

**MODELLING AND
STATE OF CHARGE ESTIMATION OF
LITHIUM-ION BATTERIES**



M.Sc. THESIS

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JULY 2021

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**LİTYUM BAZLI BATARYA HÜCRELERİNİN
MODELLEME VE ŞARJ DURUMU TAHMİNİ**

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To my mother, Sedika



FOREWORD

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ABBREVIATIONS

AI	: Artificial Intelligence
ANN	: Artificial Neural Network
ASIC	: Application Specific Integrated Circuit
BMS	: Battery Management System
BOL	: Beginning of Life
CSC	: Cell Supervisory Circuit
DOD	: Depth of Discharge
DST	: Dynamic Stress Test
ECM	: Electrical Circuit Model
EChM	: Electrical Chemical Model
EIS	: Electro-chemical Impedance Spectroscopy
EKF	: Extended Kalman Filter
ELM	: Extended Learning Machine
EOL	: End Of Life
EV	: Electric Vehicle
ESS	: Energy Storage System
FC	: Fuel Cell
GA	: Genetic Algorithm
GM	: General Motors
GPR	: Gaussian Process Regression
HEV	: Hybrid Electric Vehicle
ICE	: Internal Combustion Engine
IEC	: International Electrotechnical Commission
IEEE	: Institute of Electrical and Electronics Engineers
ISO	: International Organization for Standardization
KF	: Kalman Filter
LA	: Lead Acid
LCO	: Lithium Cobalt Oxide
LEV	: Light Electric Vehicle
LFP	: Lithium Iron Phosphate
Li-Air	: Lithium Air
Li-S	: Lithium Sulphur
LIB	: Li-ion Battery
LMO	: Lithium Manganese Oxide
MARS	: Multivariate Adaptive Regression Splines
MCU	: Module Control Unit
ML	: Machine Learning
NCA	: Lithium Nickel Cobalt Aluminium Oxide

NiCd	: Nickel Cadmium
NiFe	: Nickel-Iron
NiH	: Nickel-hydrogen
NiMH	: Nickel-metal-hydride
NiZn	: Nickel-zinc
NMC	: Lithium Nickel Cobalt Manganese Oxide
OCV	: Open Circuit Voltage
OEM	: Original Equipment Manufacturer
PF	: Particle Filter
PNGV	: Partnership for a New Generation of Vehicles
RMS	: Root Mean Square
RMSE	: Root Mean Square Error
SAC	: Standardization Administration of China
SAE	: Society of Automotive Engineers
SOC	: State of Charge
SOE	: State of Energy
SOH	: State of Health
SOP	: State of Power
SOS	: State of Safety
SMO	: Sliding Mode Observer
SSB	: Solid State Battery
SVM	: Support Vector Machine
TTC	: Two Time Constant
UL	: Underwriter's Laboratory
UMD	: University of Maryland
UN	: United Nations
USCAR	: United States Council for Automotive Research
VCU	: Vehicle Control Unit
VRLA	: Valve-Regulated Lead-Acid
VTM	: Voltage Temperature Monitoring

SYMBOLS

A	: Ampere
Ah	: Ampere-hour
C	: Capacitance
C_{tot}	: Nominal capacity of the cell in Ah
Δt	: Sampling time
i	: Current
$i(k)$: Current passing through the battery cell in Amps
$i_R(k-1)$: Current passing through R at previous state in Amps
$i_R(k)$: Current passing through R at present state in Amps
$i_1(k-1)$: Current passing through R_1 at previous state in Amps
$i_1(k)$: Current passing through R_1 at present state in Amps
$i_2(k-1)$: Current passing through R_2 at previous state in Amps
$i_2(k)$: Current passing through R_2 at present state in Amps
Ω	: Ohm
$^{\circ}\text{C}$: Degree Celcius
R	: Resistance
SOC(k)	: SOC value at current state
SOC(k-1)	: SOC value at previous state
t	: Time
T	: Temperature
τ	: Time constant
τ_1	: Time constant for first RC branch
τ_2	: Time constant for second RC branch
U(k)	: Input signal which can be a current
V_{act}	: Voltage measured from actual battery
OCV(SOC)	: Open circuit voltage of the cell
V_t	: Terminal voltage of the cell
W/kg	: Power density
Wh	: Energy
Wh/kg	: Energy density
x(k)	: State variables such as SOC, i_1 and i_2
y(k)	: Output signal from measurement



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MODELLING AND STATE OF CHARGE ESTIMATION OF LITHIUM-ION BATTERIES

SUMMARY

The electric revolution is here, and the mass adoption of Lithium-Ion Batteries (LIBs) in the automotive industry is here to stay. Ever decreasing manufacturing costs for LIBs coupled with generous government incentives to own Electric Vehicles (EVs) make the shift from ICE vehicles a very real possibility for the general populace. The need for change has never been as strongly felt as it is today and this has been reflected both in the number of EV start-ups registered globally in the last decade as well as the push for more stringent CO₂ emission legislation by governments the world over. Most of the big automotive OEMs in the American, European and Chinese market have accepted this new reality and made heavy investments to transform their current design and manufacturing methods, and while it's easy to register the change taking place in the automotive world, we must not forget the significant progress taking place in the other sectors. Electrification through the implementation of Lithium-Ion Battery packs is also being accelerated in the Electric Energy Storage (ESS) sector, Industrial Mining sector, Public Transport sector, Agriculture Industry and even in the Sports and Recreation Industry (e-bikes). Lithium-Ion Battery packs and systems are not new, the first electric and hybrid cars have been around since the 1990's. However, with time this technology has matured and by spending significant resources in research and development, we can now see high power and high energy cells on the market that are commercially feasible. This has facilitated the mass production of these battery systems and has highlighted the need for a better understanding of the systems that control and manage the health of a battery cell. With each iteration of a battery pack design, the technologies used in thermal management system (TMS), electrical management system (EMS) and the overall Battery Management System (BMS) becomes more complex and sophisticated. The BMS is a key element of a LIB pack, especially in EVs. This can be attributed to the high level of functional safety required in a passenger vehicle and the wide-ranging environments that these vehicles can be operated in. Without a robust, reliable, well-developed, and well tested BMS system, an electric vehicle's potential will be under-utilised in the best of cases and become a safety hazard in the worst of cases. However, the BMS can contribute to more than just the functional safety of a vehicle, if designed correctly it can help extend the battery life which in turns reduces ownership cost and increase driving range. There are many types of BMS on the market, but most would have a common crucial function, which is to estimate the battery pack's State of Charge (SOC). The SOC describes the usable energy as a portion of the total energy available under certain conditions and there are a number of different estimation methods currently found on the market. There are both conventional and modern methods for SOC estimation. Modern techniques create different algorithms to estimate SOC via the indirect method, but the conventional measurement techniques use the so-called direct estimation method. Another method to estimate SOC is by using machine

learning models which are created from different application-based data sets, this is also referred to as a data-driven method which uses several artificial intelligence approaches including machine learning. In the battery management systems found on the market today, particularly those in EVs since they tend to be the most complex, any one of these methods or a combination of them is used to improve battery performance. In this thesis work, in addition to conventional approach of indirect estimation using Luenberger observer machine learning techniques of Multi-Linear Regression were used result of which were compared against each other.



LİTYUM BAZLI BATARYA HÜCRELERİNİN MODELLEME VE ŞARJ DURUMU TAHMİNİ

ÖZET

Elektrik devrimi burada ve otomotiv endüstrisinde Lityum-İyon Pillerin (LIB'ler) kitlesel olarak benimsenmesi kalıcı olmaya devam ediyor. LIB'lerin azalan üretim maliyetleri ve hükümetlerin elektrikli araç kullanma yönündeki cömert teşvikleri, içten yanmalı motorlu araçlardan elektrikli araç kullanımına geçmeyi büyük kitleler için mümkün kıldı. Geçtiğimiz on yılda küresel çapta elektrikli araç start-up şirketlerindeki artış ve hükümetlerin CO2 salınımlarıyla ilgili katı kısıtlamalarına bakıldığında değişim ihtiyacı daha sert hissediliyor. Amerika, Çin ve Avrupa piyasasındaki büyük otomotiv üreticileri bu yeni gerçekliği kabul ettiler ve mevcut tasarım ve üretim yöntemlerini dönüştürmek için büyük yatırımlar yaptılar. Otomotiv dünyasındaki bu dönüşümü fark etmek zor değil, ancak diğer sektörlerdeki kaydadeğer ilerlemeleri de gözden kaçırmamak gerekir. Lityum-İyon Bataryalar ile elektrifikasyon; elektrik enerjisi depolama, endüstriyel madencilik, toplu taşıma, tarım endüstrisi ve hatta spor ve eğlence sektörlerinde (elektrikli bisikletler) hız kazandı.

Lityum-İyon Batarya paket ve sistemleri yeni değildir. İlk elektrikli ve hibrit otomobiller 1990'lerden beri kullanımdadır. Ancak bu teknoloji ciddi miktarda ar-ge kaynağı harcanarak olgunlaştırıldı. Şu anda piyasada yüksek güç ve yüksek enerji kapasiteli hücrelere rastlayabiliyoruz ve bu hücrelerin üretimi ticari açıdan uygulanabilir halde. Bu durum batarya sistemlerinin seri üretimini kolaylaştırdı ve batarya hücrelerinin sağlığını kontrol edip yöneten sistemlerin daha iyi anlaşılması ihtiyacını doğurdu. Sıcaklık yönetim sistemi, elektriksel yönetim sistemi ve tüm batarya yönetim sistemi; batarya paketlerinin her tasarım döngüsünde daha karmaşık ve daha sofistike hale geldi.

Tüm LIB paketlerinde, özellikle elektrikli araçlarda, BYS kilit elemandır. Bu durum yolcu taşımacılığında gerekli olan yüksek fonksiyonel güvenlik gereksinimi ve bu araçların geniş çevresel koşullarda çalışabilme gerekliliği ile bağdaştırılabilir. Sağlam güvenilir ve iyi geliştirilmiş bir BYS olmadan, elektrikli araçlar, en iyi ihtimalle potansiyelinin altında kullanılacaktır; en kötü ihtimalle ise güvenlik tehlikesi oluşturacaktır. Ancak iyi tasarlanmış bir BYS, yalnızca fonksiyonel güvenliğe katkıda bulunmanın ötesinde, batarya ömrünü uzatarak kullanıcıya maliyet ve sürüş menzili açısından avantaj sağlar. Piyasada bulunan sayısız BYS'lerde ortak olarak bulunan en önemli özellik, batarya paketinin “Şarj Durumu”nu hesap etmesidir. “Şarj Durumu” belli koşullar altında mevcut tüm enerjinin kullanılabilir kısmı anlamına gelir. “Şarj Durumu”nu hesaplamak için piyasada çeşitli yöntemler bulunmaktadır.

ŞD'yi hesaplamak için hem geleneksel, hem modern yöntemler bulunmaktadır. Modern teknikler çeşitli algoritmalar kullanarak ŞD'yi dolaylı yoldan hesaplar. Ancak geleneksel ölçüm yöntemleri, direk ölçüm yöntemleridir. ŞD'yi hesaplamak için kullanılan bir diğer yöntem ise çeşitli uygulama bazlı veri setlerinden devşirilen

makine öğrenimi modelleridir. Bu yöntem veriye dayalı yöntem olarak adlandırılır ve makine öğrenmesi de dahil olmak üzere çeşitli yapay zeka yaklaşımları kullanır. Piyasada bulunan güncel batarya yönetim sistemleri, bilhassa elektrikli araçlarda kullanılanlar, bu yöntemlerin birini veya aynı anda birkaçını aynı anda kullanan karmaşık sistemler halindedir. Bu tez çalışmasında, Luenberger gözlemcisi gibi geleneksel dolaylı tahmin yaklaşımına ek olarak, makine öğrenmesi teknikleri kullanılarak analizler sonrasında sonuçlar birbirleri ile karşılaştırılarak.

Gözlemci tasarımı modelleme gerektirir. Yani, batarya hüccesinin davranışını matematiksel denklemler ile göstermek gerekmektedir. Sistem tanıma bilgisi hücre modellesi için çok yararlıdır. Batarya hüccesinin çeşitli girdilere nasıl tepki verdiğini gözlemledikten sonra sistem dinamiği matematiksel olarak gösteriliyor. Gözlemcilerin gözlenebilirliğinin tespiti açısından avantajlı olduğu için elde edilen batarya hüccesinin matematiksel modeli durum uzay denklemleri şeklinde gösterilmesi tercih ediliyor. Hücre modellemesi için, ilk önce batarya dinamikleri belirlenmesi gerekmektedir. Sonrasında, dinamikleri tespit etmek için belirli testler yapılması gerekiyor. Batarya testleri, uygun test tesislerin olmasını gerektiriyor ki bu da maliyet açısından kısıtlama getiriyor. Genellikle, batarya testleri pahalıdır. Dolayısıyla, batarya modellemesi için gereken testleri yapmak ve veri elde etmek büyük bir kısıtlama. Bu tezde ABD'nin Maryland Üniversitesinin ileri mühendislik araştırma enstitüsünün yaptıkları testler sonucunda elde edilen batarya verileri kullanılmıştır.

Modelleme yapmadan önce, batarya dinamikleri öğrenmek lazım. Dolayısıyla, batarya dinamiği konusunda araştırmalardan detaylı bahsedilmiştir. Batarya dinamiği bilgileri sayesinde, elektriksel devre modeli şablon olarak seçilmiştir. Elektriksel devrenin derecesi, elemanları ve elemanlarının sınırları teorik bilgiler sayesinde belirlenmiştir. Bu yaklaşım, gerçekçi model elde etmek için özellikle önem taşıyordur. Elektriksel devre modelinin derecesi ise literatürdeki çalışmalara dayanarak seçilmiştir.

Açık kaynaktan alınmış olan test verileri ilk önce işlenmesi gerekmektedir. İlk önce, açık devre geriliminin test verileri işlendi. Bu veriler, batarya hüccesinin yük altından olmadığı durumdaki gerilimi göstermektedir. Bu gerilim batarya hüccesinin şarj durumu ile ilintilidir. Şarj durumunun azalımı ile batarya hüccesinin açık devre gerilimi de azalmaktadır. Ayrıca, açık devre gerilimi sıcaklık ile değişim göstermektedir. Dolayısıyla, belirli bir sıcaklıkta, batarya hüccesi adımlar ile deşarj edilir. Dikkate alınması gereken başka bir husus ise adımlar arasındaki bekleme sürecidir. Bu bekleme saatler kadar uzun olabilir. Beklemenin amacı hüccenin elektriksel dengeye ulaşması içindir. Analiz sonucunda açık devre gerilimi şarj durumu ve sıcaklık cinsinden başvuru çizelgesi olarak elde edilmektedir.

Batarya hüccesinin dinamiklerini gösteren diğer elemanlar ise dirençler ve kapasitörler cinsinden belirlenmektedir. Aynı şekilde, bu elemanlar şarj durumu ve sıcaklık cinsinden başvuru çizelgesi olarak elde edilmektedirler. Bu elemanlar belirli testler ile elde edilir. DCIR, DST, HPPC gibi testler kullanılabilir. Bu projede dinamik stres testi (DST) kullanılmıştır. Başvuru çizelgelerin belirlenmesi, optimizasyon yöntemleri ile mümkündür. Özetçe, batarya hüccesinin akımı ve sıcaklığı girdi olarak, batarya hüccesinin gerilimi ise çıktı olarak belirlenir. Optimizasyon problemi ise, modeldin gerilimi ve gerçekte ölçülen gerilim arasındaki en düşük mutlak hatayı döndüren başvuru çizelgelerini bulmaktan ibarettir.

Optimizasyon metodları çeşitlidirler. Bazıları, yerel veya lokal sonuçlar döndürürken, diğerleri global veya küresel sonuçlar döndürüyorlar. Bu çalışmada, popüler

optimizasyon metodlarından, genetik algoritması kullanılmıştır. Genetik algoritması özellikle mutasyon içerdiği için global sonuç bulmak için uygundur. Optimizasyon sonucunda elde edilen elektriksel devre elemanlarının başvuru çizelgeleri üç boyutlu şekil olarak gösterilmektedir.

Modelleme yapıldıktan sonra şarj durumu tahmini için Luenberger gözlemcisi kullanılmaktadır. Bu gözlemci basit bir tahmin metodudur. Durum uzay denklemler cinsinden gösterilen batarya dinamikleri gözlemci tasarımında özellikle önem taşımaktadır. Gözlenebilirlik özelliği durum uzay denklemindeki A matrisinden tespit edilebilir. Şarj durumu tahmini algoritması için tasarlanacak gözlemcinin gözlenebilirliği şarj durumu ve sıcaklığa bağlıdır. Dolayısıyla, sıcaklık ve şarj durumu bölgelerine göre gözlemcinin kat sayısı belirlenmektedir.

Şarj durumu tahmini için geliştirilen modelin ve gözlemcinin validasyonu için dinamik bir kullanım profili kullanılmaktadır. Bu tez çalışmasında, otomotivde iyi bilinen FUDS profili kullanılmaktadır. Bu profil üzerinde algoritmalar test edilecektir. İlk önce gözlemci çalışmıyorken, açık dönüde modelden hesaplanan gerilim, gerçekte ölçülen gerilim ile kıyaslanıp modelin hassasiyeti ölçülür ve yorumlanır. Aynı zamanda Coulomb hesaplama ile elde edilen şarj durumu referans olarak kaydedilir. Coulomb hesaplama yönteminde, başlangıç şarj durumu ve batarya hücresinin kapasitesine ek olarak akım ölçümünün hassasiyeti de önem taşımaktadır.

Sonraki aşamada, bilinçli olarak yanlış başlangıç şarj durumu değeri verilerek gözlemcinin performansı yorumlanacaktır. Gözlemci belli süre geçtiğinde gerçek şarj durumuna ulaşması beklenmektedir. Gerçek değere ulaşmasının hızı ise gözlemcinin kat sayısına bağlıdır fakat yüksek kat sayı dengesizliğe yol açıyor. Bu çalışmada deneyimler sonucunda kat sayılar bulunmuş ve testler ile performansı yorumlanmıştır. Sonuçlara bakıldığında hassas bir batarya hücre modeli ve dengeli ve efektif bir gözlemci geliştirildiği görülmüştür.

Şarj durumu tahmini için kullanılan bir başka yöntem de istatistiksel öğrenmeye dayalı yöntemlerdir. Günümüzde bir çok mühendislik alanlarında sıkça kullanılan makine öğrenmesi yöntemleri batarya durum tahmini için de kullanılmaktadır. Bu tez çalışmasında makine öğrenmesi yöntemi ile geliştirilen şarj durumu tahmini daha önce geliştirilmiş olan gözlemci yöntemi ile kıyaslanmıştır.

Makine öğrenmesi yöntemlerinin dengeli sonuç vermeleri için batarya dinamikleri detaylıca incelenmiştir ve sonucunda her sıcaklık için altı makine öğrenmesi modeli geliştirilmiştir. Buna ek olarak, üç çeşit makine öğrenmesi yöntemi kullanılmıştır. Geliştirilen her modelin parametreleri özetlenip validasyon testlerine tabi tutulmuştur. İlk önce, doğrusal regresyon analizi ile bir model geliştirilmiştir. Sonrasında geliştirilen model farklı bir veri setindeki değerler ile kıyaslanıp elde edilen hata polinom regresyon ile sıfırlanmaya zorlanmıştır. Regresyonda kullanılan denklemler ve parametreler çeşitlidir. Bu çalışmada akım, gerilim, sıcaklığın kuplajları ve dereceleri regresyon modelini belirlenmektedirler. Şarj durumu tahmini için ağaç bazlı yöntemler de denenmiştir fakat uygun olmadıkları tespit edildiği için sunulmamıştır. Ağaç bazlı makine öğrenmesi yöntemlerinin çalışması için veri setinin güçlü ve çeşitli olması gerekmektedir. Buna ek elde edilen ağaç modelin gerçek zamanlı sistemlerde uygulanması zorlayıcı bulunmuştur.

Son olarak, makine öğrenmesinden elde edilen sonuçlar denge ve kararlılık açısından FUDS profili ile test edilmiştir. Elde edilen sonuçlara göre öneriler verilmiştir. Bu öneriler, sanayide kullanılan yöntemler ile uyumludur.



1. INTRODUCTION

With the rise of global awareness about climate change, energy storage systems in particular batteries are believed to play a pivotal role in combating this existential threat to human kind by transforming future of energy. Batteries have been studied for a long time and Lithium-ion battery cells have proven to show better performance in terms of power and energy density compared to others. LIB are dynamic systems that need to be closely monitored in terms of available energy, health and safety. Battery Management Systems (BMS) are responsible for monitoring and controlling batteries. One important measure is available energy which is commonly referred to as State-of-Charge (SOC). It is the measure of Lithium-ion concentration. SOC is crucial in determining states of the battery which makes its estimation particularly important. There is no direct way of measuring SOC but it could be inferred from other measurements such as voltage, current and temperature. Therefore, SOC estimation requires modeling based on significant amount of data. In this chapter an overview of methods to estimate SOC including modeling and parametrization based methods as well as data-driven methods are discussed.

1.1 Purpose of Thesis

Purpose of this thesis work is to investigate and validate SOC estimation developed by modeling the battery as an Electric Circuit Model (ECM) which would be from the perspective of energy storage systems in automotive applications in particular electric vehicles. Furthermore, data-driven method i.e. Machine Learning is used to solve the problem. Advantages and disadvantages of each method is discussed.

1.2 Literature Review

Physics Nobel price winner John Goodenough introduced LIB in 1980 [1]. Ever since, significant improvements have been happened in terms of safety and cost reduction [2]. To accurately monitor and control a battery cell modeling its behavior

is substantial [3]. Among numerous modeling approaches [4] while work of Schmidt et al. proposes parametrization of lumped elements [5] Oh et. al. take the approach of multi-physics configuration [6]. ECM comes out to be the most popular representation of LIB's dynamics among scientists due to practical advantages including effort spent on development which is preferred by experts in car industry [7–11]. In addition to implementation considerations such as computation and processing demand of the model, accuracy is a matter of great importance too which calls for a challenging management of trade-offs. This constitutes the motives behind works of Fleischer et. al. [3] and Sabatier et. al. [12] in developing reduced-order model and presentation of fractional-order model in work of Mu et. al. [13]. After setting the structure of the model whether it is electrochemical, equivalent electrical circuit or any of the above-mentioned methods determining parameters are also crucial for an accurate representation of system dynamics. One way of parametrization is to Electrochemical Impedance Spectroscopy (EIS) [14]. This method relies on frequency response analysis by creating Bode and eventually Nyquist plots [7]. On the other hand, one could accomplish characterization with the help of optimization methods such as Genetic Algorithm (GA) [15], adaptive filtering, Recursive Least Squares (RLS) [16] or other methods [17] which would require well-defined tests. The ultimate goal being state estimation, it is unequivocal that scientists and researchers pay special attention to the topic [18]. States of the battery which is of importance in monitoring and controlling the battery include but are not limited to state-of-charge (SOC), state-of-health (SOH), state-of-power (SOP), state-of-energy (SOE). All the states depend on SOC which is therefore of highest importance. Figure 1.1 and figure 1.2 depict architectural view of state estimation as part of Battery Management System (BMS).

Simplest form of SOC estimation which is known as coulomb counting is presented by the work of Aylor [20]. This method has downsides which are compensated by techniques from control theory like different types of observers [21–23], variations of Kalman filters [24–32]. Data-driven methods on the other hand which have become popular in numerous fields of engineering and science are applied to obtain states of the battery directly. Artificial Neural Networks (ANN) [33], Support Vector Machines (SVM) [34] and Guassian Process Regression (GPR) [35] are some of many methods

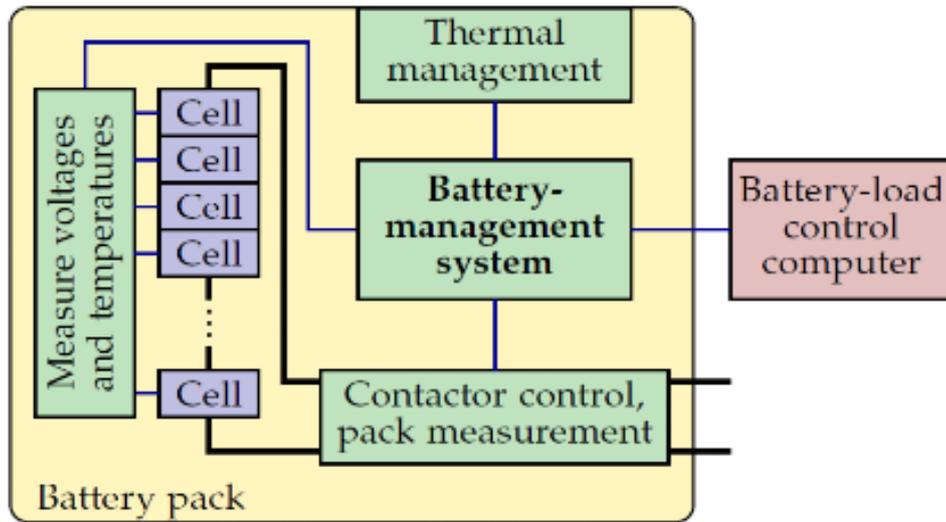


Figure 1.1 : System view of Battery Management System [19].

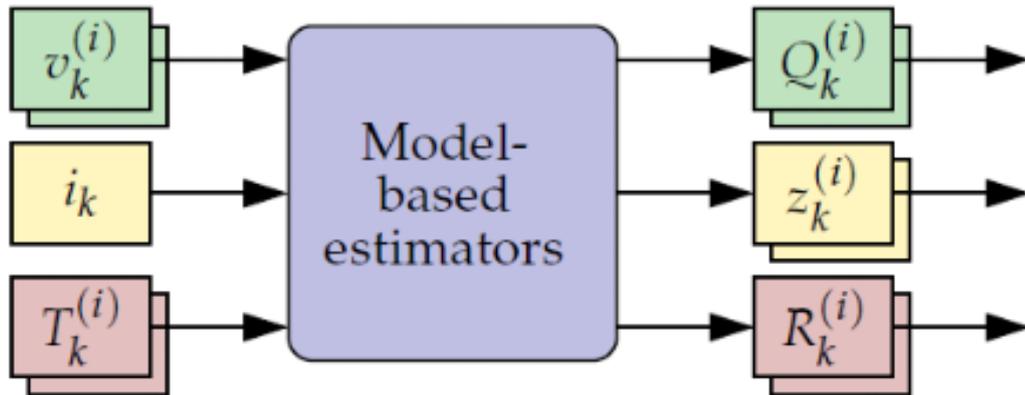


Figure 1.2 : Block functional view of state estimation of BMS [19].

that are used by scientists to solve the problem of battery state estimation. This thesis work focuses on applying an observer to estimate the SOC step by step which would give a clear picture of processes as well as challenges which would pave the way for further improvement of the algorithms. In addition to that, a machine learning algorithm is used to quantify the development effort as well as drawing attention to trade-offs that are needed to be further optimized.

2. BATTERY STATE-OF-CHARGE ESTIMATION METHODS

Among estimations that Battery Management System (BMS) performs which reveal condition of the battery, an important estimation is state-of-charge (SOC) which has direct impact on battery's remaining energy, power, cell balancing etc. From electrochemical point of view, SOC is indication of concentration of lithium ions in electrodes of the battery. However, in most applications ours included, SOC is defined as the ratio of remaining energy to total energy available. SOC can not be measured directly. Therefore, a method needs to be developed to infer SOC from quantities that could be measured from the battery. In other words, inferring the "states" from the response they would produce. In most general categorization there are three ways SOC could be estimated:

2.1 Model-Free Methods

These methods correlate real-time measurements to the SOC directly without trying to capture battery behavior from physical principles. Coulomb counting and black box approach are the two methods that follow does not rely on a pre-calibrated battery model.

2.1.1 Coulomb counting

This method is most straight forward way of obtaining SOC by keeping track of accumulated charge in the battery from the current flowing out of or to the battery. In mathematical terms this is expressed as following:

$$SOC(t) = SOC(t_0) + \frac{1}{3600C} \int_{t_0}^t i(\tau) d\tau \quad (2.1)$$

in discrete time:

$$SOC(k) = SOC(k-1) + \frac{i(k)T_s}{3600C} \quad (2.2)$$

where C is the capacity of the cell in Ah and T_s is the sampling period in seconds. This method however simple and easy to implement has significant disadvantages. Most

obvious downside is open loop nature of the estimation. As can be seen from the equations 2.1 and 2.2, SOC very much depends on initial value. In case of wrong initialization there will be no correction along the way therefore the error persists throughout the estimation period. Furthermore, capacity degradation over time and errors in current measurement will result in erroneous SOC estimation also.

2.1.2 Black box approach

As they are quite popular techniques in numerous fields, data driven methods could be used to solve battery state estimation problem also. These methods make use of data gathered from the system and try to predict their behavior under unseen circumstances rather than attempting to understand the behavior of the system from fundamental principles.. Some examples of data driven methods used for battery state estimation are Artificial Neural Networks [36], Fuzzy-based Neural Networks [37], Support Vector Machines [34] etc. Data driven methods are attractive because they reduce calibration effort significantly. However, there are challenges due to reliance on massive amount of data, stability of the algorithms and high processing power demand which makes implementation of these algorithms challenging.

2.2 Model-Based Methods

Another approach for battery state estimation is inspired by fundamental physical principles that define battery behavior. This approach requires information about the battery performance under well-defined conditions. Defining those conditions and performing corresponding tests are main challenges for this method in terms of time, cost and effort. There are mainly two widely modeling approaches for battery applications: electrical circuit model (ECM) and electrochemical model.

2.2.1 Electrical circuit model (ECM)

An electrical circuit model consisting of resistances and dynamic elements such as capacitors and inductors could be constructed to represent battery behavior. Figure 2.1 illustrates an electric circuit model of a battery cell. Circuit elements of an ECM depends on SOC and temperature. In practice this model is used in conjunction with a correction method such as observers and variations of Kalman filters that

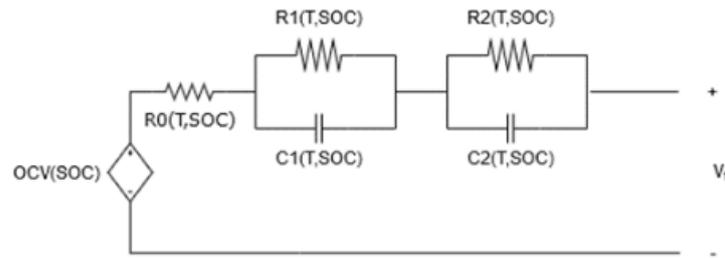


Figure 2.1 : Example of electric circuit model of the battery cell.

correlates deviation of simulated output from actual output to internal states of the model including SOC.

2.2.2 Electrochemical model

Electrochemical models make direct use of chemical reactions to arrive at an expression for SOC. This method although describing the physics behind the battery is difficult to implement in a computationally efficient way on a low cost microcontroller. However there are studies that has tried to simplify the complex mathematical expressions to arrive at computationally more feasible method.

2.3 Hybrid Methods

Aforementioned methods could be used in conjunction with each other to produce hybrid methods. Recently data driven physics based models are popular. This will result in a stable algorithm with less calibration effort. For instance parameters of an ECM could be determined by a machine learning algorithm. Hybrid methods are good ways of compensating for pitfalls of certain methods. Table 2.1 summarizes performance of discussed methods.

In this thesis work, we first use an ECM in conjunction with a state observer for SOC estimation. Later in second part we use a data driven method mainly machine learning algorithm for estimation. The results will be discussed in detail and conclusions are to be made after post analysis. The cell used for the study is from Battery Research Group of Center for Advanced Life Cycle Engineering [38]. The cell has specifications outlined in the table 2.2. An Arbin BT2000 Battery Test System has been used

Table 2.1 : Comparison of methods for battery state estimation.

Method	Accuracy/ Noise-Tolerance	Complexity	Calibration Effort	Validity over Time
Coulomb Counting	- - -	+ + +	+ + +	- - -
Data-Driven	+ +	-	+ + +	-
ECM	+ +	+ +	+	-
Electrochemical Model	+ +	- -	+	+

to retrieve data from the cell placed in a temperature chamber for setting the test temperature.

Table 2.2 : Battery Cell Specification [38].

Battery Sample	Battery Parameter	Specification
	Rated Capacity	2000 Ah
	Cell Chemistry	LNMC/Graphite
	Weight	45.0 g
	Radius	$18.33 \pm 0.07 \text{ mm}$
	Length	$64.85 \pm 0.15 \text{ mm}$

3. BATTERY DYNAMICS AND PARAMETERIZATION

In this part, an equivalent electric circuit model of the battery will be developed. However, as it would become evident, understanding the battery dynamics is crucial in developing an accurate model. Therefore, a thorough analysis of physics of the battery is outlined first.

3.1 Open-Circuit Voltage

One important characteristic of the battery is the voltage of the battery when it is disconnected from the load. SOC could be determined directly from this voltage. Therefore before visiting dynamics of the battery it is necessary to acquire this data through specific tests procedure of which are outlined in table 3.1.

Table 3.1 : OCV test procedure.

STEP	DESCRIPTION	PROFILE	DURATION	MEASUREMENT
1	Fully charging the battery	CC-CV	Depends on SOC of the battery before charging	Cut-off voltage for CC phase and then cut-off current for CV phase
2	Rest the battery	$I = 0$	> 1 hour	Voltage at the end of rest period
3	Discharge the battery	Continuous discharge current	Until 10% of capacity is removed i.e. $\Delta T = \frac{0.1 * 3600 * C_{tot}}{I}$	-
4	Rest the battery	$I = 0$	> 1 hour	Voltage at the end of rest period
5	Repeat steps 3 and 4 until minimum energy is reached or minimum voltage was observed	-	-	-

For a particular temperature, firstly battery is fully charged using Constant Current-Constant Voltage(CC-CV) procedure which is illustrated in figure 3.1. Battery is rested for long enough time usually more than an hour then voltage is measured. Battery is then discharged with constant current to remove a defined percentage of the energy. Battery is rested for more than an hour and voltage is measured. The procedure is repeated until minimum available energy is reached or minimum voltage was observed. Moreover, procedure is applied in other current direction for charge case.

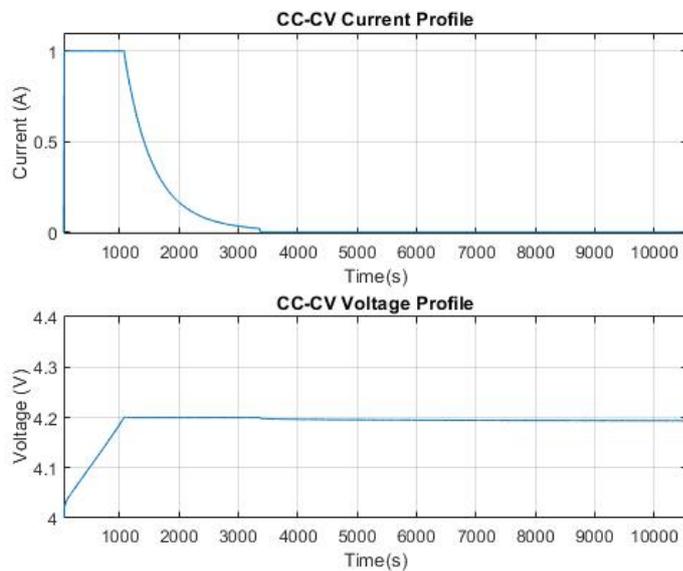


Figure 3.1 : Constant Current - Constant Voltage Profile.

For further clarity, 10% discharge of the battery energy is shown in figure 3.2.

Processing the data from the OCV test for 3 different temperatures namely; 0°, 25°, 45° and averaging them over charge and discharge curves we can construct a 2-D OCV look-up table as a function of SOC and temperature which is depicted in figure 3.3.

3.2 Battery Dynamics

Before obtaining the parameters of equivalence electric circuit model of figure 2.1 it is important to know the reasoning behind such representation so that reasonable parametrization could be obtained.

A dynamic system is defined in terms of inputs and outputs. As depicted in figure 3.4, a time dependent signal $u(t)$ is the system stimulation and $y(t)$ is the system response.

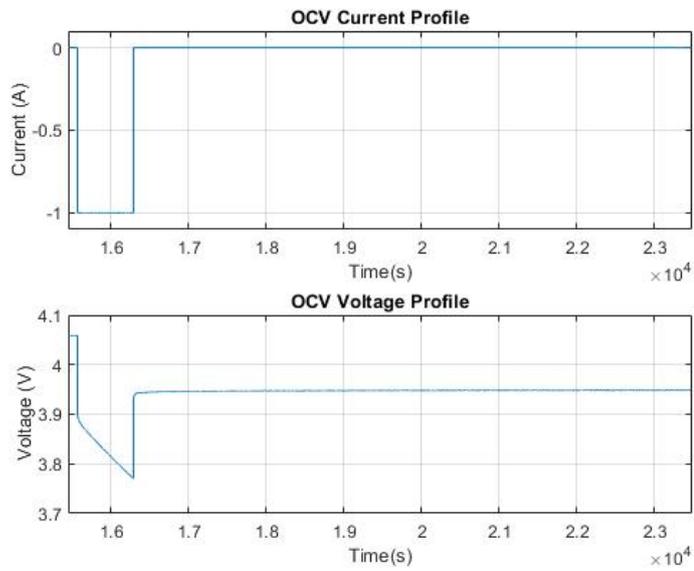


Figure 3.2 : OCV Current and Voltage Profile Example.

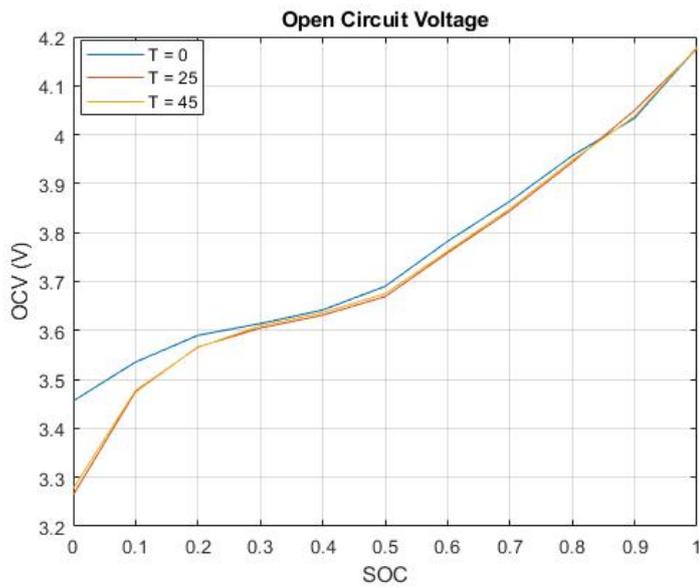


Figure 3.3 : Open Circuit Voltage Look-up Table.

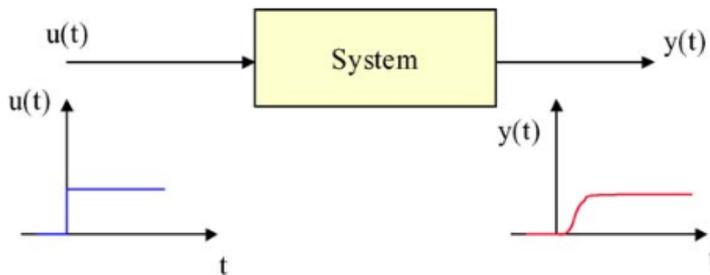


Figure 3.4 : Input and output illustration of a dynamic system [7].

System dynamics could be represented by set of differential equations $\dot{y}(t) = f(y(t), u(t))$

For batteries, it is common that current and ambient temperature would be taken as inputs while voltage, cell temperature, SOC, SOP, SOH, SOE be considered as outputs. To understand and be able to interpret dynamics of the battery it is crucial to know physical effects inside the battery resulting in responses in time and frequency domains. Different physical effects are behind time domain responses of the battery which could range from microseconds such electric and magnetic effects up to several years due to operation principles like mass transport and double-layer effects as well as operation conditions. Figure 3.5 depicts time ranges of effects due to different dynamics of the battery.

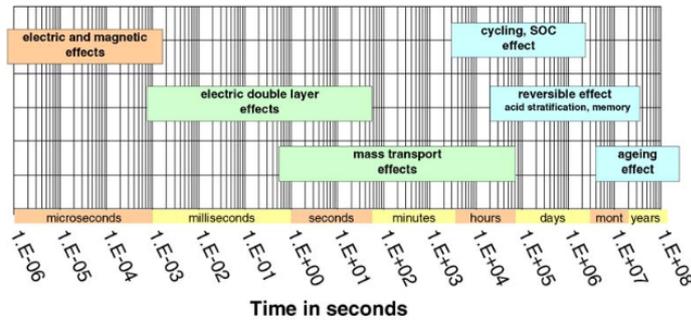


Figure 3.5 : Time effects of different dynamics of the battery [7].

3.2.1 Analysis of battery dynamics using electrochemical impedance spectroscopy (EIS)

This technology is very useful in understanding battery behavior. As shown in figure 3.6 Nyquist plot of complex impedance over a range of frequency gives good insight into internal dynamics of the battery.

Characteristics of battery impedance is mainly capacitive, therefore imaginary axis is flipped so that the curve is positioned at the upper part of the plot. Inspired by typical EIS analysis of batteries, we will construct equivalent circuit model.

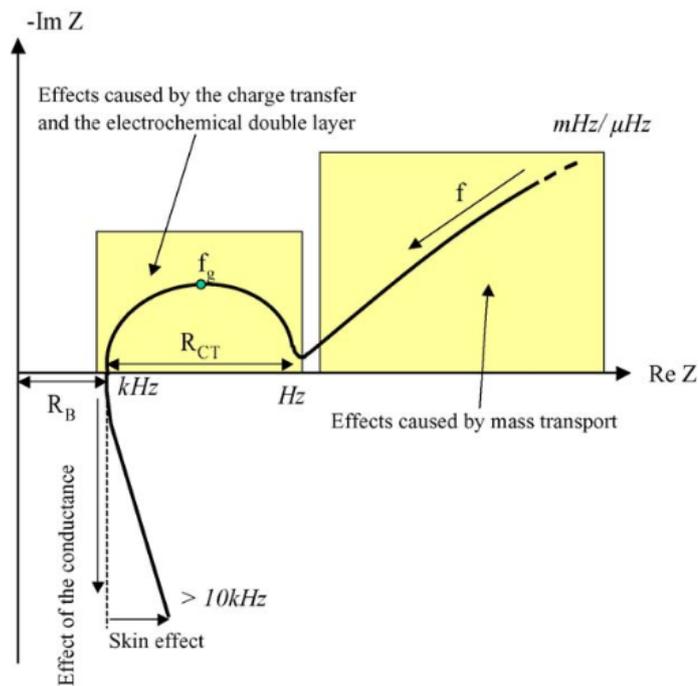


Figure 3.6 : Typical Nyquist plot of impedance of a battery [7].

3.2.2 AC resistance

This is the pure resistive effect of the battery at high frequency which is pointed in figure 3.6 as R_B

3.2.3 Butler-Volmer impedance (double-layer capacitance)

This phenomenon occurs between electrolyte and electrode. The effect is observed in porous electrodes with large surfaces and in the vicinity of the electrodes as shown in figure 3.7. Voltage of the electrode causes stored charge in the layer which behaves like a capacitor thus called double-layer capacitance.

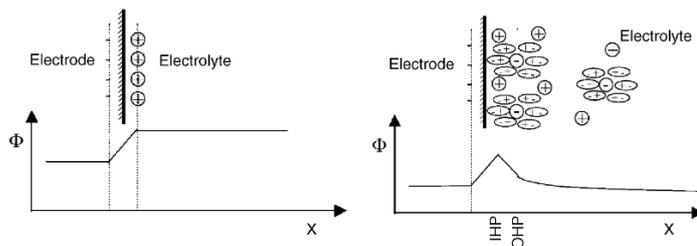


Figure 3.7 : Two models describing the double-layer capacity: on the left, the Helmholtz model and on the right, the Grahame model [7].

Among numerous modeling approaches, one commonly used in literature consists of a capacitor in parallel with a resistance as shown in figure 3.8. Charge transfer reaction is combination of electrochemical potential and charge transfer over potential which is obtained from Butler-Volmer equation. Electrochemical potential is neglected since the resistance is of 0Ω .

In the equivalent electrical circuit model, R_{CT} represents charge transfer over potential where C_{DL} is to model double-layer capacitance. Ohmic series resistance is independent of double-layer capacitance. It must be noted that R_{CT} and C_{DL} depend on SOC, temperature, ageing as well as current.

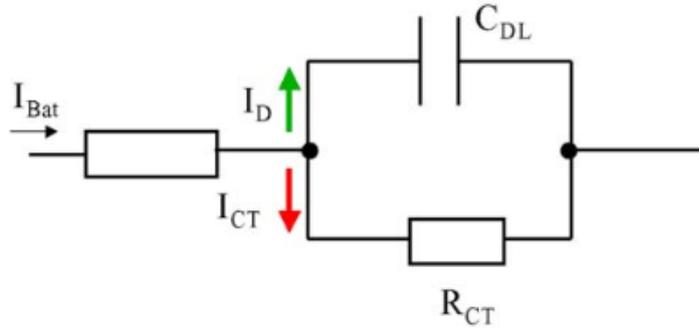


Figure 3.8 : Equivalent Circuit Model of double-layer capacitance [7].

Double-layer capacitance behaves like a low-pass filter therefore only AC currents will be carried. Revisiting Nyquist representation as of figure 3.6, cut-off frequency and time constants are obtained as

$$f_g = \frac{1}{2\pi RC} \quad (3.1)$$

and

$$\tau_{RC} = RC \quad (3.2)$$

Where f_g is the high frequency region in impedance spectrum and R is the diameter of the curve as shown in figure 3.9.

This element is what we refer to as fast dynamics in our equivalent electric circuit model and it ranges from milliseconds up to tens of seconds.

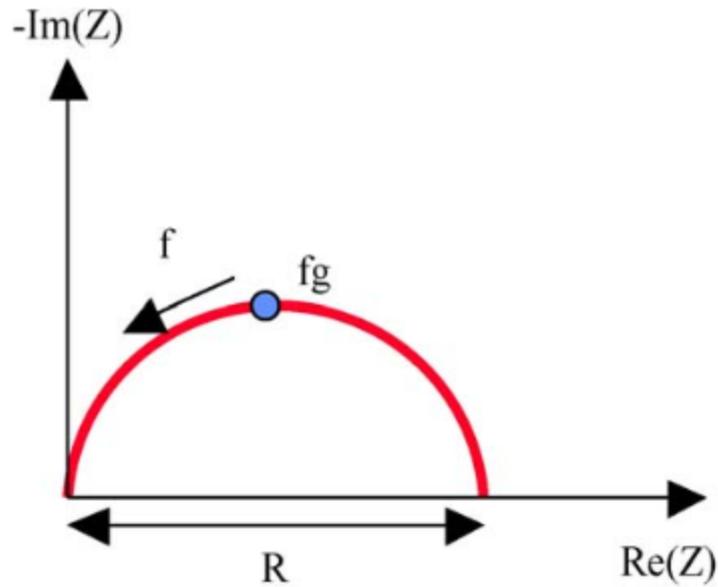


Figure 3.9 : Impedance Curve of a RC filter [7].

3.2.4 Warburg impedance

The transport of ions inside the battery happens either due to migration or diffusion. Diffusion is due to gradient in concentration which is the dominant cause for mass transport. Diffusion occurs:

- in the free electrolyte or separator
- in porous electrode which has great impact on battery dynamics
- reaction products that move to their final location
- On the surface of anode of the battery, there is a film which is referred to as Solid Electrolyte Interface (SEI) through which diffusion occurs which has great impact on behavior of the battery.

Visual depiction of diffusion inside the battery is done in figure 3.10.

Diffusion effects have life time from seconds to minutes. We will refer to this time response as slow dynamics. The time depends on electrode thickness and structure. It corresponds to low frequency (< 1 Hz) region of impedance spectrum. Furthermore, like double-layer capacity diffusion is not static and depends on temperature as well as free ions in electrolyte as well as porous structure of the electrodes. The planar plot

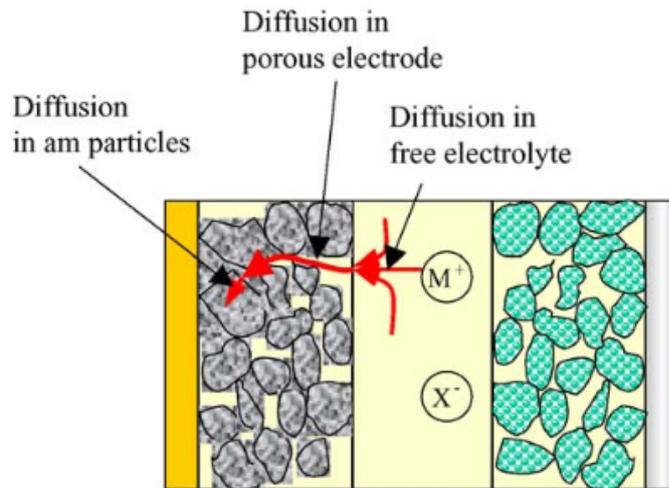


Figure 3.10 : Diffusion process inside the battery [7].

in figure 3.11 shows a semi-infinite diffusion layer with -45° phase where electrolyte reservoir is infinite. In this case Warburg impedance could be written as:

$$Z_\omega = \frac{\sigma}{\sqrt{\omega}} - j \frac{\sigma}{\sqrt{\omega}} \quad (3.3)$$

Where, Z_ω is the Warburg impedance, σ is the diffusion coefficient and ω is the angular frequency.

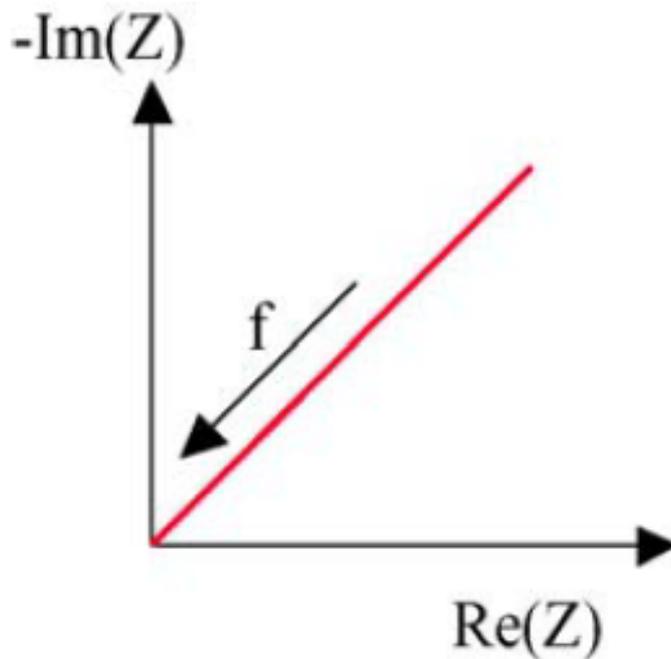


Figure 3.11 : Nyquist plot for semi-infinite diffusion layer [7].

In general, R, C, L elements are not sufficient to precisely represent diffusion however, for our application using the equation 3.3 to construct a RC filter would give acceptable results.

Figure 3.12 summarizes this section. The importance of understanding dynamics of the battery to obtain plausible and realistic model must be noted.

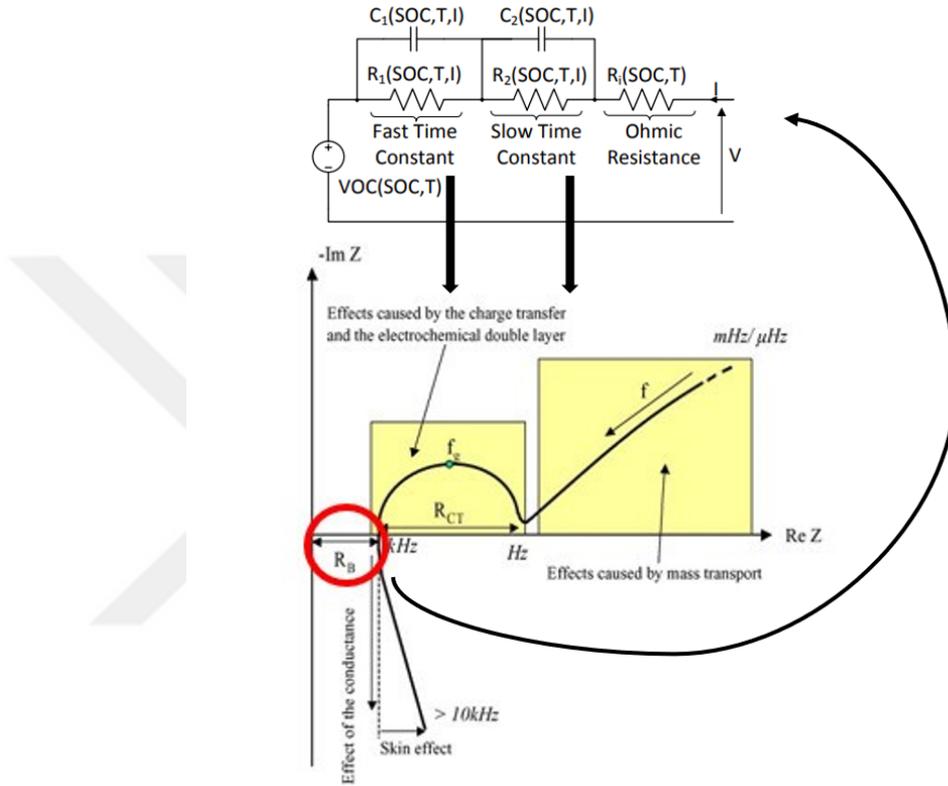


Figure 3.12 : Dynamics of the battery corresponding to equivalent electric circuit model [7, 39].

3.3 Parametrization

Having learned dependency of circuit elements on temperature and SOC, we will create 2-D look-up tables for each element. This would mean constructing an optimization problem that would run in a loop. From electric circuit theory, the solution to an RC network shown in figure 3.13 in time domain could be written as follows:

$$I_R(t) = I_R(0)e^{-\frac{t}{\tau}} + I(t)(1 - e^{-\frac{t}{\tau}}) \quad (3.4)$$

By first-order Taylor series approximation and discretizing the system one obtains:

$$I_R(k+1) = I_R(k) \frac{\tau}{\Delta t + \tau} + I(k) \frac{\Delta t}{\Delta t + \tau} \quad (3.5)$$

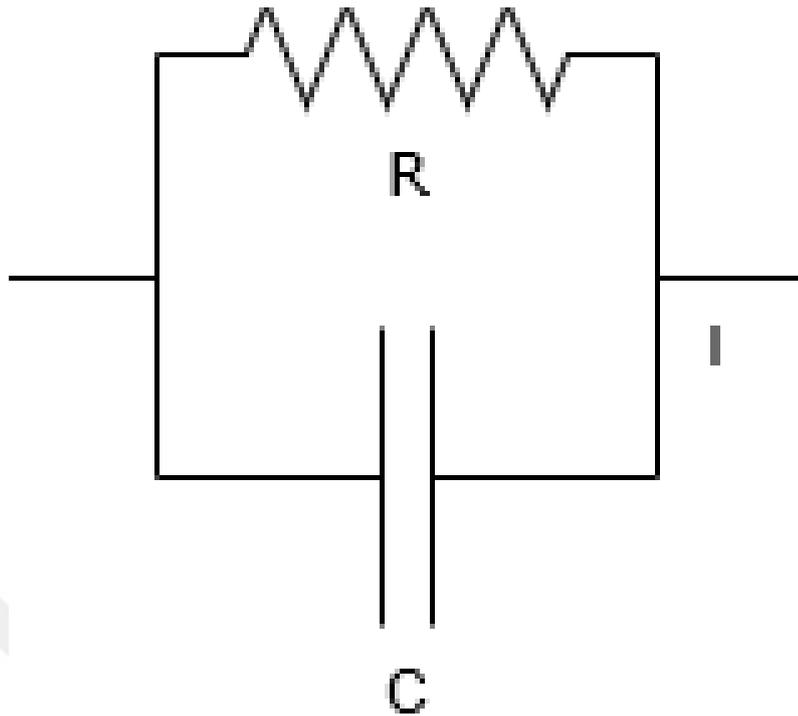


Figure 3.13 : RC Circuit.

Where Δt is the sampling time.

For a particular current profile I , current response I_R for two different time constants were shown in figure 3.14.

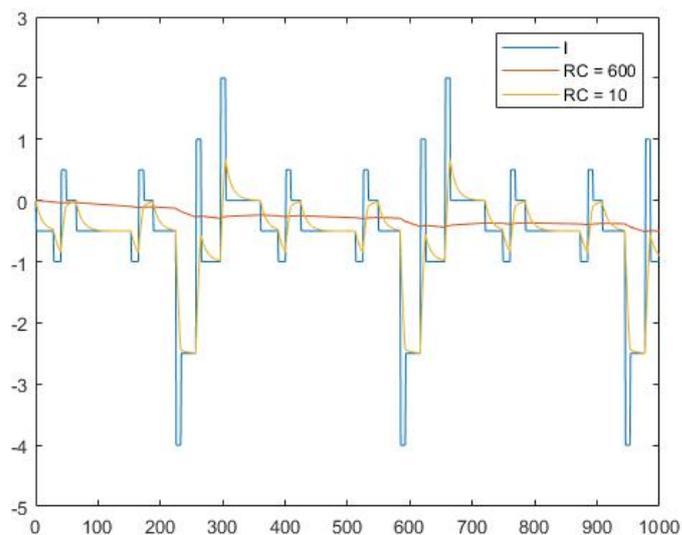


Figure 3.14 : Current response of an RC filter for different time constants.

It is clear to see slow and fast dynamics looking at the current responses. With bigger time constant current response is slower and it does not follow a dynamic current. In

light of current dynamics described in equations 3.4 3.6 the solution to circuit in figure 2.1 is straight-forward:

$$V_t = OCV(T, soc) + IR + I_1R_1 + I_2R_2 \quad (3.6)$$

it would be of use specially when designing the observer to represent the dynamics of the system in state-space:

$$\begin{pmatrix} soc_{k+1} \\ i_{1,k+1} \\ i_{2,k+1} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{\tau_1}{\Delta t + \tau_1} & 0 \\ 0 & 0 & \frac{\tau_2}{\Delta t + \tau_2} \end{pmatrix} \begin{pmatrix} soc_k \\ i_{1,k} \\ i_{2,k} \end{pmatrix} + \begin{pmatrix} \frac{\Delta t}{3600C} \\ \frac{\Delta t}{\Delta t + \tau_1} \\ \frac{\Delta t}{\Delta t + \tau_2} \end{pmatrix} I(k) \quad (3.7)$$

Now the optimization problem could be constructed in the form of:

$$\min_{x \in \mathbb{R}} \sqrt{(V_{actual} - V_t)^2} \quad (3.8)$$

where $x = \begin{pmatrix} soc_{k+1} \\ i_{1,k+1} \\ i_{2,k+1} \end{pmatrix}$

It must be noted that time constants are not considered in optimization as they can be found separately using a static profile such as those of OCV test. With doing so, accuracy of optimization result in terms of resistances are not compromised by time constants. Figure 3.15 depicts result of curve fitting to find time constant. Using the static OCV pulses time constants of 10 and 600 seconds were determined which would be used in parametrization.

Having a well-defined optimization problem at hand we use Genetic Algorithm(GA) to solve the problem of finding global minima. The optimization was run over data obtained from a Dynamic Stress Test available in [38]. Obtaining resistance values as look-up tables depending on temperature as well as SOC, figure 3.16 through 3.18

Before moving forward with validation, one clear observation is that resistance is higher in low temperature and low SOC for all three maps. Generally toward the

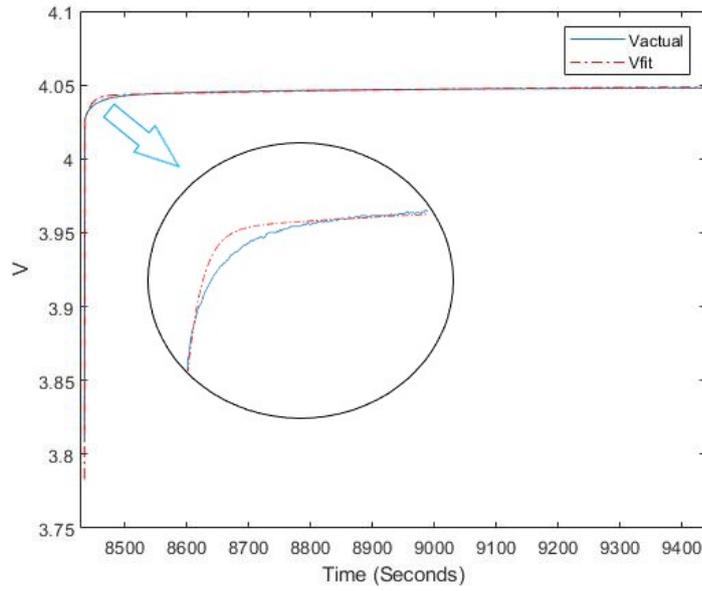


Figure 3.15 : Time constant fit.

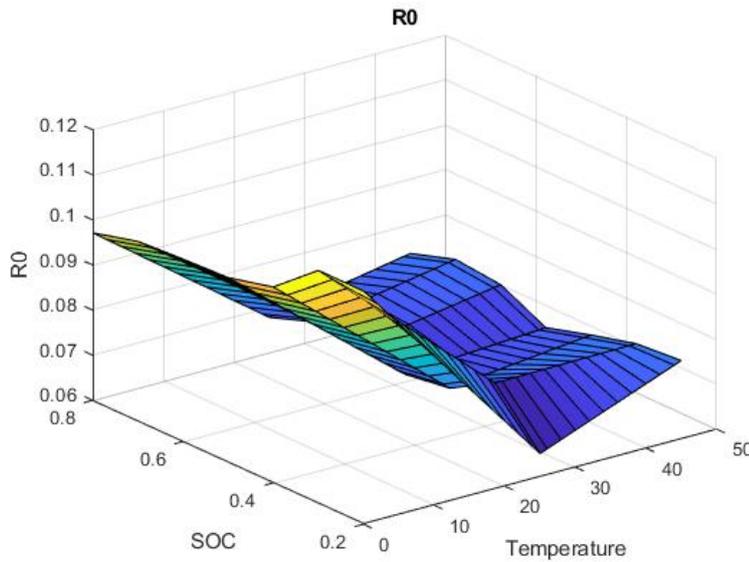


Figure 3.16 : R_0 Map.

edges of SOC, it is difficult to model the battery easily as it is highly non-linear in those regions. This conclusion is consistent with our observation of OCV maps. This information is particularly important to bear in mind while designing observer in the next section. Figure 3.19 shows accuracy of the model when a Federal Urban Driving Schedule (FUDS) [40] profile is applied.

Accuracy of the model could be summarized in terms of error distribution:

$$\mu_E = -0.0184; \sigma_E = -0.0129 \quad (3.9)$$

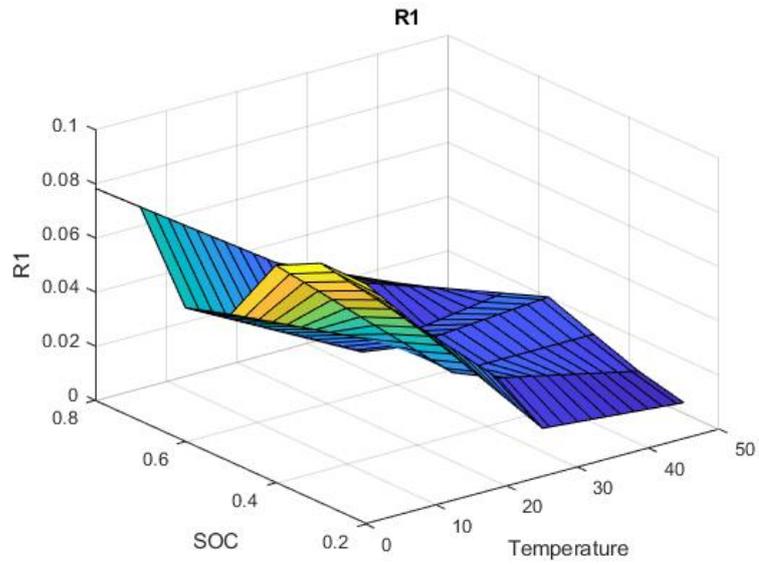


Figure 3.17 : R_1 Map.

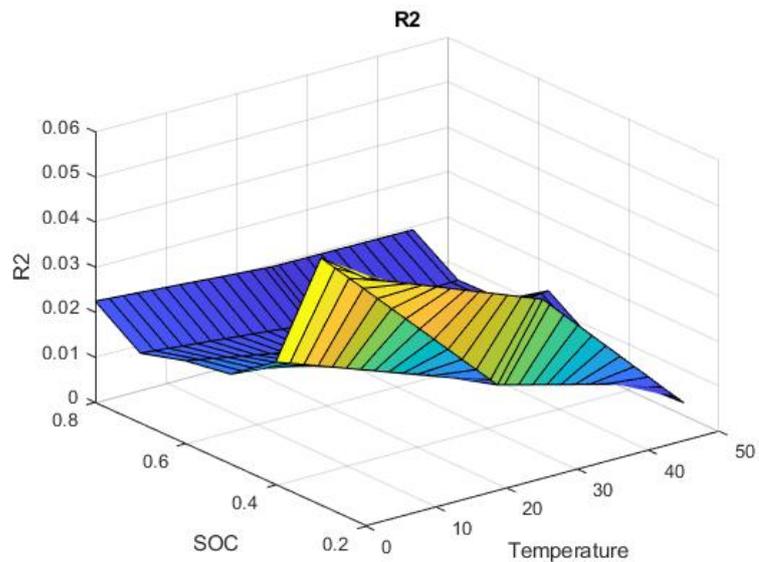


Figure 3.18 : R_2 Map.

Which indicates our model accuracy is high. In order to observe this result clearer we can zoom in to a region of voltage response. Figure 3.20 shows actual voltage measurement and voltage predicted from the model which indicates that our model represents dynamics of the battery very well.

There seems to be a constant offset between the signals which is expected due to possible wrong initial SOC value. This offset could be inferred from statistics of the error in equations of 3.9 in particular from non-zero mean. The issue of constant offset will be addressed in the following chapter by designing an observer.

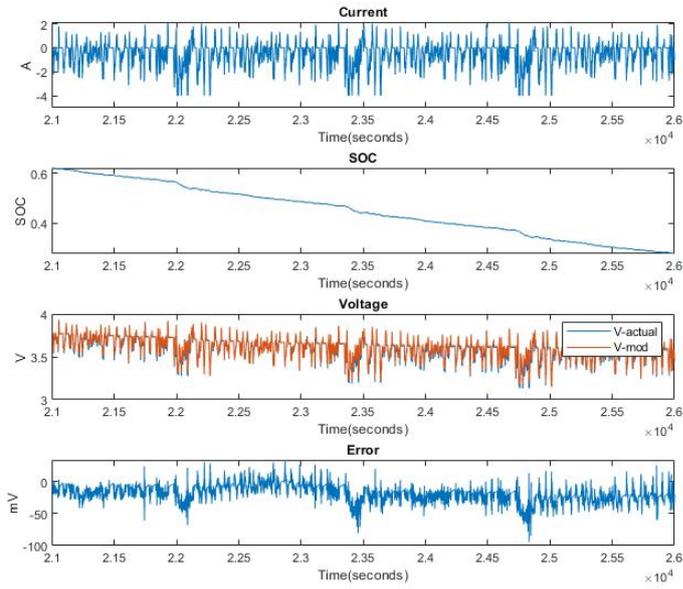


Figure 3.19 : Model Validation with FUDS profile.

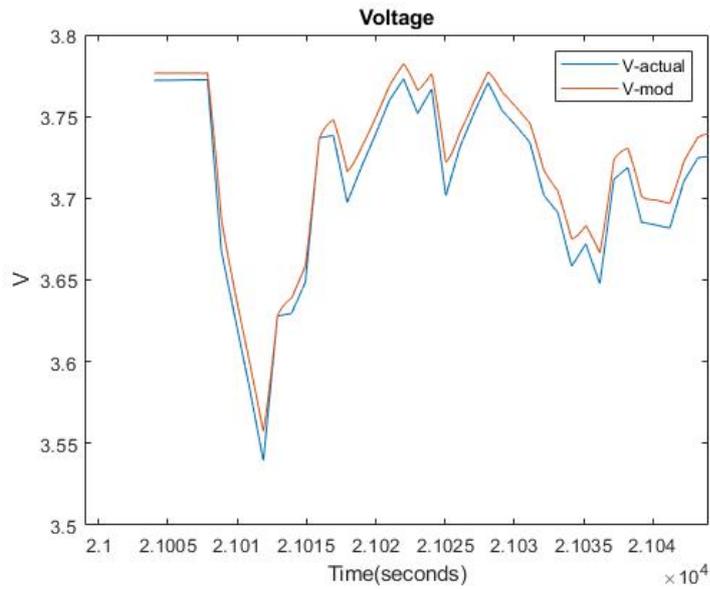


Figure 3.20 : Detailed voltage observation for model accuracy.

4. STATE-OF-CHARGE ESTIMATION USING LUENBERGER OBSERVER

As was seen from results of previous sections as well as theoretical knowledge about disadvantages of coulomb counting, wrong initialization would lead to a persistent erroneous estimation of SOC. Therefore a correction method is needed.

4.1 Luenberger Observer Design

To have a correction approach, Luenberger observer is used. This method is particularly interesting because it is computationally advantageous compared to their statistical counterparts such as Kalman Filters. For a system represented as:

$$x(k+1) = Ax(k) + Bu(k) \quad (4.1)$$

$$y(k) = Cx(k) + Du(k) \quad (4.2)$$

an observer makes use of the deviation between output actual measurement and model output prediction to correct the estimation in a closed-loop manner:

$$x(k+1) = A\hat{x}(k) + Bu(k) + L[y(k) - \hat{y}(k)] \quad (4.3)$$

Where L is the observer gain. In designing observers there is the problem of observability which needs to be paid attention to. Observability is the measure to determine whether there is enough information in terms of input and output history such that a state could be estimated. Mathematically this could be examined via observability matrix:

$$P = \begin{pmatrix} C \\ CA \\ \vdots \\ CA^{n-1} \end{pmatrix} \quad (4.4)$$

A system is observable if and only if $\text{rank}(P) = n$.

Revisiting equation 3.7 it is clear that observability of a battery system is dependent on temperature and SOC. Therefore, we will activate correction only when operating in observable region. As could be seen from the model validation results, battery behaves very non-linear in low temperature as well as edge SOC. Hence, we tune observer gain with respect to those regions. The observer designed for SOC estimation is depicted in figure 4.1.

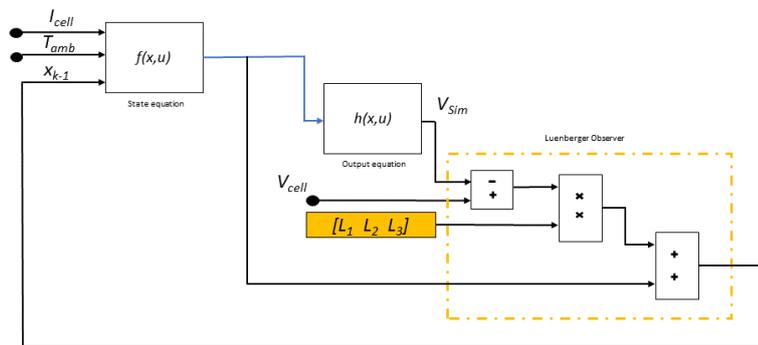


Figure 4.1 : Overview of system design with observer.

4.2 Validation

To validate this algorithm, we will look into pitfalls of coulomb counting. In other words we will intentionally start the simulation with a wrong initial SOC and observe whether it would be corrected and how long would it take to reach the actual SOC. This could be seen in figure 4.2.

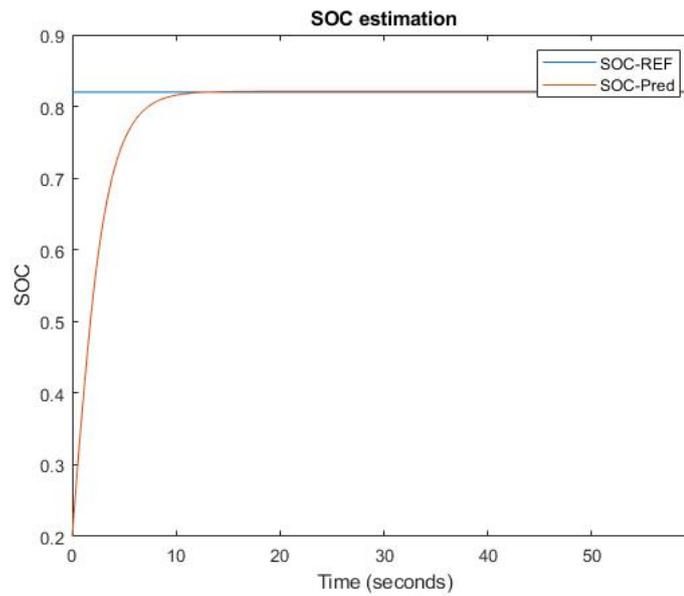


Figure 4.2 : SOC estimation performance of designed observer.

It can be seen that SOC estimation tracks the reference value after 10 seconds. For this simulation the observer gain was chosen very low i.e. $L = [0.01 \ 0.01 \ 0.01]$. Larger gain would result in faster convergence however overshoot was observed that would lead to unstable estimation at times.

In this part we accomplished to implement a SOC estimator by modeling a LIB cell from understanding of physics and developed a stable observer to cover drawbacks and closing the estimation loop. Although the results were convenient however one might find the process effortful. In next chapter a data driven method is implemented which would be beneficial in minimizing calibration effort.



5. STATE-OF-CHARGE ESTIMATION USING MACHINE LEARNING

In this chapter, machine learning is used to estimate SOC. Expectation is that calibration effort would be minimum however demand for data and processing power would be high. Since validation and verification is major concern specially in automotive industry, machine learning model method is chosen to follow physical principles of the battery. Revisiting OCV plot of figure 3.3 it is seen that battery dynamics could be split in different regions based on temperature and SOC: based on temperature we divide the regions by two:

- Low temperature i.e. $T = 0^\circ$
- Normal temperature i.e. $T > 20^\circ$

Based on SOC we can split the region in three:

- Low SOC i.e. $SOC < 0.2$
- Medium SOC i.e. $0.2 \leq SOC \leq 0.8$
- High SOC i.e. $SOC > 0.8$

Therefore there will be six models for in total.

Furthermore, a structure of the models could be changed as well.

5.1 Method I

First SOC is predicted using a linear regression:

$$SOC_{pred} = c_0 + c_1I + c_2T + c_3V \quad (5.1)$$

Using Multi-Linear Regression method, coefficients were obtained and the model is used to obtain error on test data which could be minimized using Polynomial-Linear Regression:

$$SOC_e = SOC_{act} - SOC_{pred} \quad (5.2)$$

$$SOC_e = c_1V + c_2V^2 + c_3V^3 \quad (5.3)$$

Validation result of one model out of six is shown in figure 5.1 and coefficients of all models for low and normal temperatures are outlined in tables 5.1 and 5.2 respectively.

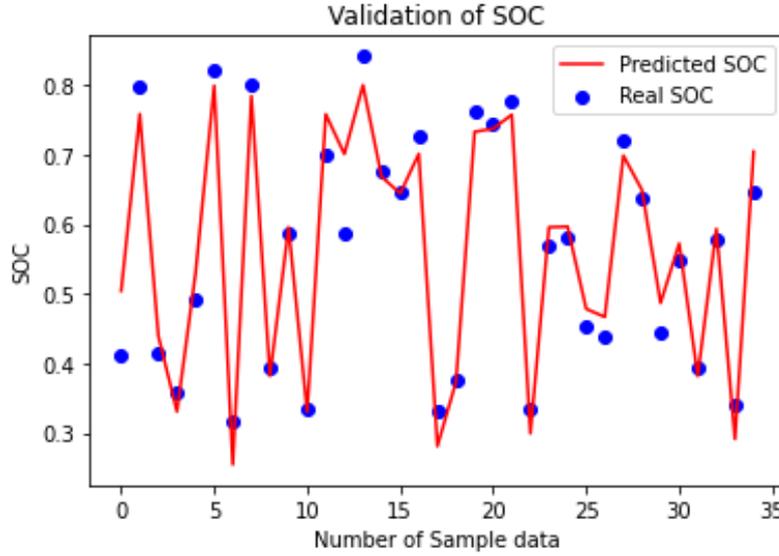


Figure 5.1 : Validation for $0.2 \leq SOC \leq 0.8$ and $T = 25^\circ$.

Table 5.1 : Coefficients of the model for $T = 0^\circ$.

Coefficients	$0.2 \leq SOC \leq 0.8$	$SOC < 0.2$	$SOC > 0.8$
$c_0 + c_4$	4.034	-12.486	-1.903
c_1	-0.160	-0.052	-1.903
c_2	0	0	0
$c_3 + c_5$	-39.526	11.884	0.695
c_6	11.668	-3.834	0
c_7	-1.105	0.420	0

5.2 Method II

In this method in addition to parameters already included in previous method, power i.e. $I \times V$ is considered. Equations 5.7 through 5.6 represent the regression problem.

$$SOC_{pred} = c_0 + c_1I + c_2T + c_3V + c_4IV \quad (5.4)$$

Table 5.2 : Coefficients of the model for $T > 20^\circ$.

Coefficients	$0.2 \leq SOC \leq 0.8$	$SOC < 0.2$	$SOC > 0.8$
$c_0 + c_4$	81.263	-11.305	276.949
c_1	-0.124	-0.033	-0.066
c_2	-0.001	0	0
$c_3 + c_5$	-72.485	12.034	-208.590
c_6	21.968	-4.291	52.296
c_7	-1.993	0.510	-4.351

$$SOC_e = SOC_{act} - SOC_{pred} \quad (5.5)$$

$$SOC_e = c_1V + c_2V^2 + c_3V^3 \quad (5.6)$$

Similar to previous methods six models were trained and validation result for one out of six is shown in figure 5.2

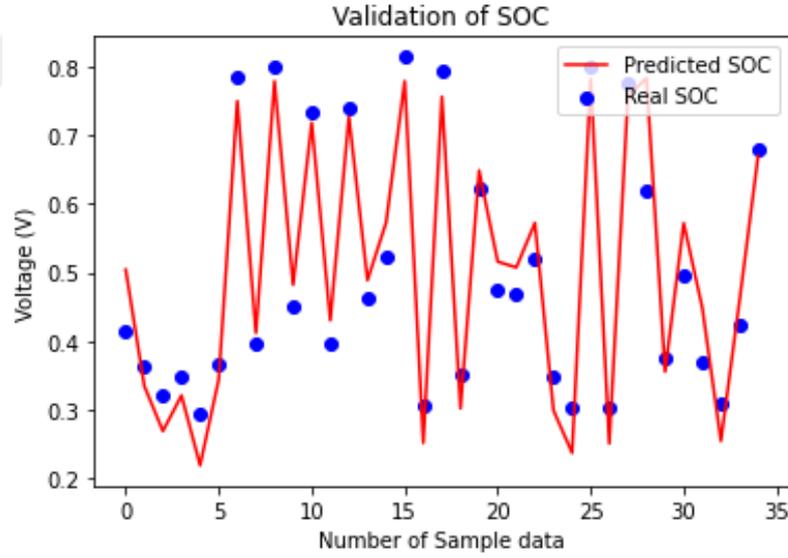


Figure 5.2 : Validation for $0.2 \leq SOC \leq 0.8$ and $T = 25^\circ$.

5.3 Method III

Finally the problem is constructed in one stage:

$$SOC_{pred} = c_0 + c_1I + c_2T + c_3V + c_4V^2 + c_5V^3 + c_6IV \quad (5.7)$$

Validation for this method is shown in figure 5.3

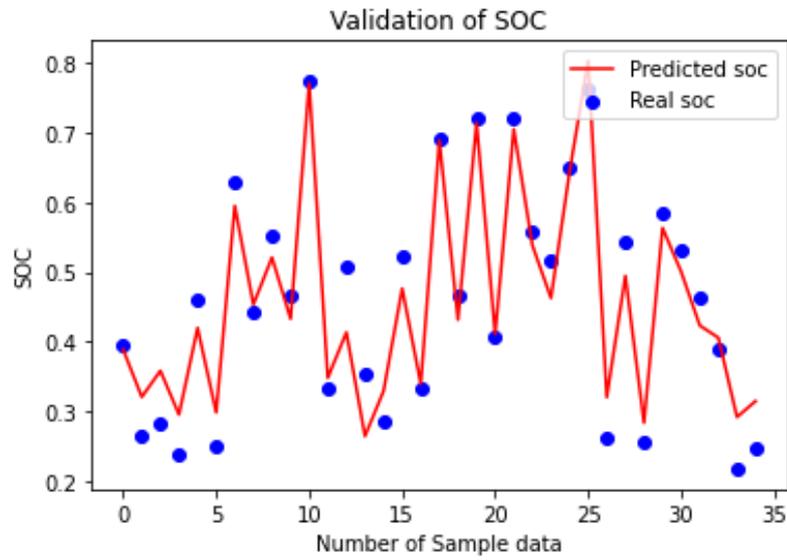


Figure 5.3 : Validation for $0.2 \leq SOC \leq 0.8$ and $T = 25^\circ$.

In spite of advantages in calibration effort data driven methods are prone to unstable results. Testing the algorithm with a dynamic profile is done and the result is shown in figure 5.4

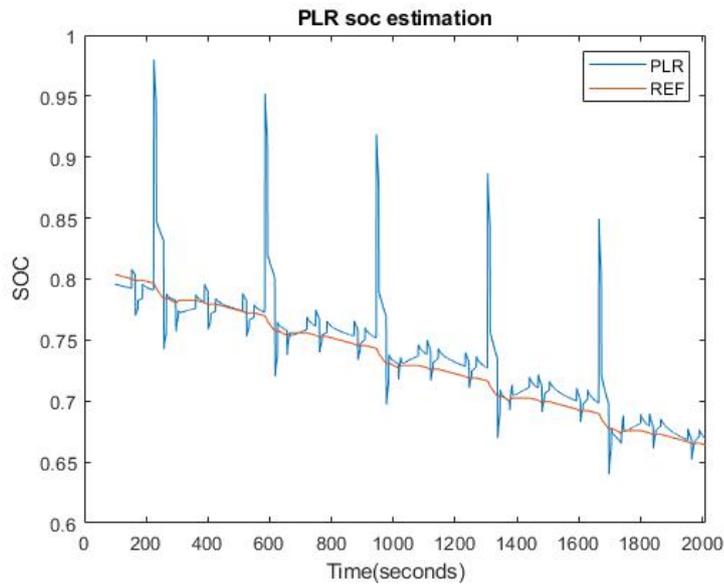


Figure 5.4 : Validation of Polynomial Linear Regression on FUDS profile.

6. CONCLUSIONS AND RECOMMENDATIONS

The results show that although calibration effort is more in using ECM compared to data-driven method, it is more accurate and stable. Furthermore, since it is not a black box, algorithms based on ECM are verifiable which makes them applicable in safety critical applications such as automotive and aviation.

It is suggested that data-driven techniques be used for calibration and modelling of the battery dynamics which would reduce calibration effort significantly. Furthermore, there is high potential in determining dynamics of the battery from chemical point of view with the help of data-driven methods.



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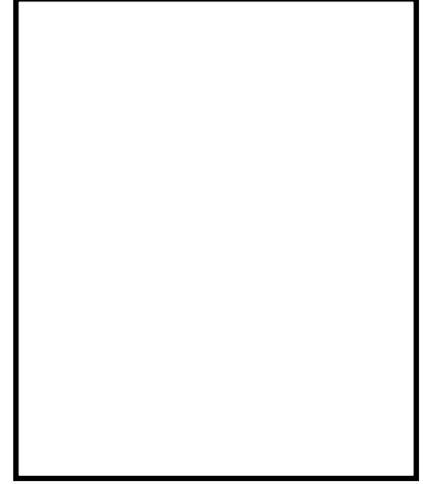
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