.16 and Figure 4.17 below, while there is no significant change in generated heat, the temperature distribution is decreasing with the increase of thickness of the negative electrode.

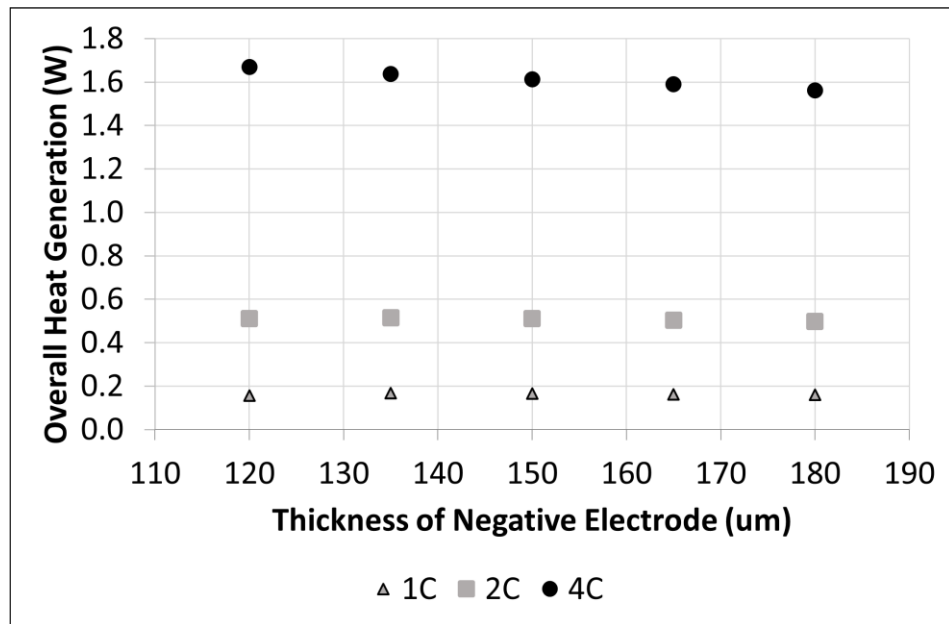


Figure 4.16: Overall heat generation graph at the thickness of the negative electrode.

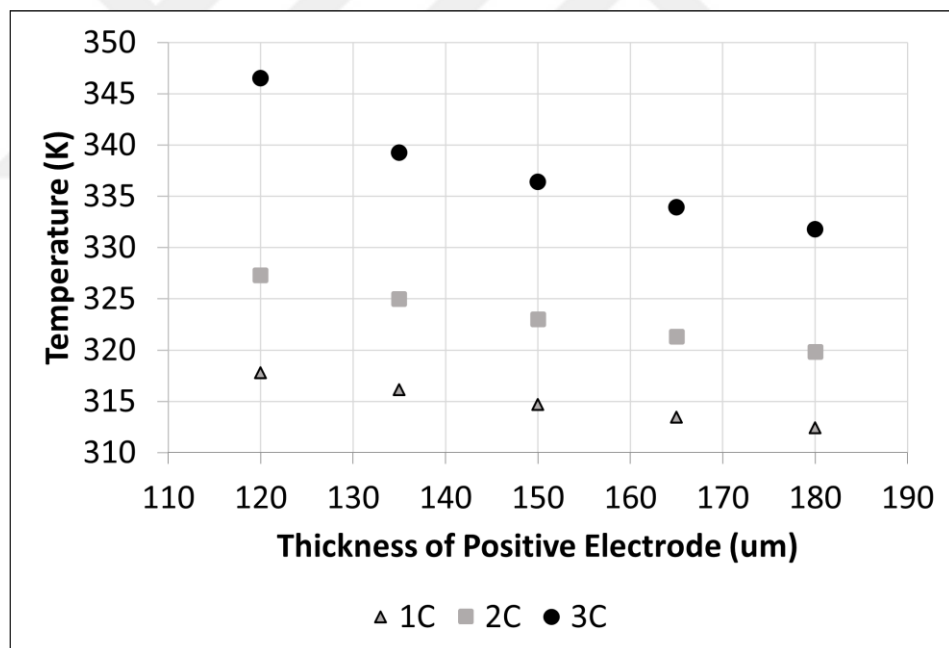


Figure 4.17: Average temperature graph at the thickness of the negative electrode.

5. CONCLUSION

In this thesis, a 3D coupled electrochemical-thermal model of the pouch-type lithium-ion battery is developed and validated with experimental results in the literature. 20 Ah LFP / Graphite type lithium-ion battery is selected to analyze both chemical and geometric parameters that affect heat generation and temperature distribution of the battery cell. Parameters such as, the change of the porosity of electrodes ($\epsilon_{s,pe}, \epsilon_{s,ne}$), lithium concentration of electrodes ($c_{s,max,pe}, c_{s,max,ne}$), the salt concentration of electrolyte ($c_{l,0}$), and the change of thickness of electrodes (δ_{pe}, δ_{ne}) are analyzed with the range of -20%, -10%, +10%, and +20%, and the results on heat generation and temperature distribution are shared. The results of analyzed parameters are given below in the list:

- The change in the porosity of electrodes has a significant effect on overall heat generation. Decreasing the porosity of the positive electrode reduces the heat generation and temperature of the cell substantially. That effect increases with the increase of current rates.
- Change of lithium concentration of positive electrode is the second significant parameter on heat generation. That parameter also affects cell capacity directly.
- A change in the lithium concentration of the negative electrode has almost no effect on heat generation.
- The salt concentration of electrolyte has an insignificant effect on heat generation (i.e. the maximum measured heat generation change is around 4% at a 4C rate).
- The thickness of the positive electrode is the third parameter that has a great influence on heat generation. Thickness also changes the cell capacity as well as the lithium concentration of the positive electrode parameter.
- The thickness of the negative electrode almost has no effect on the heat generation of the cell. Despite that, increasing the thickness of the negative electrode decreases the overall cell temperature distribution.

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