# Analyzing the Behavior of Li-B Electrothermal Voltage and Capacity Loss under Varying Temperatures and Discharge rates

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# Analyzing the Behavior of Li-B Electrothermal Voltage and Capacity Loss under Varying Temperatures and Discharge rates

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**Abstract:** *Lithium batteries are preferred for electric vehicles due to their high energy density, power output, rechargeability, efficiency, durability, and positive environmental impact. To enhance energy density of Li-B, electrochemical models are carefully designed after analyzing at changing charging and discharging behaviors to improve the efficiency. However, the complex structure arising from numerous physical parameters hampers better analysis of key battery parameters. This paper presents an electrothermal model in which batter's dynamic electrical parameters are simulated using Impedance-based Chen and Mora electrical equivalent circuit while thermal characteristics are simulated using the Bernard's Heat equation. Besides, accurate battery voltage is calculated using voltage compensation offset. Moreover, using the proposed model, the study investigates the impact of different ambient temperatures and charge/discharge rates on battery voltage. Additionally, a semi-empirical model is also proposed here to assesses the lifespan of Li-B by accounting two of the major Capacity Losses i.e., Calendar Loss and Cycle Loss. Similarly, the proposed battery-life-prediction model is also used to analyze behavior of battery parameters under varying temperatures and discharge rates.*

**Keywords:** Battery Electrothermal Model; Battery Capacity Loss Model; Voltage Compensation offset.

## 1. INTRODUCTION

Lithium-ion Batteries (Li-B) are widely used in most electronic applications and Electric Vehicles (EV) due to their advantages, which include higher energy density, greater voltage capacity, and a lower self-discharge rate.

Different types of lithium batteries have complicated charging and discharging processes based on their electrical and thermal characteristics due to their varying electrochemistry. Keeping in view of the significance of these electrical and thermal aspects of Li-B , there has been a substantial amount of research done in recent years to enhance the electrical and thermal modeling of Li-B at various degrees of precision and complexity [1]. Electrochemical , mathematical, and electrical methodologies are typically used to base Li-B modeling. The electrochemical models focus on a physical approach that primarily optimize the design parameters and improve the physical characteristics of batteries. These models simulate the battery temperature profile while charging and discharging using the current and cell voltage, but they are complex numerical and require huge simulation time. [2]

Mathematical models on the other hand are too abstract to accurately predict the battery capacity or efficiency and are only applicable in certain circumstances. Besides, these devices lack cell voltage profiles during the charging and discharging scenarios and bears 5-20% of inaccurate results. [3], [4]

Electrical models employ electrical equivalent circuits for Li-B and integrate the circuit elements(resistors, capacitors and voltage sources) These models produce cell voltage profile with 1.5% error based on temperature limits during charging and discharging scenarios but cannot generate temperature profiles during both scenarios. [5] Therefore, mathematical, and electrochemical models have a limited ability to predict the energy profile of a real battery, which restricts their use to specific design tasks. Whereas electrical models are well-known for producing more accurate I-V information results than mathematical and electrochemical models.[2], [6]

Besides, the development of battery life models to predict capacity loss in Li-B has received a lot of attention now adays to avoid business risks. In this regard, several capacity loss models have also been developed based on aging mechanisms, such as parasitic side reactions, SEI formation, and increase in resistance. However , experimental data is essential to effectively monitor the concept behind the aging mechanism for developing a reliable battery life prediction model. [7]

Therefore, an electrothermal model of Li-B voltage and temperature during charging and discharging is presented in the first section of this paper where the battery voltage is computed based on the state of charge (SOC) level, and then the battery temperature is determined using a simulated open-circuit voltage. [1]

Similarly, in order to understand the aging mechanism and to forecast the life of Li-B , a semi-empirical capacity loss model accounting calendar loss and cycle loss in Li-B [7] is also highlighted here in the second section. Finally, the battery's behavior is analyzed in terms of its parameters on MATLAB using these models under varying rates and temperatures.

## 2. LI-B ELECTROTHERMAL MODEL

The Li-B Electrothermal model is a mathematical representation of Li-B using its electrical and thermal characteristics to analyze the battery's dynamic parameters i.e., voltage and temperature under different operating conditions. This paper presents the electrothermal model where the battery voltage and the temperature profile is generated in accordance with the SOC level for each charging and discharging modes following the flowchart in Fig1. This section is divided into two subsections: the first sub-section explains the battery electrical model and the second sub-section discusses the battery temperature model.

### 2.1 Battery Electrical Model

The battery voltage or the potential difference between the two battery terminals is calculated here using the Chen and Mora (CM) electrical equivalent circuit as shown in figure.1 which is an impedance-based electrical circuit accounting for bulk resistance ,charge transfer reaction ,short-term and long-term transient effects and unlike conventional electrical circuits, it helps in achieving the detailed internal behavior of all battery parameters. [1] The formula expresses the battery voltage ( $V_{bat}$):

$$V_{bat} = V_{oc} - I_{bat} \times Z_{eq} + \Delta E(T) \quad (1)$$

Where, $V_{oc}$ is the open-circuit voltage, $I_{bat}$ is the battery current, $Z_{eq}$ is the internal impedance and ΔE(T) is the voltage compensation offset and is initially assumed as 0.2

The open- circuit voltage represents the maximum voltage generated by voltage in open circuit conditions and is dependent on SOC level, it can be expressed as:

$$Voc_{(SOC)} = -1.031\,e^{(-35SOC)} + 3.685 + 0.2156SOC - 0.1178SOC^2 + 0.3201SOC^3 \quad (2)$$

Where SOC is the State of Charge and is calculated using the Coulomb Counting method as:

$$SOC = SOC_{ini} - \frac{n}{Cc}\int Ibat\,dt \quad (3)$$

Where, SOCini is the initial state of charge, $n$ is the Coulomb's efficiency constant ($n$= 1 for discharge and $n$ <=1 for a charge ), $C_c$ is the nominal capacity, and $I_{bat}$ is taken +ve $I_{bat}$ for discharge and -ve $I_{bat}$ for charge.

The electrical elements, series resistance Rs, short transient capacitance Cts, short transient resistance Rts, long transient capacitance Ctl and long transient resistance Rtl as illustrated in the battery electrical equivalent circuit in Figure1 are dependent on SOC and therefore can be expressed as:

$$Rs_{(SOC)} = 0.1562e^{(-24.37SOC)} + 0.07446 \quad (4)$$

$$Cts_{(SOC)} = -752e^{(-13.51SOC)} + 703.6 \quad (5)$$

$$Rts_{(SOC)} = 0.3208e^{(-29.14SOC)} + 0.04669 \quad (6)$$

$$Ctl_{(SOC)} = -6056e^{(-27.12SOC)} + 4475 \quad (7)$$

$$Rtl_{(SOC)} = 6.603e^{(-155.2SOC)} + 0.04984 \quad (8)$$

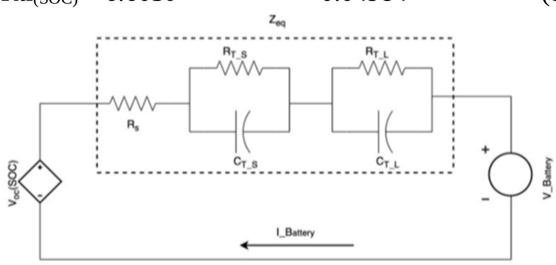



Figure 1. Chen & Mora Battery Electrical Equivalent Circuit

The internal Impedance $Z_{eq}$ of Electrical Circuit in Figure 1 can be calculated as:

$$Z_{ts} = \frac{RtsXts}{\sqrt{(Rts^2 + Xts^2)}} \quad (9)$$

Where, $R_{ts}$ and $X_{ts}$ are Short-term transient resistance and Short-term transient reactance respectively.

$$X_{ts} = 1/2\pi fC_{ts} \quad (10)$$

Where, f is the frequency in Hz and $C_{ts}$ is the Short-term transient Capacitance.

$$Z_{tl} = \frac{RtlXtl}{\sqrt{(Rtl^2 + Xtl^2)}} \quad (11)$$

Where, $R_{tl}$ and $X_{tl}$ are Long-term transient resistance and Long-term transient reactance respectively.

$$X_{tl} = 1/2\pi fC_{tl} \quad (12)$$

Where, f is the frequency in Hz and $C_{tl}$ is the long-term transient capacitance.

$$Z_{eq} = R_s + Z_{ts} + Z_{tl} \quad (13)$$

### 2.2 Battery Temperature Model

The proposed battery temperature model is based on following Bernard's heat generation equation which covers all factors affecting the change in temperature inside Li-B. [8]

$$M \times C_P\, \boldsymbol{dT/dt} = Q_{gen} - h \times A(T - T_A) \quad (14)$$

Where M is the mass of the battery cell, $C_p$ is the specific heat capacity , $Q_{gen}$ is the total heat generation, h is the heat transfer coefficient , A is the area , T is the cell temperature and $T_A$ is the ambient temperature.

Total heat generation $Q_{gen}$ inside the battery cell is the sum of irreversible heat $Q_{irrev}$ and reversible heat sources $Q_{rev}$. therefore , $Q_{gen}$ can be expressed as:

$$Q_{gen} = Q_{irrev} + Q_{rev} \quad (15)$$

whereas the irreversible heat source is calculated as follows:

$$q_{irrev} = I_{bat}\,(V_{bat} - V_{oc}) \quad (16)$$

The reversible heat source is calculated as follows:

$$Qrev = I_{bat} \times T(\boldsymbol{dVoc/dT}) \quad (17)$$

where $\boldsymbol{dVoc/dT}$ expresses the change in entropy due to electrochemical reactions during the charging and discharging cycle. This entropy change can be measured using an electrochemical thermodynamic measurement system ETMS where experimental entropy results are assessed to achieve set of polynomial equations as mentioned in [1] to simulate the $\boldsymbol{dVoc/dT}$ based on SOC level during each charging and discharging scenarios. Using equations 16. and 17. Irreversible and reversible heat sources are calculated to obtain the simulated total heat generation and subsequent achievement of simulated temperature profile using equation 14. for each charging and discharging scenarios.

Moreover , this paper also presents the calculation of voltage compensation offset E(T) based on cell temperature using a curve for equilibrium potential against cell temperature from [9] to obtain a unique equilibrium potential or Voltage compensation offset for a specific cell temperature. Figure 2 shows temperature-dependent equilibrium potential curve.
The calculated E(T) is used in the battery electrical model above to calculate the actual cell voltage.

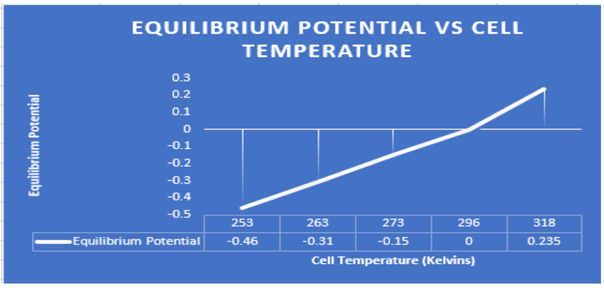



Figure 2. Temperature-dependent Equilibrium Potential Curve [9]

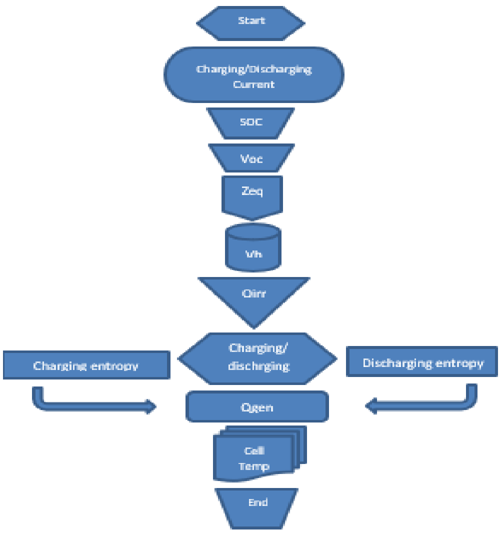



Figure 3. Flow chart of Battery Electrothermal Model

## 3.LI-B CAPACITY LOSS MODEL

The capacity fade model presented here is based on the identification of responsible factors behind aging behaviors in Li-B by analyzing the capacity trend data and discharge profiles during cycle test experiment described in [7]- which concluded the following two major contributors of lithium loss in Li-B.

i.) .Loss of lithium ions due to high temperature.
ii.) Lithium loss is due to high discharge rates at low temperatures.

Keeping in view of the above two primary influencers, a semi-empirical capacity loss model is devised in terms of a calendar loss model and cycle loss model to incorporate these major experimental parameters.

### 3.1 Calendar Loss Model

Calendar loss defines the irreversible self- discharge capacity loss. The loss of lithium during the development of the solid-electrolyte interphase (SEI) at the graphite negative electrode is the primary cause of this type of capacity loss. As [10]–[12] since the growth of SEI is a diffusion limited process which makes calendar loss a function of $time^{1/2}$. Besides, as [13]–[15] SEI growth is also a thermally triggered one and can be simulated using the Arrhenius equation. Thus, it finally concludes that Calendar Loss can be modelled using time and temperature [12], [14], [16] as follows:

$$Cal_{loss(\%)} = A\exp\left(-\frac{Ea}{R\times T}\right)t^{0.5} \quad (18)$$

Where $Cal_{loss(\%)}$, is the calendar loss in percentage, A is the pre-exponential factor, Ea is the activation energy, R is the Universal gas constant, T is the absolute temperature and t is the time in days.

The equation (9) can be simplified as:

$$\ln(Cal_{loss(\%)}) = \ln(A\times t^{0.5}) - (\frac{Ea}{R\times T}) \quad (19)$$

Furthermore , from equation (10) , fitting parameters are determined using single step optimization technique to plot the logarithmic percentage of calendar loss as a function of inverse temperature[4] to finally develop the calendar loss model as :

$$Cal_{loss(\%)} = 14876\exp(\frac{-24500}{8.314\times T})t^{0.5} \quad (20)$$

The above equation (11) shows that calendar loss is dependent on time and temperature.

### 3.2 Cycle Loss Model

The cycle Loss is calculated by subtracting the calendar loss from the total capacity loss in [7] and the percentage of cycle capacity loss is plotted against the throughput energy values, finding a direct relation of cycle-induced capacity loss with the rates and following a linear trend with time and rates, which also comes in conformity with the [17] Therefore, to develop an empirical relation between cycle loss and rate, cycle loss is plotted as a function of rate and rate effect is fitted by an exponential function to generate the cycle model as :

$$Cyc_{loss(\%)} = B1\exp(B2\times I_{rate})Ah \quad (21)$$

Where $Cycl_{loss(\%)}$ is the cycle loss in percentage ,Irate represents the current charge/discharge rate B1 is the pre-exponential factor whereas B2 is the exponential factors, and Ah represents the battery throughput energy Ah and can be expressed as:

$$Ah = Cr\times DoD\times N_c\times E_{rt} \quad (22)$$

Here, Cr denotes the rated capacity , DoD is the Depth of Discharge ,$N_c$ is the No. of life cycles and $E_{rt}$ is the round-trip efficiency (which can be obtained from the manufacturer's datasheet)

Moreover, to find the impact of temperature on cycle loss, the pre-exponential and exponential factors were plotted as a function of temperature which illustrated the linear trend in exponential factor B2 decreasing with increasing temperature whereas the relation between the pre-exponential factor B1 and temperature could not be developed as the B1 showed higher values on both lower and higher temperatures. However, a second-order polynomial equation is developed in [7] to achieve the empirical fitting of B1 and B2 , calculating the cycle loss which is as follows:

$$Cyc_{loss(\%)} = (aT^2 + bT + c)\exp[(dT + e)I_{rate}]Ah \tag{23}$$

Where a,b,c,d,e are the coefficients, their respective experimental values from [7] are inserted into equation.23 to obtain the final cycle loss model which is as follows:

$$Cyc_{loss(\%)} = (8.61 \times 10^{-6}T^2 - 5.13 \times 10^{-3}\,T + 7.63 \times 10^{-1})\exp[(-6.7 \times 10^{-3}T + 2.35)I_{rate}]Ah \tag{24}$$

### 3.3 Total Capacity Loss in Li-B

The total capacity loss in Li-B is the sum of calendar loss and cycle loss. Therefore, the total Capacity Loss Model is achieved by adding the equation 20. and equation 24. as:

$$Cap_{loss(\%)} = [\,(14876\exp(\frac{-24500}{8.314 \times T}) \times t^{0.5}) + (8.61 \times 10^{-6}T^2 - 5.13 \times 10^{-3}T + 7.63 \times 10^{-1})\exp\{(-6.7 \times 10^{-3}T + 2.35)I_{rate}\}Ah\,] \tag{25}$$

The predicted values in the above Capacity Loss model Eq.25 are within $\pm 5\%$caapcity loss of the measured values and is based on temperature and discharge/charge rates, Therefore, capacity loss in Li-B can be predicted under different temperatures and different rates.

## 4. RESULTS

The formulations of both the aforesaid models (Li-B Electrothermal Model and Li-B capacity Loss Model ) were checked using MATLAB under different scenarios to establish the facts.

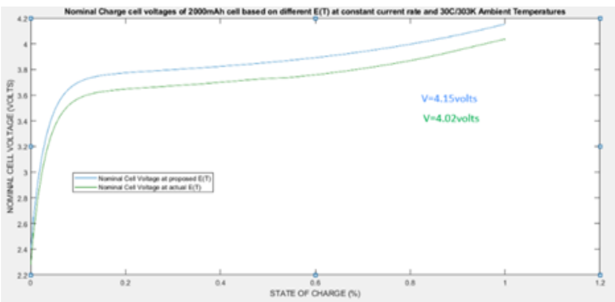
### 4.1 Li-B Electrothermal Model

#### 4.1(a) Simulating Nominal Cell Voltage against SOC

In order to simulate the nominal cell voltage based on SOC level during charge and discharge scenarios, parameters, as illustrated in Table.1, were assumed to generate charge and discharge nominal cell voltage profiles based on proposed and calculated voltage compensation offsets and were analyzed based on different values of voltage compensation offsets.Figure 4 and Figure 5 shows the nominal voltages for charging/discharging scenarios respectively.

Table 1:Parameters and the values for Electrothermal Model

Figure 4. Nominal Cell Voltage during Charging Scenario



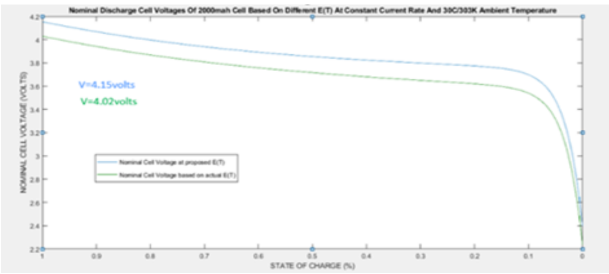




Figure 5. Nominal Cell Voltage during discharge scenario

| Parameters | Values |
|---|---|
| Rated Capacity Cr | 2Ah |
| SOCini Charging | 0% = 0 |
| SOCini Discharging | 100= 1 |
| Charge/Discharge rate (100%) | 2Amp |
| Ambient temperature $T_A$ | 303K |
| Initial Cell surface temperature Tc | 305K |
| Proposed Voltage Compensation offset E(T) | 0.2 |

#### 4.1(b) Simulating Cell Temperature against SOC

The 2Ah cell temperature was simulated at all SOC levels from 0% - 100% (Charging) and from 100% - 0% (discharging) based on parameters mentioned in Table.1 to achieve the charge and discharge temperature profiles at proposed and calculated voltage compensation offsets. Figure 6 and Figure 7 shows the cell temperature during charging/discharging respectively.

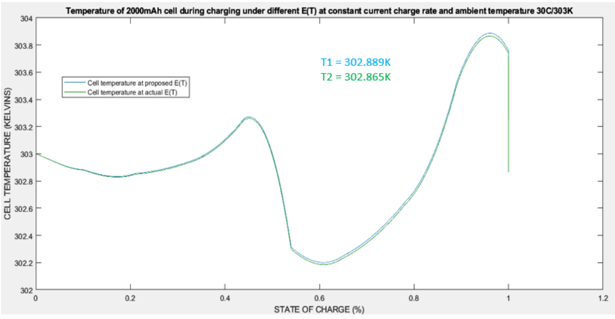



Figure 6. Cell Temperature during constant rate Charging Scenario

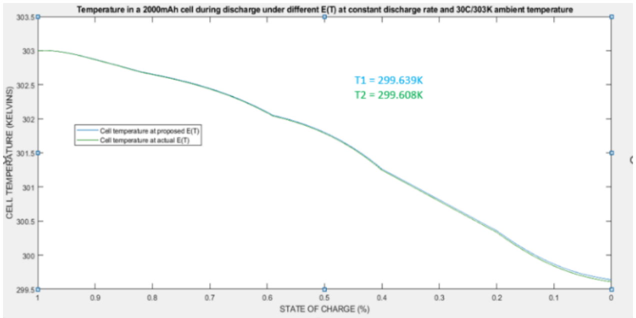



Figure 7. Cell Temperature during Discharging Scenario

#### 4.1(c) Simulating Nominal Cell Voltage at Different Discharge rates

In order to analyze the behavior of the 2Ah battery cell and the parameters in Table.1 and using an electrothermal model at different discharge constant current rates, the cell voltages obtained for each

| Parameters | Values |
|---|---|
| Rated Capacity of cell | 2Ah |
| Ambient Temperature | 34C/307K |
| Discharge time | 3600seconds |
| Depth of Discharge ( DOD ) | 80% |
| Round Trip Efficiency (Ert) | 95% |
| Rate of discharge (100%) | 2A |

discharge rates of 0.25C,0.5C, 0.75C and 1C were simulated against all SOC levels during discharge modes at an Ambient temperature of 30C/303K. The curve of cell voltage simulation at different discharge rates is shown in Figure8

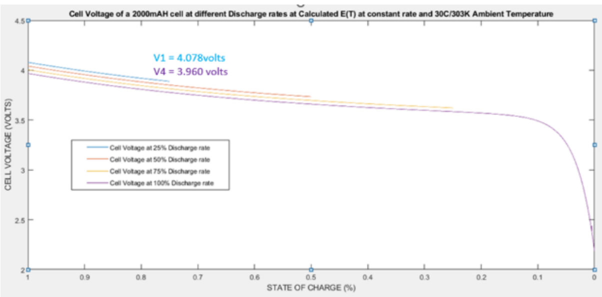



Figure 8. Cell Voltage at different discharge rates

**4.1(d) Simulating Cell Voltage at different Ambient Temperatures.**

The behavior of 2Ah battery cell was further analyzed using the parameters in Table.1 for the electrothermal model under different temperatures by simulating the cell voltage against all SOC levels during discharge at different ambient temperatures (-13C/260K, -3C/270K, 20C/293K, 30C/303K). The voltage curves obtained under different ambient temperatures are shown in Figure 9

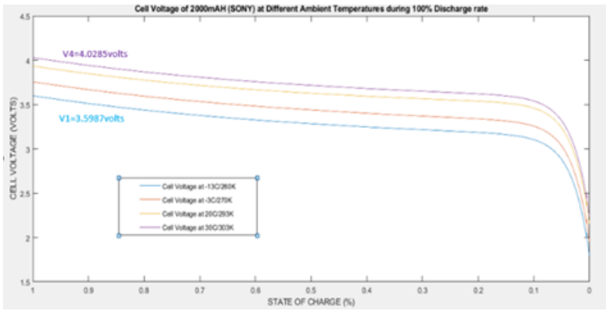



Figure 9. Cell Voltage at different ambient temperatures

## 4.2 Li-B Capacity Loss Model

The ageing behavior in 2Ah cell having parameters as mentioned in Table.2 was analyzed after achieving the Calendar loss and Cycle loss using the proposed Capacity Loss Model and simulating them under different conditions as mentioned below.

**4..2(a) Simulating Capacity Loss at Different Discharge rates**

Inorder to examine the impact of different discharge rate on the total capacity loss in 2Ah cells, data obtained using the capacity loss model was simulated for different discharge rates of 0.25C,0.5C,0.75C,1C for one half cycle of length 3600seconds. Figure8 shows the total capacity loss in a 2Ah cell after one-half cycle under different discharge rates.

Table 2: Parameters and their values for Capacity Loss Model

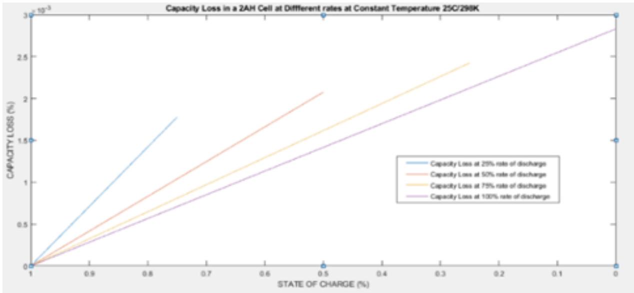



Figure 10. Capacity Loss at different discharge rates

**4.2(b) Simulating Capacity Loss at Different Ambient Temperatures**

Similarly, in order to evaluate the impact of a range of temperatures on the life of 2Ah cell, Simulations for a length of 3600seconds were carried out for each half cycle at different ambient temperatures of 18C/291K, 32C/305K, 44C/317K. Figure11 shows the capacity loss under different ambient temperatures.

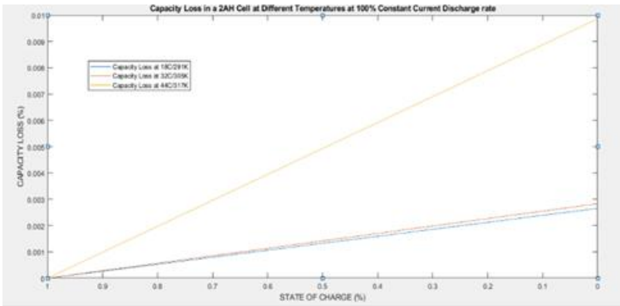



Figure 11. Capacity Loss at different Ambient Temperatures

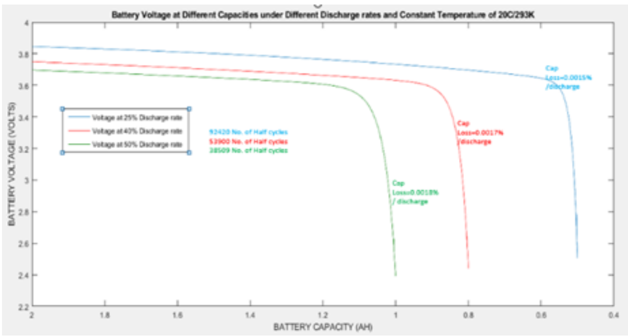



Figure 12. Cell Voltages against rated capacity after capacity loss at different discharge rates.

**4.2(c) Simulating Impact of Capacity Loss on Cell Voltage under different Discharge rates**

Furthermore, inorder to investigate the impact of capacity loss on cell voltage in the same 2Ah cell, discharge simulations were carried out till 50% of the rated capacity at three different discharge rates of 0.25C,0.4C, and 0.5C. Figure12 shows the cell voltage profiles against the rated capacity after cumulative capacity loss at each discharge rate.

## 5.CONCLUSION

This paper tried not only to formulate an electrothermal model for Li-B by which fundamental battery parameters can be analyzed under different charging and discharging scenarios instead of relying on time-consuming electrochemical methods, but also a life prediction model for Li-B is also presented ,which analyzes both the cycle loss and calendar loss during aging mechanisms under varying temperatures and discharge rates. Finally , after achieving the simulation results , it is concluded that during discharge at varying temperatures and discharge rates the assumed 2Ah Li-B exhibited the increase in cell voltage at highest temperature and lowest discharge rate respectively. Similarly , the capacity loss in 2Ah Li-B increased significantly at higher temperatures and higher discharge rates.

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