



POLITECNICO DI MILANO

DEPARTMENT OF INDUSTRIAL AND INFORMATION ENGINEERING
MASTER OF SCIENCE IN AUTOMATION AND CONTROL ENGINEERING

**DESIGN AND EXPERIMENTAL VALIDATION OF A BACKSTEPPING
STATE OBSERVER FOR A LI-ION CELL ELECTROCHEMICAL
MODEL**

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Master Thesis

by

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Abstract

Lithium-ion batteries are used for Electric vehicles and Hybrid electric vehicles as a key technology because of their high power and high energy density. In most applications, a battery is managed by a Battery Management System (BMS). A BMS guarantees safe operation conditions for Li-ion battery by managing the current, voltage, state of charge and temperature of the cell. To improve the efficiency of the battery and to avoid safety problems, accurate estimation of the state of the battery, which is a challenging task, is necessary within the BMS.

In the present work a single particle model (SPM) of a production Lithium-ion cell is presented, and its parameters are identified based on experimental data. Based on this model, a partial differential equation (PDE) backstepping observer is designed for the estimation of the gradient of Lithium concentration along the radius of particle and of battery SoC. Then, the performances of the proposed observer are validated for 2C constant current test and 2C pulse discharge test to demonstrate that the backstepping observer successfully estimates SoC and Lithium concentration along the particle radius (in simulation). The results show that bulk SoC estimation error lower than 1% is reached for both tests. Also, it is confirmed in simulation that the proposed observer is robust with respect to noise on voltage measurement and uncertain model parameters. In the latter scenario, several parameters are varied in the observer model from 50% to 98% of their original value. The SoC estimation error is less than 1.1% for all tests, also in these conditions. Finally, the observer is validated with experimental tests, in which an SoC estimation error of less than 3% after convergence is obtained.



Astratto

Le batterie agli ioni di litio (Li-ion) sono utilizzate per veicoli elettrici e veicoli ibridi elettrici come tecnologia chiave grazie alla loro elevata densità di potenza e di energia. Nella maggior parte delle applicazioni, una batteria è gestita da un sistema di gestione della batteria (Battery Management System, BMS). Un BMS garantisce condizioni di funzionamento sicure per la batteria Li-ion gestendo la corrente, la tensione, lo stato di carica e la temperatura della cella. Per migliorare l'efficienza della batteria e per evitare problemi di sicurezza, è necessaria una stima accurata dello stato della batteria all'interno del BMS, la qual cosa rappresenta un compito tecnologicamente impegnativo.

Nel presente lavoro viene presentato un Single Particle Model (SPM) di una cella agli ioni di litio in produzione, i cui parametri sono identificati a partire da dati sperimentali. Sulla base di questo modello, si progetta un osservatore backstepping per equazioni alle derivate parziali (Partial Differential Equations, PDEs), per la stima del gradiente di concentrazione del litio lungo il raggio della particella e del SoC della batteria. Quindi, le prestazioni dell'osservatore proposto sono convalidate per test a corrente costante pari a 2C e test di scarica a impulsi a 2C, per dimostrare che l'osservatore backstepping stima con successo il SoC e la concentrazione di litio lungo il raggio della particella (in simulazione). I risultati mostrano che per entrambi i test è stato raggiunto un errore di stima del SoC concentrato inferiore all'1%. Inoltre, è confermato nella simulazione che l'osservatore proposto è robusto rispetto al rumore sulla misura della tensione e all'incertezza parametrica del modello. In quest'ultimo scenario, vari parametri sono variati nel modello dell'osservatore dal 50% al 98% del loro valore originale. L'errore di stima del SoC è inferiore all'1.1% per tutti i test, anche in queste condizioni. Infine, l'osservatore è convalidato con test sperimentali, nei quali si ottiene un errore di stima del SoC inferiore al 3% dopo la convergenza.



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1 Introduction

1.1 Motivation

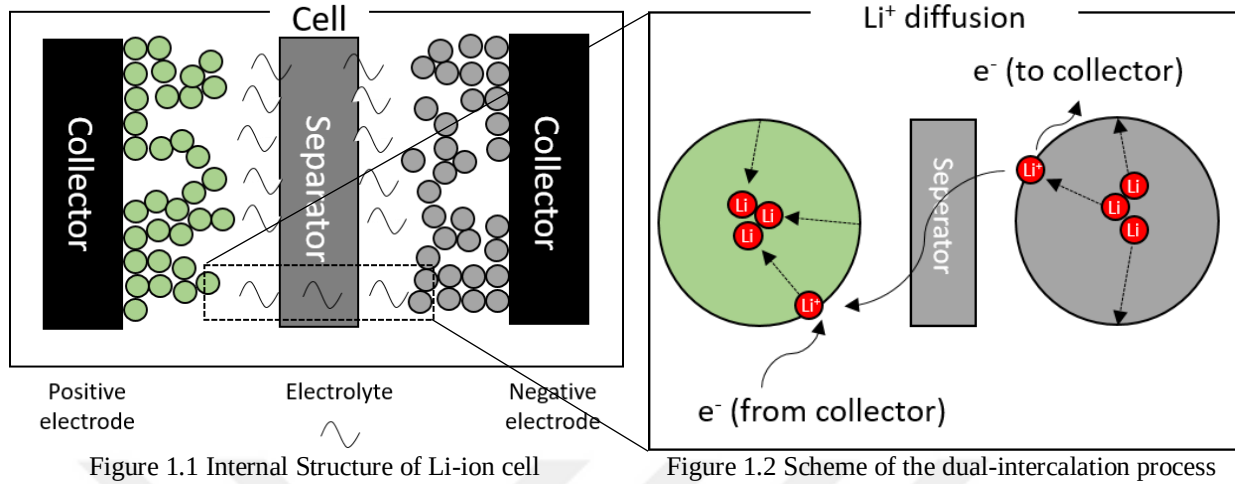
Nowadays, Lithium-ion cells are used for several applications like cell phone, laptop and many other consumer electronics. Besides their use in these applications, they are also the most common solution for electric vehicles (EVs) and hybrid electric vehicles (HEVs) thanks to their high power, high energy density and low self-discharge. In most applications, Li-ion cells need an advanced Battery Management System (BMS). The scope of a BMS is to avoid safety problems and avoid harmful operating conditions, which can cause anticipated battery aging. BMS for Li-ion batteries requires a model that represents battery dynamics, and by improving model accuracy, parameter identification techniques and state estimation methods, a sophisticated BMS can be obtained. For this purpose, the research about modelling, parameter identification and state estimation of Lithium-ion batteries has grown considerably over the past decade.

1.2 State of the art

A Li-ion cell mainly has three components: a negative electrode, positive electrode, and a separator (Figure 1.1). Both electrodes have a lattice structure that can store Lithium. A separator is a porous medium that separates the positive electrode from the negative electrode, and it allows only the Lithium-ions to flow through it, as an electrical insulator. During discharge, Lithium diffuses to the surface of active material particles of the negative electrode and it undergoes the electron generating reaction. The Lithium ions dissolve in the electrolyte and moves to the positive electrode by crossing the separator, while electrons which are divided from Lithium are conducted to the current collector by the solid lattice. After both Lithium ions and electrons reach the positive electrode, they are reabsorbed in the active material particles. This process is called *dual-intercalation* and it is demonstrated in Figure 1.2

There are several Li-ion battery models in the literature. They are divided into three major classes in terms of their complexity and accuracy: white box or electrochemical models, gray box or electro equivalent circuit models and black box models [1]. Today, most BMSs use Equivalent circuit models (ECMs) [2] [3]. Equivalent circuit models use electrical components such as voltage generator, resistors and capacitances, to describe the response of the battery terminal voltage to a given input current. These models are accurate for low currents, computationally efficient and simple. However, they do not represent the chemical reactions that happen in the battery, and they are not accurate for high current.

In order to model the chemical processes inside the cell which is necessary to know the local value of states to pose limits on parasitic reactions and in order to obtain a more accurate model, electrochemical models are used. Several electrochemical models exist (Single Particle Model (SPM), Pseudo 2 Dimensional (P2D) Model, Pseudo 3 Dimensional (P3D) Model and Stress Models) and they differ greatly according to their complexity and computational requirements. The



most well-known electrochemical models in the literature are P2D model, which consists of several partial differential equations (PDEs), and SPM, which is an approximation to the P2D model. P2D model adopted in papers such as [4] [5] [6] [7] [8] [9] can predict internal state variables of the battery accurately; however, there is a huge trade-off between accuracy of the model and computational cost. Also, P2D parametrization is a complex task, with the risk of losing physical meaning for electrochemical parameters when running some automatic identification procedure [10] [11]. Most approaches find a reduction of this model and develop observers for reduced-order model to reduce computational burden. As an example, [12] employs a polynomial approximation for the diffusion equations in the solid material, and assumes electrolyte concentration to be constant. Furthermore, [5] proposed an impedance model for solid phase diffusion and applied finite element methods to electrolyte phase. However, most popular reduced-order model is probably SPM [14]. SPM assumes each electrode as a single spherical particle and neglects the electrolyte dynamics. Some papers which are related to SPM model are [13] [14].

In the literature, P2D model-based estimations of Lithium concentrations in batteries have been developed using linear Kalman Filter [7], Extended Kalman filter [4], Unscented Kalman Filter [9]. Although these observers can accurately estimate the internal state variables of a battery, they suffer from computational time and observer structural complexity. In contrast to P2D model-based estimation techniques, state estimation designs for SPM can significantly reduce the computational cost and can easily be implemented due to their simple mathematical structure. One of the studies about SPM based estimation of Lithium-ion concentration is [14] that estimates Lithium concentration profiles along particles radius and bulk State of Charge (SoC) using a Sliding Mode Observer (SMO) on a SPM. Another study about SPM based estimation of Lithium concentration is [13]. This approach allows to estimate not only SoC, but also state in any point along radius of the particle. Also, it is mathematically well formulated and supported by standard proofs for PDEs systems. Moreover, this approach does not consider a temperature model, which may give an important contribution to the electrochemical part especially at medium-high currents. Later, these authors extended the SPM by including electrolyte dynamics (Single particle model with electrolyte dynamics (SPMe)) and applied a backstepping PDE observer again [15].

In conclusion, there are many research works in the literature about Lithium-ion battery modelling and state estimation. The main challenge is to enable an accurate model for low and medium-high current, which can also predict internal state variables correctly, to obtain a computationally efficient estimation algorithm.

1.3 Main Contributions and Results

The purposes of present work are to obtain a SPM Lithium-ion battery model which matches with experimental data and to develop a PDE backstepping observer for the estimation of the gradient of Lithium concentration along the radius of particle and of battery SoC. Scientific contributions presented in this thesis are summarized as follows:

- The SPM model is experimentally validated by using a Li-ion battery cell produced by Samsung. Two types of test are performed: constant current test and pulse current test with increasing amplitude. A trade-off is found between getting an accurate model for constant current discharge test and getting an accurate model for pulse current test. Hence, an automatic optimization is run via `fmincon` function in Matlab environment to find electrochemical parameters D_s , R_f , k_p and k_n and to obtain best possible trade-off. The results achieved from constant current test at different C-rates and pulse current test are shown in Figure 1.3 and Figure 1.4, respectively.
- A backstepping PDE observer on a SPM is developed for Lithium concentration estimation along the particle radii and battery SoC estimation. Many works about SPM in the literature only estimates SoC, not stoichiometry. The mathematical approach by Moura [13] is followed to design the observer, but here the observer is implemented on top of the SPM formulation by Bizeray [16].
- In the design of SPM, a temperature model is included in the Lithium-ion battery model. The mathematical proof of observer convergence with a bulk model of temperature is not provided here, but it is validated in simulations and experiments. As shown in Figure 1.5, the proposed observer can converge not only surface concentration, but also inner states along r . Figure 1.6 shows that SoC can be successfully estimated by the observer, and the estimation error is less than 0.6%. Moreover, the proposed observer can still close to the true value of SoC, even in the presence of uncertainty in model parameters as illustrated in Figure 1.7. The RMS error is only 0.78% after 320s.

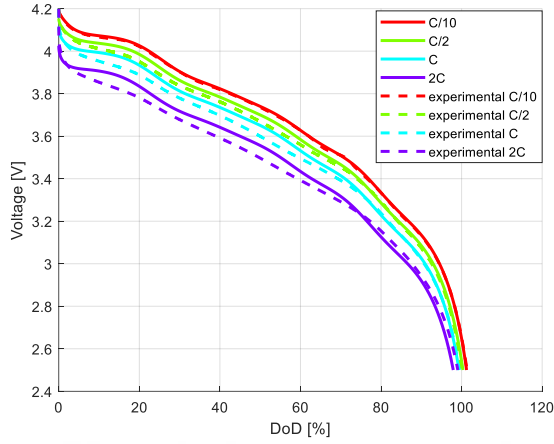


Figure 1.3 Voltage – DoD graph for different C-rates

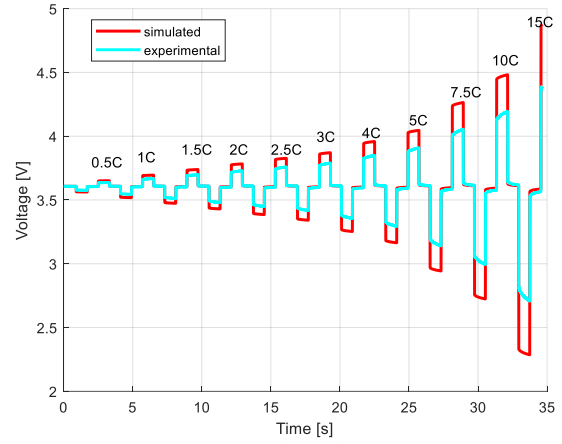


Figure 1.4 Voltage response for pulse current test

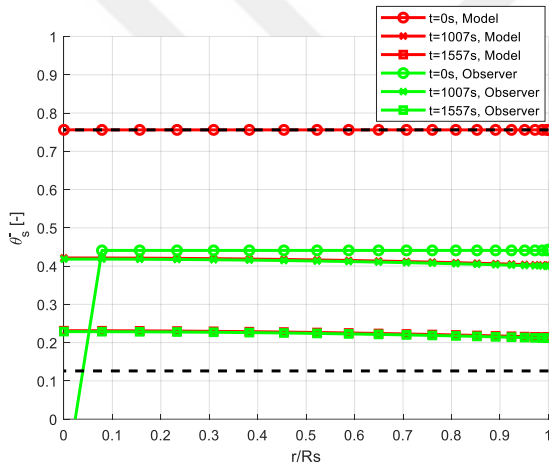


Figure 1.5 Stoichiometry along r

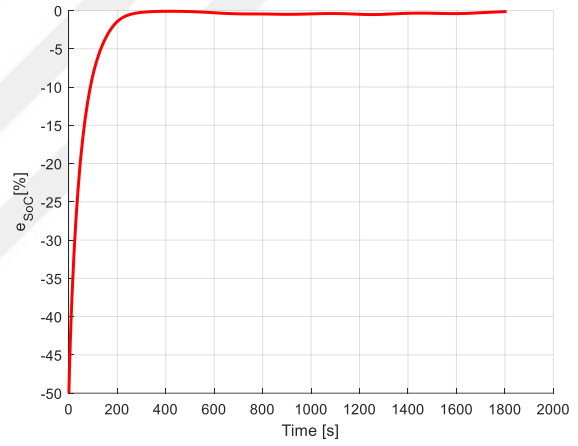


Figure 1.6 SoC estimation error

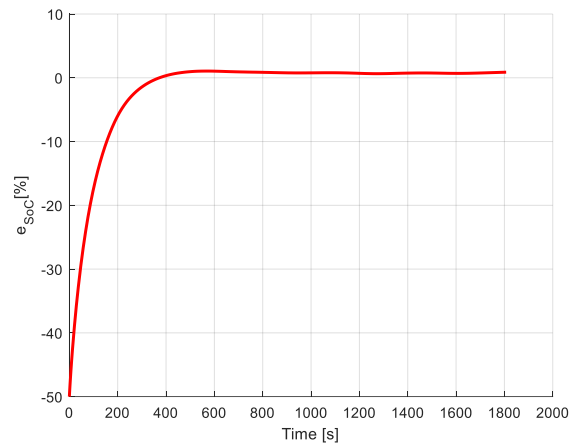


Figure 1.7 SoC estimation error with parameter uncertainty in D_s

- The proposed observer is validated experimentally using Samsung cell. Two tests are performed: constant current test at 2C and 2C pulse discharge test. Both the tests are launched with a 50% initial SoC error. For constant current test, the RMS error is 2.92% in the last 800s of the test. For pulse current test, SoC estimation error is less than 5% after 680s, and the RMS error is 3.3% after that time. The SoC estimation figures as shown in Figure 1.8 and Figure 1.9, respectively

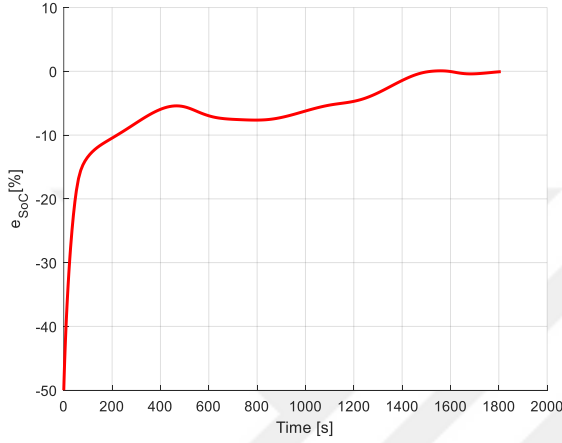


Figure 1.8 SoC estimation error for 2C constant current test

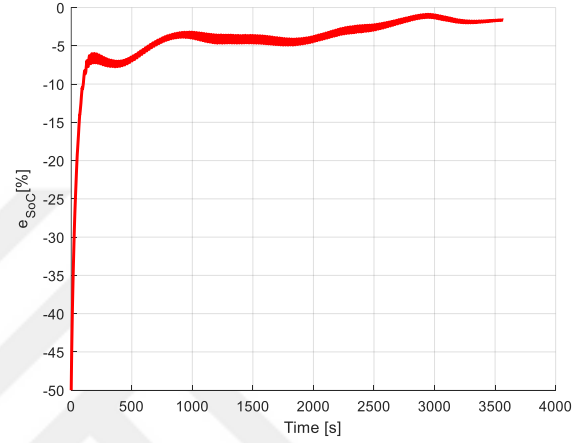


Figure 1.9 SoC estimation error for 2C pulse discharge test

1.4 Outline

Chapter 2 covers the electrochemical modelling approach, presenting pseudo two dimensional (P2D) and single particle model (SPM), including a comparison of *Lionsimba* simulator and *Spectral li-ion SPM* simulator which are respectively based on P2D and SPM Li-ion battery model and are made freely available on the internet by the authors. Then, electrochemical parameters of a Li-ion cell produced by Samsung are identified in chapter 3. This chapter is followed by an explanation of the proposed observer design and implementation process of the observer using Chebyshev orthogonal collocation method in chapter 4. In Chapter 5, SoC estimation results for simulation and experimental tests are presented using the proposed observer. In Chapter 6, the results are summarized and conclusions are drawn.



2 Modelling

In this chapter, the P2D and SPM models equations will be presented and implemented numerically in Matlab by using available toolboxes. Finally, these two models will be compared in terms of computational time and accuracy.

2.1 P2D Battery Model

The P2D model consists of several partial differential algebraic equations (PDAEs). The considered diffusion dynamics are those occurring across the battery film thickness, indicated as longitudinal direction x , and inside the spherical particles, along the radial direction r . The conservation equations are summarized in Table 2-1. In these equations, c_s is the concentration of Lithium in the solid phase; c_e is the Lithium ions concentration in electrolyte phase; i_s represents the electronic current in solid phase; i_e is ionic current in electrolyte phase; ϕ_s and ϕ_e are the solid phase potential and the electrolyte phase potential respectively. Also, D_s is the solid phase diffusion coefficient; F is Faraday's constant; a_s is specific interfacial area of an electrode; D_e^{eff} is the effective diffusion coefficient; t_+^0 is transference number of Lithium ions with respect to the velocity of solvent which is assumed as constant; σ^{eff} is the effective conductivity; κ^{eff} is the effective ionic conductivity, and κ_D^{eff} is the effective diffusion conductivity. A is the electrode plate area; $\delta_{n,p,s}$ are respectively the negative and positive electrode and separator thicknesses; L is the overall film thickness. R_s is the radius of the active material spherical particles.

The Butler-Volmer kinetics equations describes the molar flux j^{Li} at the active material particle surface:

$$j^{Li} = a_s j_0 \left[\exp\left(\frac{\alpha_a F}{RT} \eta\right) - \exp\left(\frac{\alpha_c F}{RT} \eta\right) \right] \quad (2.1)$$

where $\alpha_{a,c}$ are the anodic and cathodic transfer coefficients of electrode reaction respectively; R is the universal gas constant; T is temperature; j_0 is the exchange current density. The reaction overpotential η is obtained as:

$$\eta = \phi_s - \phi_e - U(c_{se}) \quad (2.2)$$

Where the thermodynamic equilibrium potential U is a nonlinear function of the surface concentration. The gradients of i_s and i_e along x are related to j^{Li} as follows:

$$\begin{aligned} \frac{\partial i_s}{\partial x} &= -j^{Li} \\ \frac{\partial i_e}{\partial x} &= j^{Li} \end{aligned} \quad (2.3)$$

These equations are subject to the following constraints inside the separator x :

$$\begin{aligned}
\frac{\partial i_s}{\partial x}(x) &= \frac{\partial i_e}{\partial x}(x) = 0 \\
i_s(x) &= 0 \\
i_e(x) &= \frac{I}{A}
\end{aligned} \tag{2.4}$$

Finally the terminal cell voltage is given by:

$$V = \phi_s(x = L) - \phi_s(x = 0) - \frac{R_f}{A} I \tag{2.5}$$

Where, R_f is the electrode surface film resistance.

Table 2-1 Electrochemical model conservation PDAEs

Species: solid phase	
$\frac{\partial c_s}{\partial t} = \frac{D_s}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial c_s}{\partial r} \right)$	
$\left. \frac{\partial c_s}{\partial r} \right _{r=0} = 0$	
$D_s \left. \frac{\partial c_s}{\partial r} \right _{r=R_s} = -\frac{j^{Li}}{a_s F}$	
Species: electrolyte phase	
$\frac{\partial \epsilon_e c_e}{\partial t} = \frac{\partial}{\partial x} \left(D_e^{eff} \frac{\partial c_e}{\partial x} \right) + \frac{1 - t_+^0}{F} j^{Li}$	
$\left. \frac{\partial c_e}{\partial x} \right _{x=0} = 0$	
$\left. \frac{\partial c_e}{\partial x} \right _{x=L} = 0$	
Charge: solid phase	
$i_s = -\sigma^{eff} \frac{\partial \phi_s}{\partial x}$	
$\left. \frac{\partial \phi_s}{\partial x} \right _{x=\delta_n} = \left. \frac{\partial \phi_s}{\partial x} \right _{x=\delta_n+\delta_s} = 0$	
$-\sigma^{eff} \left. \frac{\partial \phi_s}{\partial x} \right _{x=0} = -\sigma^{eff} \left. \frac{\partial \phi_s}{\partial x} \right _{x=L} = \frac{I}{A}$	
Charge: electrolyte phase	
$i_e = -k^{eff} \frac{\partial \phi_e}{\partial x} - k_D^{eff} \frac{\partial}{\partial x} \ln(c_e)$	
$\left. \frac{\partial \phi_e}{\partial x} \right _{x=0} = 0$	
$\left. \frac{\partial \phi_e}{\partial x} \right _{x=L} = 0$	

Thermal model equations are shown in Table 2-2: where Q_{ohm} , Q_{rev} and Q_{rxn} are the ohmic, reversible and reaction generation rates respectively; σ_{eff} is solid phase conductivity; κ_{eff} is electrolyte conductivity; c_p is the lumped specific heat of the cell and ρ is the cell bulk density.

Table 2-2 Thermal model equations and boundary conditions

Thermal model at positive and negative electrodes	
$\rho c_p \frac{dT}{dt} = \frac{d}{dx} \left[\lambda_i \frac{dT}{dx} \right] + Q_{ohm} + Q_{rxn} + Q_{rev}$ $-\lambda_a \frac{dT}{dx} \Big _{x=0^-} = -\lambda_p \frac{dT}{dx} \Big _{x=0^+}$ $-\lambda_n \frac{dT}{dx} \Big _{x=L^-} = -\lambda_z \frac{dT}{dx} \Big _{x=L^+}$	
Thermal model at separator	
$\rho c_p \frac{dT}{dt} = \frac{d}{dx} \left[\lambda_i \frac{dT}{dx} \right] + Q_{ohm}$ $-\lambda_p \frac{dT}{dx} \Big _{x=\delta_p^-} = -\lambda_s \frac{dT}{dx} \Big _{x=\delta_p^+}$ $-\lambda_s \frac{dT}{dx} \Big _{x=\delta_p+\delta_s^-} = -\lambda_n \frac{dT}{dx} \Big _{x=\delta_p+\delta_s^+}$	
Heat source terms (Anode and Cathode)	
$Q_{ohm} = \sigma_{eff,i} \left(\frac{d\phi_s}{dx} \right)^2 + \kappa_{eff,i} \left(\frac{d\phi_e}{dx} \right)^2 + \frac{2\kappa_{eff,i}RT}{F} (1 - t_+) \frac{d \ln c_e}{dx} \frac{d\phi_e}{dx} \quad i \in \{p, n\}$ $Q_{rxn} = F a_i j \eta_i \quad i \in \{p, n\}$ $Q_{rxn} = F a_i j T \frac{dU_i}{dT} \Big _{T_{ref}} \quad i \in \{p, n\}$	
Heat source terms (Separator)	
$Q_{ohm} = \kappa_{eff,i} \left(\frac{d\phi_e}{dx} \right)^2 + \frac{2\kappa_{eff,i}RT}{F} (1 - t_+) \frac{d \ln c_e}{dx} \frac{d\phi_e}{dx} \quad i = s$	

2.1.1 Lionsimba Simulator

In the present section, numerical implementation of P2D model is investigated by using *Lionsimba* toolbox. *Lionsimba* is a toolbox for the simulation of P2D model, developed by Torchio et al. [8]. In order to solve the differential algebraic equations (DAEs), *Lionsimba* toolbox uses IDA solver which reduces computational time. Moreover, *Lionsimba* toolbox allows the users to choose three different current type: galvanostatic input current (constant current (dis)charge), variable input current and potentiostatic (allows to impose voltage). In *Lionsimba* toolbox, the governing

equations described above are discretized by using finite volume method. The cell is discretized along x in $N_{n,p,s}$ elements for the negative and positive electrode and separator respectively.

With the help of *Lionsimba*, several tests are carried out to understand the toolbox capabilities in terms of computational time and accuracy. In the following section, some simulation results are shown for different scenarios.

2.1.2 Simulation Results

Firstly simulation results for constant current discharge at 5C (150A) are shown. The *Lionsimba* simulator is starting from SoC = 90%, since it is the maximum value accepted by the simulator. The simulator is based on the following discretization: $N_r=50$, $N_n=N_s=N_p=10$.

As it can be seen from Figure 2.2, the cell is not empty at the end of simulation, however the *Lionsimba* simulator stopped because of cut-off voltage which is 2.5V as shown in Figure 2.1.

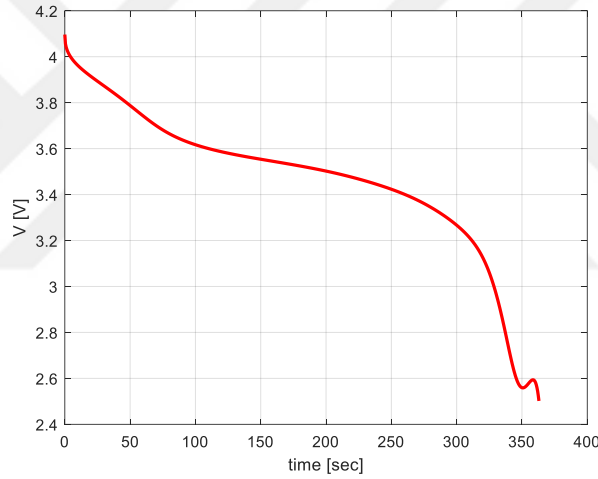


Figure 2.1 Voltage profile for 5C constant current discharge

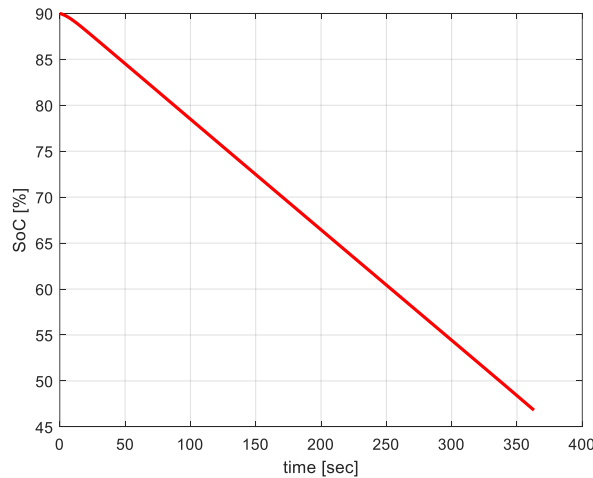


Figure 2.2 SoC results for 5C constant current discharge

A few distributed variables are shown in the following, to give an overlook to how the P2D model can describe inner cell phenomena and physical gradients. The surface solid-phase concentration is presented in Figure 2.3 at time $t=60s$, and the molar flux in Figure 2.4. Concentration along solid-phase particle radius is shown in Figure 2.5 for a particle in negative electrode close to separator. Solid-phase potential is presented in Figure 2.6 at different points in x , which show that there is no significant gradient.

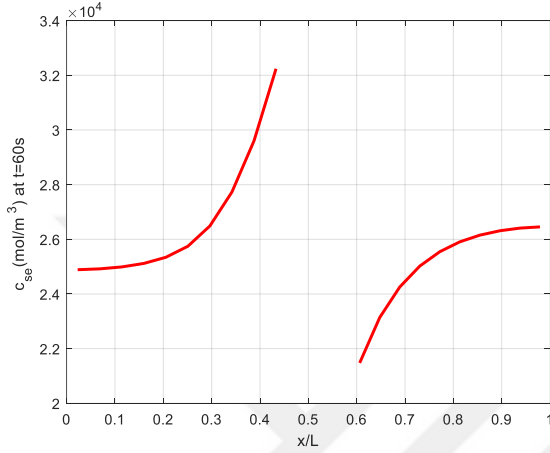
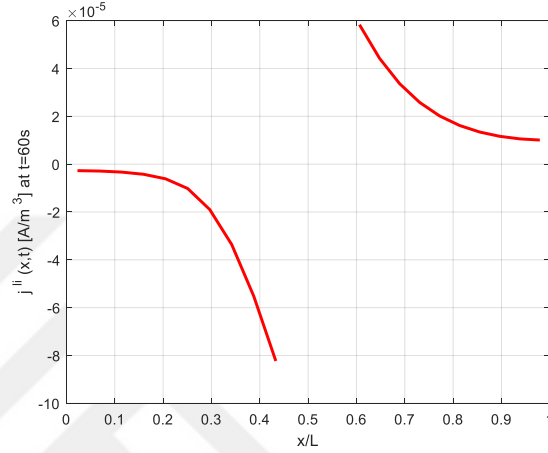
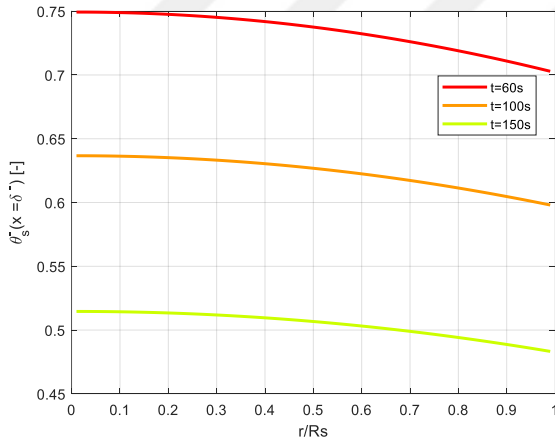
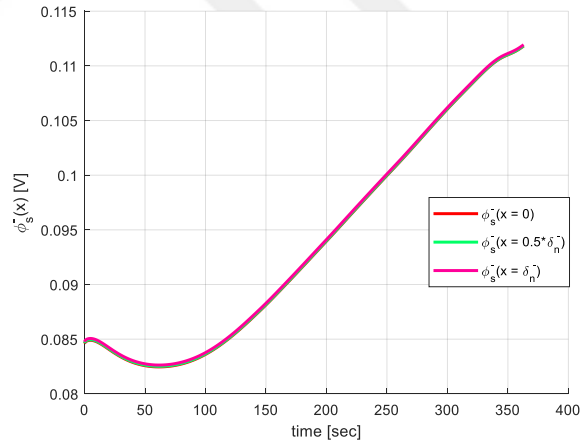
Figure 2.3 Surface concentration at $t=60s$ Figure 2.4 Ionic flux at $t=60s$ Figure 2.5 Stoichiometry along r in negative electrode at separator

Figure 2.6 Solid phase potential in negative electrode at current collector, middle and separator

Figure 2.7, temperature results are shown for 5C constant current test. As expected for the discharge test at high C rates, temperature is increasing along with simulation time. However, the change on amplitude of temperature is not realistic. Lithium-ion battery cell usually works up to $60^\circ C$, but in that case it reaches to $120^\circ C$ since there is no cut-off temperature in *Lionsimba* toolbox.

In the second scenario, a more dynamic test is considered. A pulse input current designed with increasing amplitude as shown in Figure 2.8. The simulator is starting from SoC = 50%.

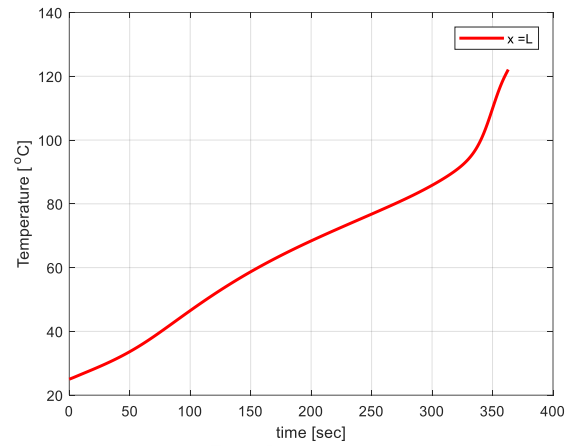


Figure 2.7 Temperature graph at negative current collector

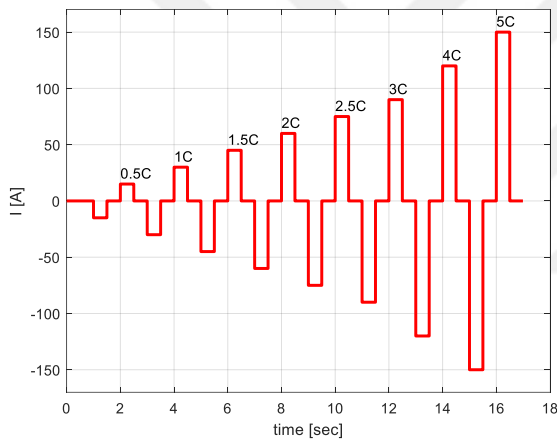


Figure 2.8 Pulse input current profile with increasing amplitude

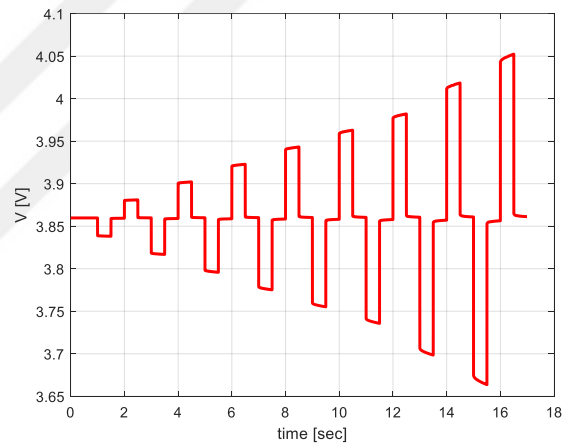


Figure 2.9 Voltage response to given input current

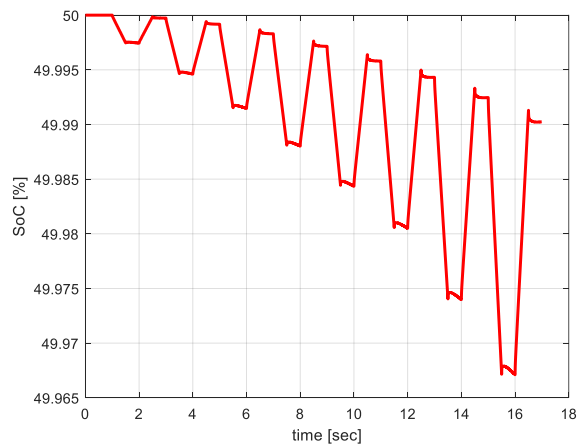


Figure 2.10 SoC result for pulse input current

As it can be seen from Figure 2.8, the maximum amplitude of pulse current is 5C. It is observed that when pulse current test is performed higher C-rates than 5C, *Lionsimba* simulator stops due to solver problem.

Figure 2.10 demonstrates SoC result for the given pulse input current. If there is no charge or discharge operations for a battery, SoC has to be constant. However, as illustrated in Figure 2.10 even when the cell is rest (zero input current), SoC moves a little for a while, which is unexpected behaviour.

2.2 Single Particle Model

Single Particle Model describes electrochemical dynamics like Lithium transport, reaction kinetics and thermal reactions that take place inside the battery. There is only one solid spherical particle in each electrode. Also, the electrolyte diffusion and migration dynamics are neglected. Since the electrolyte dynamics are neglected and the number of particle inside the electrode is just one, implementation of SPM is easier than the implementation of P2D Model, but accuracy is typically reduced to lower current ranges (for example, up to 2-3C).

In the SPM, diffusion in each electrode is ruled by Fick's law in spherical coordinates:

$$\frac{\partial c(r, t)}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(D_{s,i}(T) r^2 \frac{\partial c(r, t)}{\partial r} \right) \quad (2.6)$$

The boundary conditions at the particle center and surface are, respectively:

$$\begin{aligned} \left. \frac{\partial c(r, t)}{\partial r} \right|_{r=0} &= 0 \\ D_{s,i}(T) \left. \frac{\partial c(r, t)}{\partial r} \right|_{r=R_s} &= -j_{Li} \end{aligned} \quad (2.7)$$

j_{Li} is the molar flux at particle surface, the relationship between j_{Li} and I in each electrode are given by:

$$j_{Li,p} = \frac{-I}{a_{s,p} F A \delta_p}; j_{Li,n} = \frac{+I}{a_{s,n} F A \delta_n} \text{ and } a_{s,i} = \frac{3\epsilon_{s,i}}{R_{s,i}} \quad i \in \{p, n\} \quad (2.8)$$

The overpotential η can be computed from the inversion of Butler-Volmer equation:

$$\eta_i = \frac{2RT}{F} \sinh^{-1} \left(\frac{j_{Li,i}}{2 * i_{0,i}} \right) \quad (2.9)$$

where the exchange current density $i_{0,i}$ is:

$$\begin{aligned} i_{0,i} &= k_i(T) \times F \times \sqrt{c_e^{avg}} \times \sqrt{c_{s,i}^{surf}} \times \sqrt{c_{s,i}^{max} - c_{s,i}^{surf}} \\ k_i(T) &= k_{i,ref} \times e^{Ea_i * R \left(\frac{1}{T_{ref}} - \frac{1}{T} \right)} \end{aligned} \quad (2.10)$$

Finally, output voltage equation is given by:

$$V = U_p(\theta_p, T) - U_n(\theta_n, T) + \eta_p - \eta_n - R_f I \quad (2.11)$$

The thermal model is a simple bulk thermal model, in which temperature dynamics are described by following equations:

$$\rho c_p \frac{dT}{dt} = \dot{q}_{gen} + \dot{q}_{conc} \quad (2.12)$$

with a convective boundary condition:

$$\dot{q}_{conc} = -\frac{hA_c(T - T^{amb})}{V_c} \quad (2.13)$$

The total heat generation rate per unit volume $\dot{q}_{gen}$ is:

$$\begin{aligned} \dot{q}_{gen} &= \dot{q}_{rev} + \dot{q}_{rx} + \dot{q}_c \\ &= -\frac{i_{app}}{L} T \left(\frac{dU_p}{dT} - \frac{dU_n}{dT} \right) + \frac{i_{app}}{L} (\eta_n - \eta_p) + \frac{R_c A i_{app}^2}{V_c} \end{aligned} \quad (2.14)$$

where, c_p is the lumped specific heat of the cell; ρ is the cell bulk density; $\dot{q}_{rev}$, $\dot{q}_{rx}$ and $\dot{q}_c$ are reversible, reaction and ohmic heat contributions respectively; V_c is the cell volume; h is the convective heat transfer coefficient; A is electrode surface area; T^{amb} is ambient temperature; i_{app} is the current density which is equal to $\frac{I}{A}$.

2.2.1 Spectral li-ion SPM simulator

In present work, *Spectral li-ion SPM* which is developed at the Department of Engineering Science of the University of Oxford is investigated [16]. By using *Chebyshev orthogonal collocation* spectral method, the SPM is discretized. The idea of the method is that PDEs approximated solution can be expressed by a sum of Chebyshev polynomials that interpolates the solution at the discretizing Chebyshev nodes defined on a normalize domain [-1 1]. Chebyshev differentiation matrices allows to bring the model to state space form, and to include boundary conditions at the surface and core elements. This form of the model can thus be solved using a standard ODE solver, for example ODE45 in Matlab. For more details on the numeric implementation, investigate to [16].

2.2.2 Simulation Results

As in *Lionsimba* simulator, two different scenario are carried out for *Spectral li-ion SPM* simulator. In the first scenario, constant current discharge of a Lithium-ion battery is simulated at 2C (5.8A). Initial state of charge is chosen as 100%. Voltage-time graphic, SoC-time graphic and Voltage-DoD (depth of discharge) graphic are shown in Figure 2.11, Figure 2.12 and Figure 2.13 respectively. Note that the original electrochemical parameters for each simulator were retained, so these tests rely on a different test with respect to *Lionsimba* toolbox.

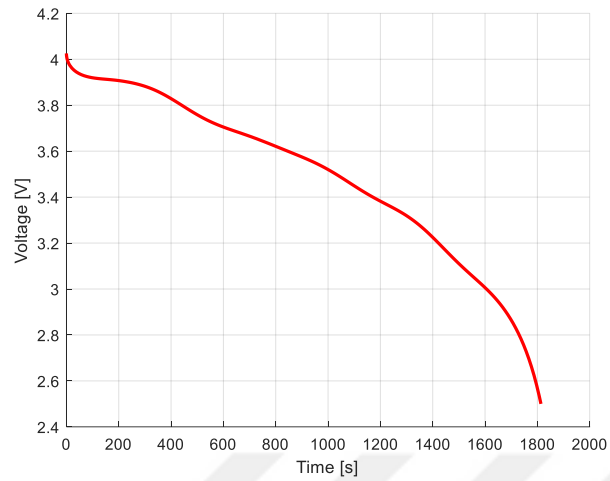


Figure 2.11 Voltage response for 2C constant current discharge

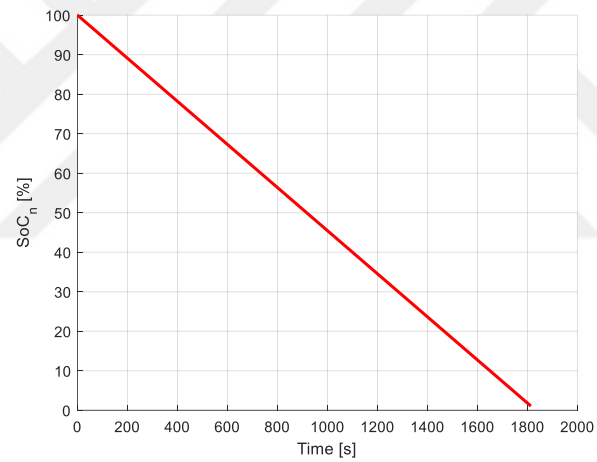


Figure 2.12 SoC result for 2C constant current discharge

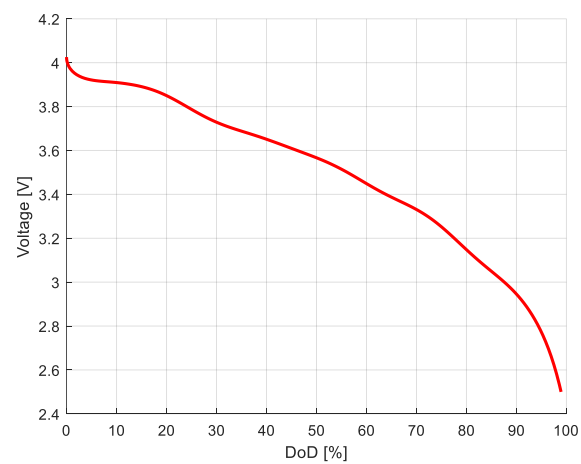


Figure 2.13 Voltage – DoD graph

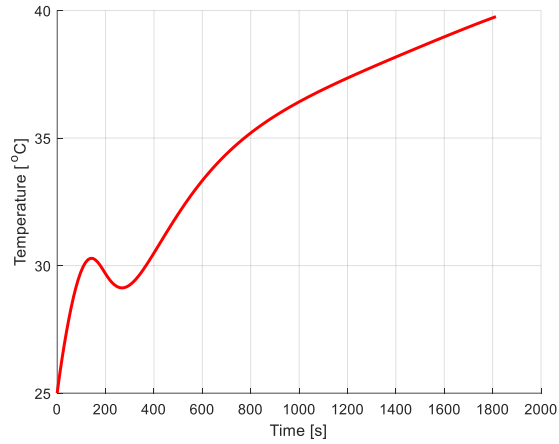


Figure 2.14 Temperature graph for 2C constant current discharge

In the second scenario, a pulse test with increasing amplitude (from 0.5C to 15C) is applied to the *Spectral li-ion SPM* simulator. Applied current is shown in Figure 2.15 and Voltage-time and SoC-time graphics are shown in Figure 2.16 and Figure 2.17 respectively.

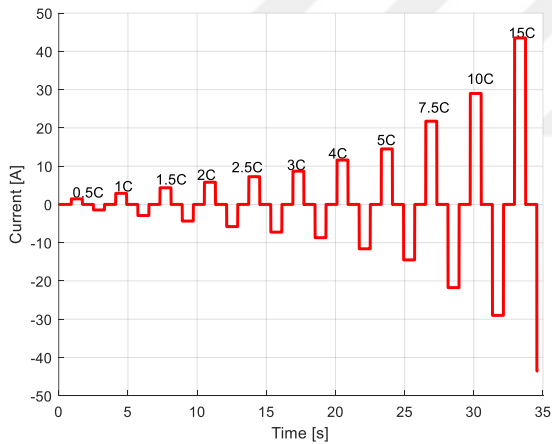


Figure 2.15 Pulse current with increasing amplitudes level

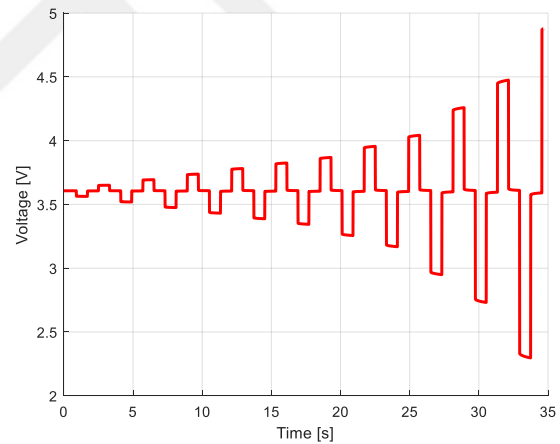


Figure 2.16 Voltage results for pulse input current

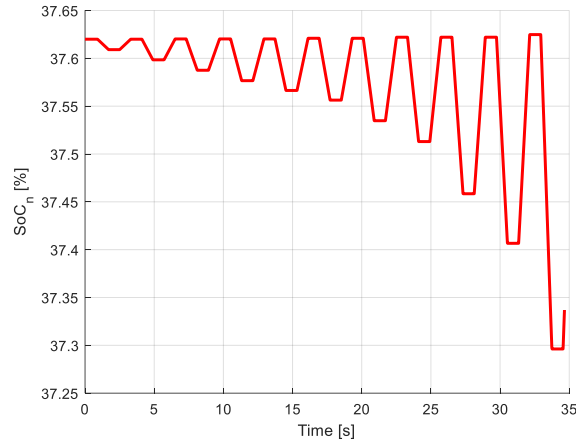


Figure 2.17 SoC – Time graph for pulse current test

2.3 Comparison of *Spectral li-ion SPM Simulator* and *Lionsimba Simulator*

In Table 2-3, advantages and disadvantages of *Spectral li-ion SPM simulator* and *Lionsimba simulator* are compared. By taking into account the pros and cons explained in the Table 2-3, it is decided to use *Spectral li-ion SPM simulator* to model Samsung (INR 18650-30Q) cell. In next chapter, parameter identification of Samsung cell by using *Spectral li-ion SPM simulator* model will be carried out. Then, this model will be used to implement a backstepping observer in chapter 4 (Observer design).

Table 2-3 Comparison of *Spectral li-ion SPM simulator* and *Lionsimba simulator*

	<i>Lionsimba Simulator</i>	<i>Spectral li-ion SPM Simulator</i>
Accuracy	Accurate	Accurate for low-medium currents
Computational load	Computationally efficient (thanks to IDA solver)	Computationally efficient
Model	Detailed model of electrochemical reactions	Approximated model to P2D model, no gradient along x direction
Observer Implementation	Implementation of Observer is more difficult	Implementation of Observer is simple
Other problems (1)	It suffers from pulse current test at high current because of solver problem	-
Other problems (2)	There are oscillations on voltage response for constant current test higher than 5C, because stoichiometry in positive electrode at separator is getting closer the maximum	-



3 Parameter Identification

In this chapter, identification of model parameters is presented. Experiments are performed on a commercial Li-ion cell produced by Samsung. Some of the nominal parameters provided by the manufacturer are given in Table 3-1. Then, the value of parameters of the electrochemical SPM is found so that the model response resembles the experimental data with sufficient accuracy. As a first step, the model parameters are divided into two parts: static and dynamic parameters. The former group includes parameters responsible for quasi-static or instantaneous behaviors of the cell; the latter group includes parameters determining the transient responses of the cell to an input current. Internal resistance (R_f) and capacity (Q) of the cell are directly obtained from experimental measurements (However, internal resistance (R_f) is readjusted by numerical optimization to improve accuracy of model). Some of the electrochemical parameters are adopted from the literature which are shown in Table 3-2 [16]. Other parameters (Diffusion coefficient (D_s), solid-phase volume fractions ($\epsilon_{sp,sn}$) and reaction rate constants ($k_{p,n}$)) are adopted from the literature as an initial guess, then adjusted as necessary to match the model and experimental data.

Table 3-1 Nominal Specification of Samsung Cell

<i>Item</i>	<i>Specification</i>
Maximum Voltage	4.2 V
Nominal Voltage	3.6 V
Cut-off Voltage	2.5 V
Capacity (Q)	2.95 Ah
Cell dimension: height	Max 65 mm
Cell dimension: diameter	Max 18.4 mm

Table 3-2 List of parameters used in Simulations from Literature

<i>Symbol</i>	<i>Unit</i>	<i>Description</i>	<i>Value</i>
L	m	Electrode thickness	1.68×10^{-4}
A_s	m^2	Electrode active surface area	0.0982
R_s	m	Particle radius	Anode: 12.5×10^{-6} Cathode: 8.5×10^{-6}
c_e^{avg}	mol/m^3	Average electrolyte concentration	1000
c_s^{max}	mol/m^3	Maximum solid phase concentration	Anode: 30556 Cathode: 51555
C_p	$J/(kg K)$	Specific heat	750
ρ	kg/m^3	Cell bulk density	1626
h	$W/(m^2 K)$	Convective heat transfer coefficient	30

3.1 Experimental Setup

An Arbin test bench is used for the battery charge/discharge test. It has the capability to run any current input profile with high precision, while measuring voltage and surface temperature of the cell. Figure 3.1 shows the all experimental setup with PC, cells, Arbin test bench, thermocouples and wire connections from a general view Figure 3.2 demonstrates the Samsung cell, the cell holder, thermocouple and wire connections from a closer look.



Figure 3.1 Experimental Setup

In the following, static parameters (internal resistance, solid-phase volume fraction and thermodynamic equilibrium potential) are first determined, by fixing an initial guess for some of the dynamic parameters. Then, the dynamic parameters are computed by running a numeric optimization algorithm, which also includes internal resistance for increased accuracy.

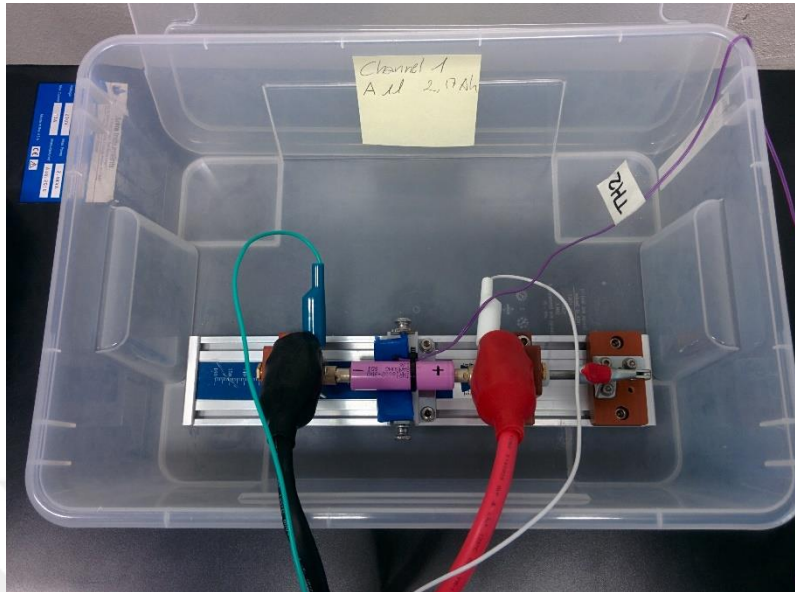


Figure 3.2 Samsung cell, cell holder, thermocouple and wire connections

3.2 Static Parameters

3.2.1 Internal Resistance

To evaluate the internal resistance, a pulse current test which has numerous pulses and rest periods with two level of current (Figure 3.3), low 1C (2.9A) and high 10C (29A), is applied to the battery and voltage response is measured (Figure 3.4).

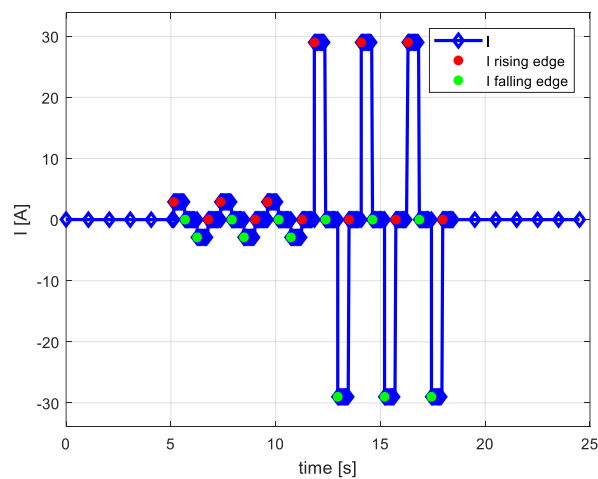


Figure 3.3 Input Current

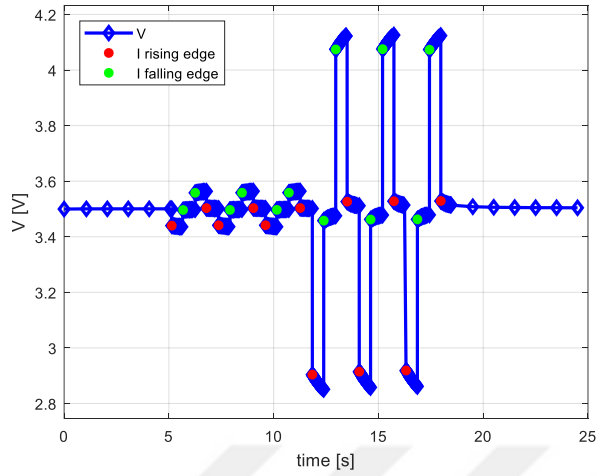


Figure 3.4 Voltage Response

Initially, the value of R_f is estimated under a simple hypothesis:

$$R_f^{est} = \frac{\Delta V}{\Delta I} \quad (3.1)$$

According to the hypothesis, when a step input is applied, the initial change on voltage response at $t = 0^+$ is completely due to internal resistance. Hence, voltage and current rising and falling edges are isolated and analyzed separately. This value is taken as an initial guess in the numerical optimization presented in section 3.3, by removing this initial hypothesis.

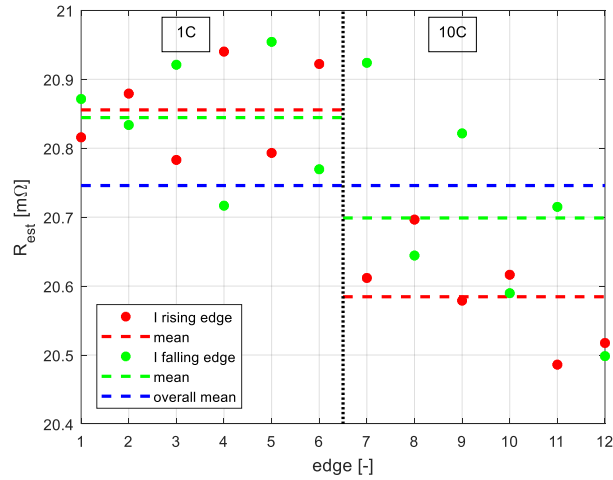


Figure 3.5 Internal resistance analysis for low/high current and rising/falling edge

As it can be seen from the Figure 3.5, there is no significant variation among rising/falling edges and 1C and 10C, thus one value can be taken. Firstly, mean values of R_f^{est} are found for low current and high current. Then, overall mean value of R_f^{est} is found as 20.746mΩ.

3.2.2 Solid-Phase Volume Fraction

For C/10 constant current discharge test (quasi-static conditions), the cell capacity with first parameters guess is too low. In fact, SoC in negative electrode gets to 0 too early when compared to experimental test duration, and then goes below 0. Thus, the amount of Lithium available in solid phase needs to be increased in that electrode. By a simulation sensitivity study, as shown in Figure 3.6, the volume fraction is finally selected as 1.32 of its nominal.

$$\epsilon_{sp,sn1} = 1.32 \times \epsilon_{sp,sn nominal} = 1.32 \times 0.5052 = 0.6669 \quad (3.2)$$

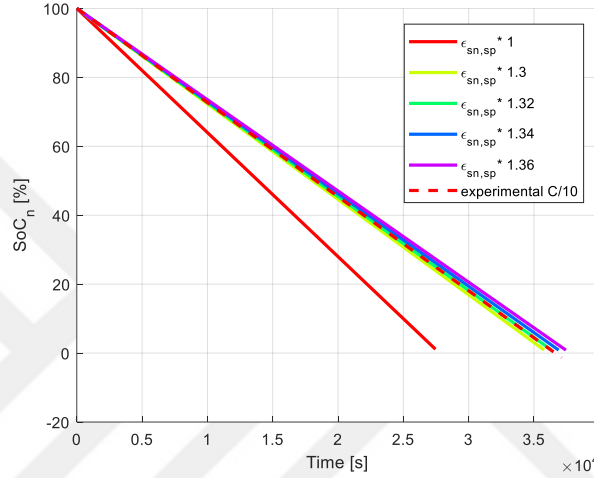


Figure 3.6 SoC – Time graphs for different ϵ

As it can be seen from the Figure 3.6, when $\epsilon_{sp,sn}$ are chosen as 1.32 times of their nominals, SoC response of experimental and model are reaching 0% SoC at the same time.

3.2.3 Determination of Thermodynamic Equilibrium Potential

After internal resistance and electrode volume fraction are defined, thermodynamic equilibrium potential function is found with same C/10 test. Diffusion coefficients ($D_{sp,sn}$) are firstly set to a value large enough, so as internal concentration gradients along r can be neglected temporarily. This value is 5 times the nominal value found in the literature. Figure 3.7 and Figure 3.8 show internal concentration gradients along r for different ($D_{sp,sn}$) values.

$$D_{sp,sn} = 5 \times D_{sp,sn nominal} = 5 \times 1.95e - 13 = 5e - 14 \quad (3.3)$$

The thermodynamic equilibrium potential of negative electrode, called U_n , is taken from literature [16] and adjusted. U_n is a nonlinear function of negative electrode surface stoichiometry, called θ_n . Then, thermodynamic equilibrium potential function for positive electrode, called U_p which is function of positive electrode surface stoichiometry (θ_p), is identified on differential data of measured V and U_n . However, if U_n as defined in Bizeray's paper [16] is used, when it is summed with experimental voltage to compute U_p , it is not possible to get a monotonically decreasing function. Because of that, stoichiometry at SoC = 0% in negative electrode is increased from 0.0065 to 0.126 [17].

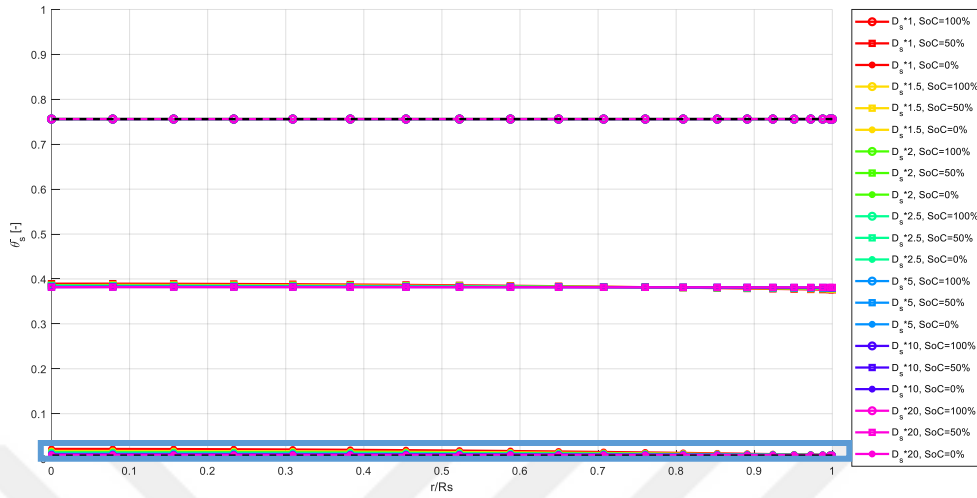
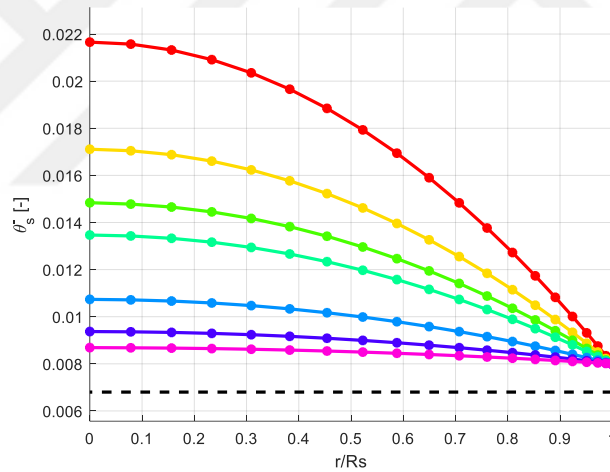

 Figure 3.7 Stoichiometry at different time instant for different D_s


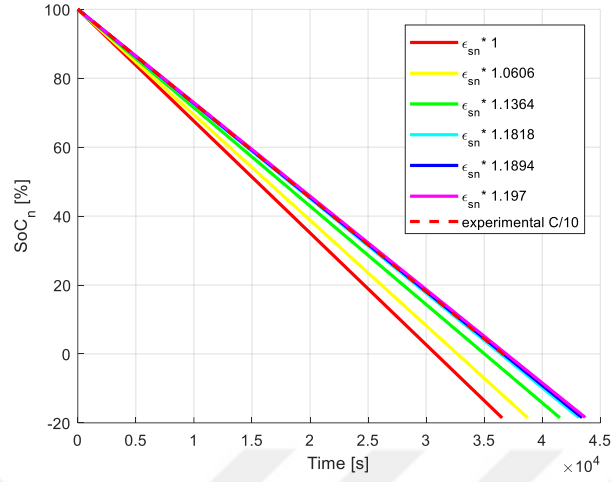
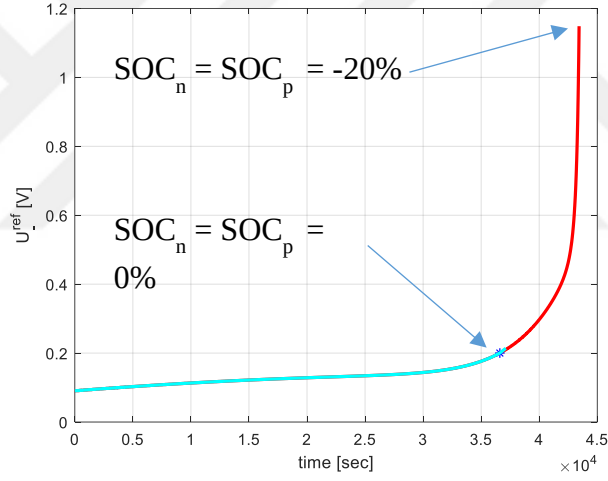
Figure 3.8 Stoichiometry (a zoom to Figure 5)

Since, in negative electrode the value of stoichiometry at SoC = 0% is changed, it is needed to adjust the volume fraction for negative electrode again. By repeating same procedure, for C/10 constant current discharge test, the volume fraction for negative electrode is finally found as;

$$\epsilon_{sn\ 2} = 1.1894 \times \epsilon_{sn\ 1} = 1.1894 \times 0.6669 = 0.7932 \quad (3.4)$$

Figure 3.9 shows SoC results for different ($\epsilon_{sn\ 2}$) values.

In Figure 3.10, the red line is the U_n for C/10 constant current discharge test. Simulation is run with no stopping condition on SoC; then SoC = 0 is chosen as final time instant for simulation and lower cut-off voltage is enforced at this point by properly defining U_p as described below .


 Figure 3.9 SoC – Time graphs for different ϵ

 Figure 3.10 U_n - Time graph

After these final touches, equation 2.11 is inverted as follows to find U_p :

$$U_p = V_{exp} + U_n + \eta_n + R_f I - \eta_p \quad (3.5)$$

note that, although resistive and overpotential contributions are in the order of mVs here, they are still considered in the equation of U_p for improved accuracy.

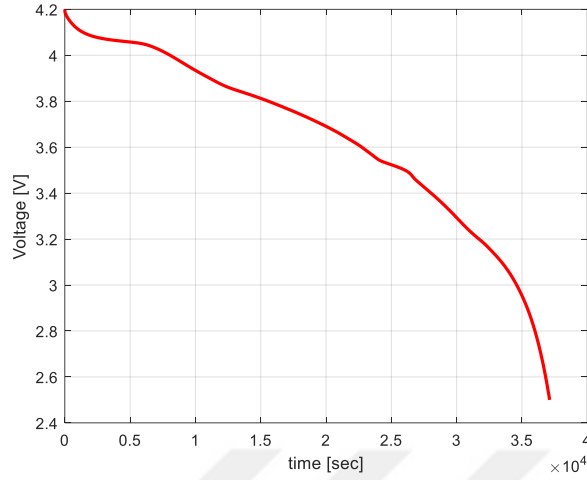
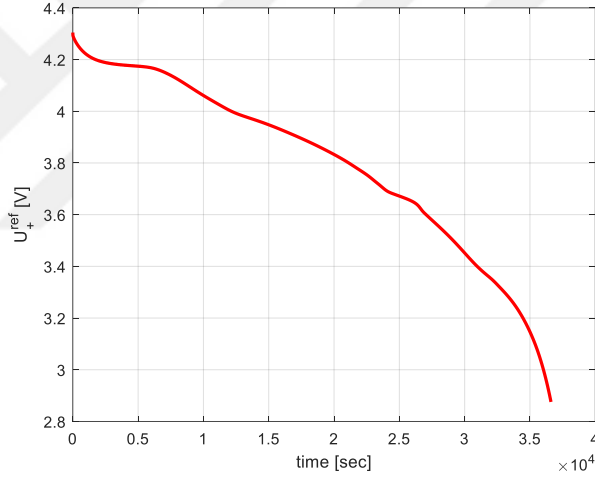


Figure 3.11 Experimental Voltage – Time graph


 Figure 3.12 U_p - Time graph

θ_p vector is created uniformly (because the test is quasi-static) between 0.465 (stoichiometry at SoC = 100%) [16] and 0.8933 (stoichiometry at SoC = 0%) [16]. Then, the data are fitted by means of curve fitting tool in Matlab. Fourier series expansion is used to define U_p as a function of θ_p . The parameters of U_p function can be found in Appendix A

$$\begin{aligned}
 U_p = & a0 + a1 \times \cos(\theta_p \times w) + b1 \times \sin(\theta_p \times w) \\
 & + a2 \times \cos(2 \times \theta_p \times w) + b2 \times \sin(2 \times \theta_p \times w) \\
 & + a3 \times \cos(3 \times \theta_p \times w) + b3 \times \sin(3 \times \theta_p \times w) \\
 & + a4 \times \cos(4 \times \theta_p \times w) + b4 \times \sin(4 \times \theta_p \times w) \\
 & + a5 \times \cos(5 \times \theta_p \times w) + b5 \times \sin(5 \times \theta_p \times w) \\
 & + a6 \times \cos(6 \times \theta_p \times w) + b6 \times \sin(6 \times \theta_p \times w) \\
 & + a7 \times \cos(7 \times \theta_p \times w) + b7 \times \sin(7 \times \theta_p \times w) \\
 & + a8 \times \cos(8 \times \theta_p \times w) + b8 \times \sin(8 \times \theta_p \times w)
 \end{aligned} \tag{3.6}$$

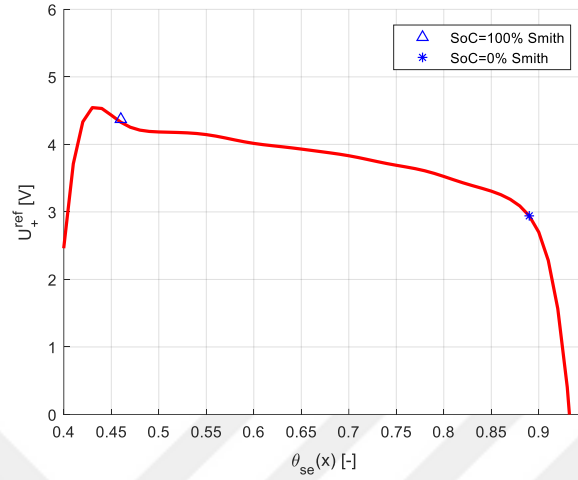

 Figure 3.13 U_p graph as a function of θ_p

Figure 3.13 shows Open circuit potential function as a function of θ_p . Also, stoichiometry limits at SoC=100% and at SoC=0% are shown with blue markers.

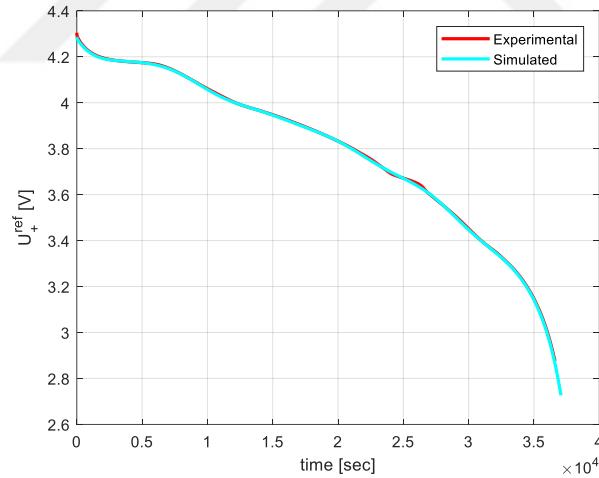

 Figure 3.14 Experimental U_p and U_p from C/10 simulation results

Figure 3.14, a validation of the identified U_p is shown: the experimental data obtained from equation 3.5 are plotted in red, while the empirical function of equation 3.6 is shown in blue. The two curves only show negligible differences over the entire test.

3.3 Parameter Identification with Optimization Toolbox

After U_p is identified, a final automatic optimization is performed to improve the estimates of parameters D_s and R_f , and to find the value of the last parameters k_p and k_n . The parameter identification procedure has been designed as follows:

- 1) A set of experimental data has been chosen for the parametric identification routine
- 2) A cost function which minimizes the error between model and experimental results is defined.

Parameter identification on a single test (constant current discharge test or pulse test) leads to a very good match between model and experimental data, but these parameters do not fit other experimental data. In order to obtain true parameters which lead to a good fit for both constant current discharge test and pulse test, a cost function which utilizes both tests data at the same time is selected and it is defined as:

$$J = \alpha J1 + (1 - \alpha)J2 \quad (3.7)$$

where,

$$J1 = \frac{1}{T_{sim,2C}} \times \int (V_{sim,2C} - V_{exp,2C})^2$$

$$J2 = \frac{1}{T_{sim,pulse}} \times \int (V_{sim,pulse} - V_{exp,pulse})^2 \quad (3.8)$$

$V_{sim,2C}$: Model voltage response of 2C constant current discharge test

$V_{exp,2C}$: Experimental battery voltage response of 2C constant current discharge test

$V_{sim,pulse}$: Model voltage response of pulse current test

$V_{exp,pulse}$: Experimental battery voltage response of pulse current test

$T_{sim,2C}$: Simulation time of 2C constant current discharge test

$T_{sim,pulse}$: Simulation time of pulse current test

α : Weight factor

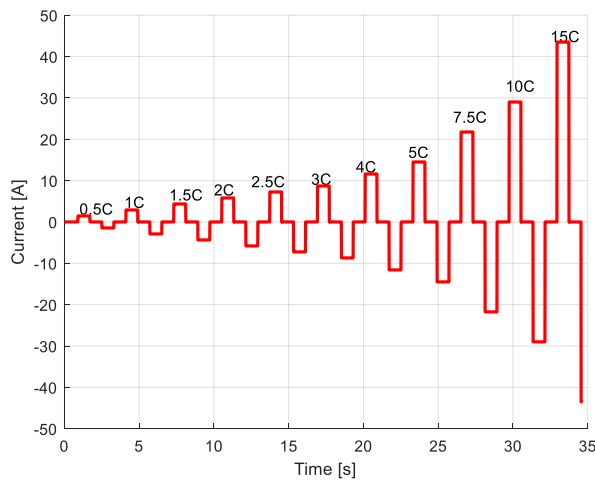


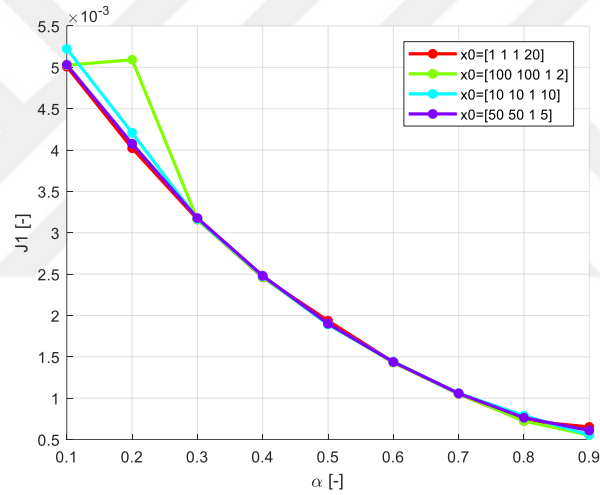
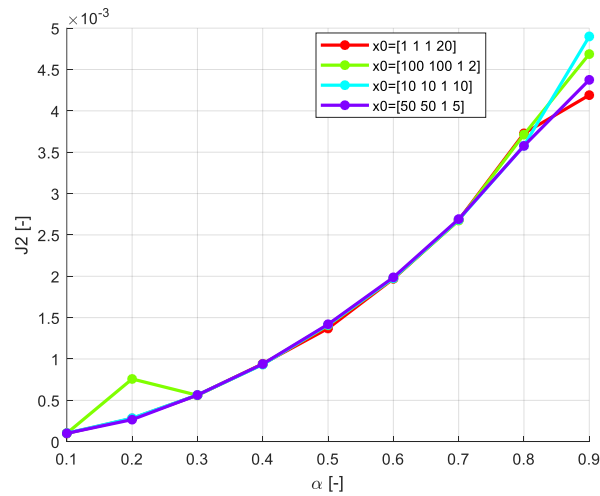
Figure 3.15. Pulse test current profile

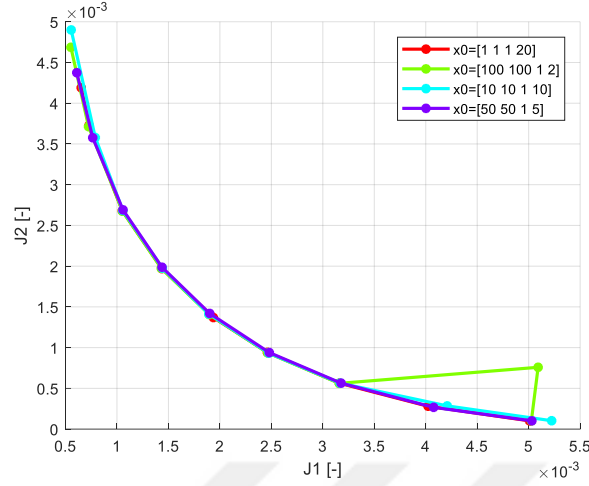
The minimization has been conducted by using fmincon function from Matlab optimization toolbox. Four different initial point are chosen for optimization to test algorithm sensitivity and robustness to x_0 and they are shown in Table 3-3.

Table 3-3 Initial points for optimization

	k_p	k_n	R_f	D_s
x_0^1	$1 \times k_{p,nominal}$	$1 \times k_{n,nominal}$	$1 \times R_{f,nominal}$	$20 \times D_{s,nominal}$
x_0^2	$100 \times k_{p,nominal}$	$100 \times k_{n,nominal}$	$1 \times R_{f,nominal}$	$2 \times D_{s,nominal}$
x_0^3	$10 \times k_{p,nominal}$	$10 \times k_{n,nominal}$	$1 \times R_{f,nominal}$	$10 \times D_{s,nominal}$
x_0^4	$50 \times k_{p,nominal}$	$50 \times k_{p,nominal}$	$1 \times R_{f,nominal}$	$5 \times D_{s,nominal}$

For 9 values of α (between 0.1 and 0.9), several tests are carried out and a total of 36 tests are shown and compared in the following figures.


 Figure 3.16 J1 – α graph for different x_0

 Figure 3.17 J2 – α graph for different x_0


 Figure 3.18 J1 – J2 graph for different x_0

As it can be seen from the Figure 3.16, if α is chosen around 0.9, the optimization toolbox tries to minimize $J1$ mainly. Optimization toolbox finds the parameters which lead to obtain more accurate model for 2C constant current discharge.

If α is low, the optimization toolbox tries to minimize $J2$ which is related to pulse current test. Because of that $J2$ is an increasing function of α (Figure 3.17). So, the lower is α , the more accurate is the model for pulse current test.

Moreover, according to Figure 3.18, it can be easily stated that initial point does not affect the results of optimization toolbox much. The only noticeable difference is for $\alpha = 0.2$ with $x_0^1 = [100 \ 100 \ 1 \ 2]$ and it is because of local minimum problem.

Since $\alpha = 0.5$ is the closest point the zero (Euclidean distance from axes origin), it is chosen as optimal and the parameters which are found with initial conditions $x_0^1 = [1 \ 1 \ 1 \ 20]$ are used.

$$[k_p \ k_n \ R_f \ D_s] = [72.4136 \times k_{p,nominal}, 72.9638 \times k_{n,nominal}, 1.3979 \times R_{f,nominal}, 7.2181 \times D_{s,nominal}]$$

3.4 Validation of Model

The parameters obtained by optimization toolbox are applied to *Spectral li-ion SPM* simulator. The model and experimental results are compared for both constant current discharge and pulse current discharge.

Figure 3.19 shows voltage responses at constant discharge current of C/10, C/2, 1C and 2C from 100% initial SoC condition and voltage responses are plotted as a function of depth of discharge (DoD).

The model is very accurate in the entire DoD range for C/10 and C/2, however the accuracy is less for 1C and 2C, in particular in the middle (DoD 10% - 70%).

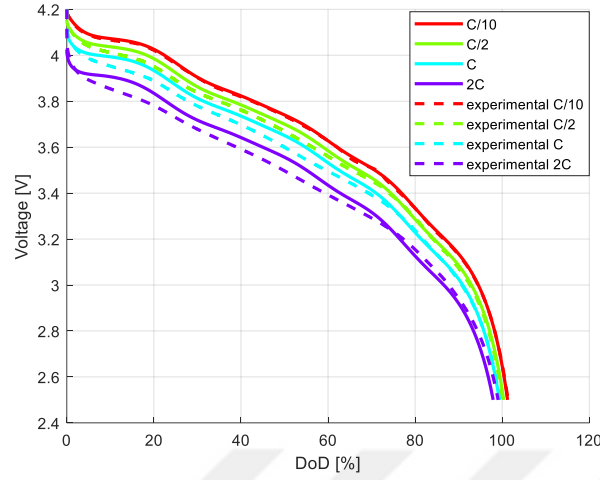


Figure 3.19 Voltage-DoD graph for different C-rates

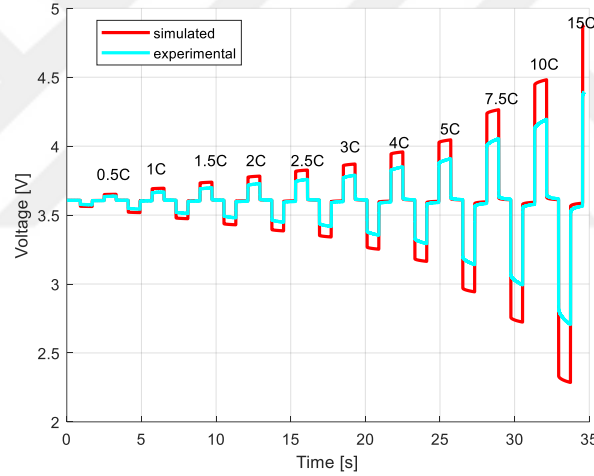


Figure 3.20 Voltage – Time graph for pulse current test

Figure 3.20 shows voltage response comparison of experimental and model data. The error between model and experimental for high C rates is bigger than 0.1V (after 5C it is bigger than 0.2V). However, it is not our main concern because, the focus of this work is only on currents up to 3C. Voltage response after 3C is just shown for completeness of information.

Although the error for high C rates is not a problem, the error on voltage response is still not negligible for lower than 3C. It is around 30mV for 0.5C and it is getting larger for the C rates higher than 0.5.

There is trade-off between getting an accurate model for constant current discharge test and getting an accurate model for pulse current test. Therefore, finding an accurate model for both constant current discharge test and pulse current test is really difficult. So, the model parametrization which is found by optimization toolbox is assumed as best possible trade-off and used for observer design in the next chapter.



4 Observer Design

In this chapter, the design of a state estimation algorithm based on backstepping observer method for partial differential equations (PDEs) is shown on a single particle model (SPM). SPM with two electrodes explained in Chapter 2 is reduced to one electrode by neglecting the cathode diffusion dynamics, and the reduced SPM (only one electrode) is used to ease the design of observer. A backstepping observer for PDEs is applied to the reduced SPM, and detailed explanation of implementation process of the backstepping observer using Chebyshev orthogonal collocation method is introduced.

4.1 The reduced SPM

In order to reduce the SPM, one can exploit the property of Lithium mass conservation. In fact, the SPM guarantees that the moles of Lithium in the solid phase is conserved [13]. The total Lithium moles inside the cell can be found as follow:

$$n_{Li} = \frac{\epsilon_s^+ L^+ A}{\frac{4}{3} \pi (R_s^+)^3} \int_0^{R_s^+} 4\pi r^2 c_s^+(r, t) dr + \frac{\epsilon_s^- L^- A}{\frac{4}{3} \pi (R_s^-)^3} \int_0^{R_s^-} 4\pi r^2 c_s^-(r, t) dr \quad (4.1)$$

By using the conservation of Lithium and neglecting diffusion dynamics, the surface concentration at cathode can be explained in terms of surface concentration at anode:

$$c_{ss}^+(t) = \frac{1}{\epsilon_s^+ L^+ A} [n_{Li} - \epsilon_s^- L^- A c_{ss}^-(t)] \quad (4.2)$$

$c_{ss}^+(t)$ on the voltage equation is replaced by $\alpha c_{ss}^-(t) + \beta$, where:

$$\alpha = \frac{\epsilon_s^- L^-}{\epsilon_s^+ L^+} \text{ and } \beta = \frac{n_{Li}}{\epsilon_s^+ L^+ A}$$

Finally, the voltage equation (4.3) of SPM with one electrode is:

$$\begin{aligned} V(t) = & \frac{RT}{\alpha^+ F} \sin h^{-1} \left(\frac{I(t)}{2a^+ AL^+ i_0^+ (\alpha c_{ss}^-(t) + \beta)} \right) \\ & - \frac{RT}{\alpha^- F} \sin h^{-1} \left(\frac{I(t)}{2a^- AL^- i_0^- (c_{ss}^-(t))} \right) \\ & + U_p(\alpha c_{ss}^-(t) + \beta) - U_n(c_{ss}^-(t)) - RI \end{aligned} \quad (4.3)$$

After SPM with one electrode is obtained, it is compared with SPM with two electrodes to show that SPM with one electrode is sufficiently accurate compared to SPM with two electrodes. Constant current test at C/10, C/2, 1C and 2C, and pulse current test are performed in both models, and the simulation results are shown in Figure 4.1 and Figure 4.2, respectively. As shown in Figure 4.1 and Figure 4.2, there is just negligible differences between these models.

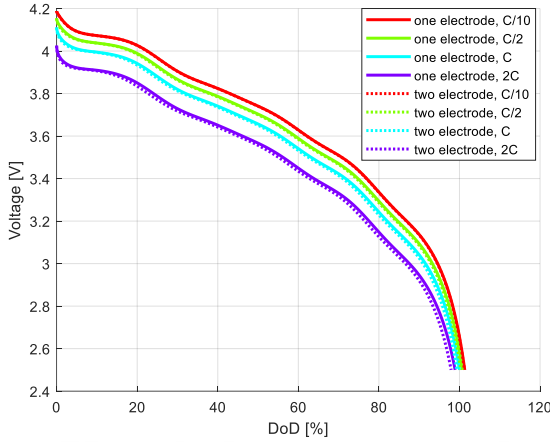


Figure 4.1 Voltage – DoD for different C-rates

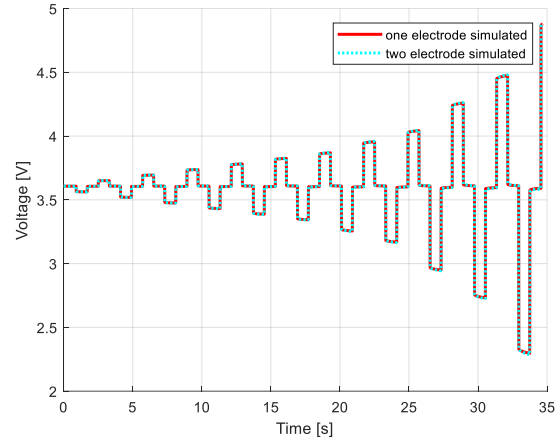


Figure 4.2 Voltage – Time graph for pulse current test

4.2 Backstepping Observer Design

The observer development process is summarized as follows:

- 1) Perform normalization and state transformation for the diffusion equation
- 2) Design a backstepping observer
- 3) Implement backstepping observer to Bizeray's model presented in Chapter 2 simplifier earlier to one electrode.
- 4) Implement the observer in Matlab

In the first two steps, the approach and symbols presented by Moura [13] are followed; in the latter two, the approach and symbols presented by Bizeray are used [16].

4.2.1 Model Normalization

Diffusion equation in negative electrode is governed by the following Fick's law in spherical coordinates and two Neuman boundary conditions at the core and surface of negative electrode as already presented Chapter 2:

$$\frac{\partial c_s^-}{\partial t}(r, t) = D_s^- \left[\frac{2}{r} \frac{\partial c_s^-}{\partial r}(r, t) + \frac{\partial^2 c_s^-}{\partial r^2}(r, t) \right] \quad (4.4)$$

$$\frac{\partial c_s^-}{\partial r}(0, t) = 0, \quad \frac{\partial c_s^-}{\partial r}(R_s^-, t) = -\frac{R_s^- I(\bar{t})}{D_s^- F a^- A L^-} \quad (4.5)$$

The radial r and time t coordinates are rescaled in order to simplify the mathematical structure of the observer, as follows:

$$\bar{r} = \frac{r}{R_s^-} \quad \bar{t} = \frac{D_s^-}{(R_s^-)^2} t \quad (4.6)$$

which results in the following PDE and boundary conditions:

$$\frac{\partial c_s^-}{\partial \bar{t}}(\bar{r}, \bar{t}) = \frac{2}{\bar{r}} \frac{\partial c_s^-}{\partial \bar{r}}(\bar{r}, \bar{t}) + \frac{\partial^2 c_s^-}{\partial \bar{r}^2}(\bar{r}, \bar{t}) \quad (4.7)$$

$$\frac{\partial c_s^-}{\partial \bar{r}}(0, \bar{t}) = 0, \quad \frac{\partial c_s^-}{\partial \bar{r}}(1, \bar{t}) = -\frac{R_s^- I(\bar{t})}{D_s^- F a^- AL^-} \quad (4.8)$$

Then, a state transformation is performed to eliminate the first order partial derivative term in the spherical diffusion equation:

$$c(\bar{r}, \bar{t}) = \bar{r} c_s^-(\bar{r}, \bar{t}) \quad (4.9)$$

Thus producing the following PDE plant:

$$\frac{\partial c}{\partial \bar{t}}(\bar{r}, \bar{t}) = \frac{\partial^2 c}{\partial \bar{r}^2}(\bar{r}, \bar{t}) \quad (4.10)$$

with Dirichlet and Robin boundary conditions:

$$\begin{aligned} c(0, \bar{t}) &= 0 \\ \frac{\partial c}{\partial \bar{r}}(1, \bar{t}) - c(1, \bar{t}) &= -\frac{R_s^-}{D_s^- F a^- AL^-} I(\bar{t}) \end{aligned} \quad (4.11)$$

4.2.2 Design of Backstepping Observer

The main idea of backstepping observer is to find gain kernel PDE that makes the plant equivalent to an exponentially stable target system. In fact, stability of the target system translates into stability of the closed loop system consisting of the plant plus boundary feedback [13]. Next, in order to find a solution of gain kernel PDE, gain kernel PDE is converted to an integral equation, and output injection gains can be computed.

The observer is the copy of the plant which is shown above plus boundary state error injection:

$$\frac{\partial \hat{c}}{\partial \bar{t}}(\bar{r}, \bar{t}) = \frac{\partial^2 \hat{c}}{\partial \bar{r}^2}(\bar{r}, \bar{t}) + p_1(\bar{r}) \tilde{c}(1, \bar{t}) \quad (4.12)$$

$$\begin{aligned} \hat{c}(0, \bar{t}) &= 0 \\ \frac{\partial \hat{c}}{\partial \bar{r}}(1, \bar{t}) - \hat{c}(1, \bar{t}) &= -\frac{R_s^- I(\bar{t})}{D_s^- F a^- AL^-} + p_{10} \tilde{c}(1, \bar{t}) \end{aligned} \quad (4.13)$$

The boundary state error is defined as follow:

$$\tilde{c}(1, \bar{t}) = \varphi(V(\bar{t}), I(\bar{t})) - \hat{c}(1, \bar{t}) \quad (4.14)$$

φ is the inverse of the system output function, which doesn't need to be inverted here, since the plant boundary state is computed by using a lookup table. The inputs of lookup table are voltage V and current I and the output is surface concentration c_{ss}^- . The block diagram of the observer is shown in Figure 4.3.

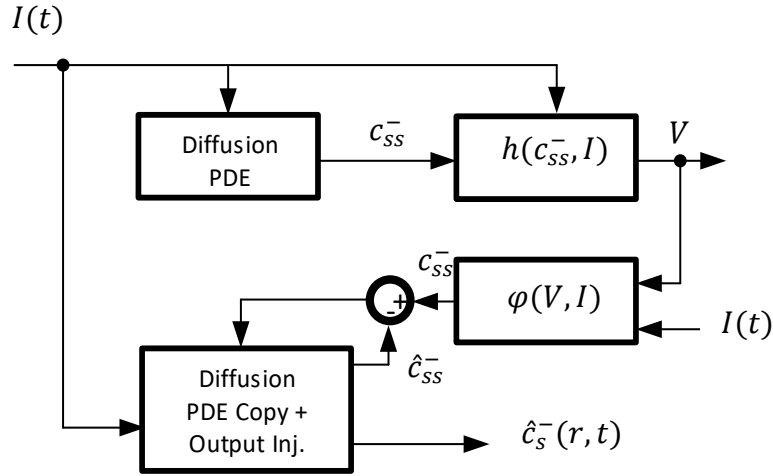


Figure 4.3 Block diagram of the observer

The backstepping approach is applied to design the output injection gains $p_1(\bar{r})$ and p_{10} . First denote the observer error as:

$$\tilde{c}(\bar{r}, \bar{t}) = c(\bar{r}, \bar{t}) - \hat{c}(\bar{r}, \bar{t}) \quad (4.15)$$

subtracting observer structure from model structure produces the estimation error dynamics:

$$\frac{\partial \tilde{c}}{\partial \bar{t}}(\bar{r}, \bar{t}) = \frac{\partial^2 \tilde{c}}{\partial \bar{r}^2}(\bar{r}, \bar{t}) + p_1(\bar{r})\tilde{c}(1, \bar{t}) \quad (4.16)$$

$$\tilde{c}(0, \bar{t}) = 0$$

$$\frac{\partial \tilde{c}}{\partial \bar{r}}(1, \bar{t}) - \tilde{c}(1, \bar{t}) = -\frac{R_s^- I(t)}{D_s^- F a^- A L^-} + p_{10}\tilde{c}(1, \bar{t}) \quad (4.17)$$

Following the procedure that are explained in Moura's paper [13], output injection gains are found:

$$p_1(\bar{r}) = -\frac{\lambda \bar{r}}{2x} \left[I_1(x) - \frac{2\lambda}{x} I_2(x) \right] \quad (4.18)$$

$$x = \sqrt{\lambda(\bar{r}^2 - 1)} \quad (4.19)$$

$$p_{10} = \frac{3 - \lambda}{2} \quad (4.20)$$

λ is tunable reaction coefficient, and it is the only tuning parameter of the observer ($\lambda < \frac{1}{4}$) [13]. $I_1(x)$ and $I_2(x)$ are the first and second order modified Bessel functions of the first kind, respectively. And the Bessel functions are given as:

$$I_1(x) = \sum_{m=0}^{\infty} \frac{\left(\frac{x}{2}\right)^{2m+1}}{m!(m+1)!} \text{ and } I_2(x) = \sum_{m=0}^{\infty} \frac{\left(\frac{x}{2}\right)^{2m+2}}{m!(m+2)!} \quad (4.21)$$

The modified Bessel functions are expressed as series of infinite terms, but finite numbers are needed to implement Bessel functions in Matlab. After a sensitivity study, it is figured out that $M_{max} = 10$ is adequate to implement Bessel functions correctly.

$$I_1(x) = \sum_{m=0}^{M_{max}} \frac{\left(\frac{x}{2}\right)^{2m+1}}{m!(m+1)!} \text{ and } I_2(x) = \sum_{m=0}^{M_{max}} \frac{\left(\frac{x}{2}\right)^{2m+2}}{m!(m+2)!} \quad (4.22)$$

4.2.3 Implementation of Backstepping Observer to Bizeray's Model

To simplify the model implementation, in both Moura's model and Bizeray's model, the authors perform normalization and state transformation in spherical diffusion equation. In order to implement backstepping observer which is explained in Moura's paper to Bizeray's model correctly, the spherical diffusion equations are written so as to obtain same normalization of radial r and time t coordinates and states. In this way, the scaling factor of output injection gains $p_{1,B}(\bar{r})$ and $p_{10,B}$, to be implemented on Bizeray model, can be found to be applied to $p_{1,M}(\bar{r})$ and $p_{10,M}$.

Diffusion equations are shown in Moura's and Bizeray's paper respectively:

$$\frac{\partial c}{\partial \bar{t}}(\bar{r}, \bar{t}) = \frac{\partial^2 c}{\partial \bar{r}^2}(\bar{r}, \bar{t}) + p_{1,M} \tilde{c}_1 \quad (4.23)$$

$$\frac{\partial u}{\partial t}(x, t) = \frac{D_s^-}{(R_s^-)^2} \frac{\partial^2 u}{\partial x^2}(x, t) + p_{1,B} \tilde{u}_1 \quad (4.24)$$

where:

$$u = rc \text{ and } x = \frac{r}{R_s^-} \quad (4.25)$$

Firstly, to eliminate the coefficient of second order partial derivative in Bizeray's model, the equation is multiplied with $\frac{(R_s^-)^2}{D_s^-}$ and:

$$\frac{(R_s^-)^2}{D_s^-} \frac{\partial u}{\partial t}(x, t) = \frac{\partial^2 u}{\partial x^2}(x, t) + \frac{(R_s^-)^2}{D_s^-} p_{1,B} \tilde{u}_1 \quad (4.26)$$

After that, in Moura's model, time $\bar{t}$ and radial $\bar{r}$ are converted to their original coordinates t and r . Also variable c is changed with u :

$$c = \frac{u}{r} \quad \bar{r} = \frac{r}{R_s^-} = x \quad \bar{t} = \frac{D_s^-}{(R_s^-)^2} t \quad (4.27)$$

By considering the change of coordinates and state defined above, it is obtained that:

$$\frac{(R_s^-)^2}{D_s^-} \frac{\partial \frac{u}{R_s^-}}{\partial t}(x, t) = \frac{\partial^2 \frac{u}{R_s^-}}{\partial x^2}(x, t) + p_{1,M} \frac{\tilde{u}_1}{R_s^-} \quad (4.28)$$

Next, the equation above is multiplied by R_s^- :

$$\frac{(R_s^-)^2}{D_s^-} \frac{\partial u}{\partial t}(x, t) = \frac{\partial^2 u}{\partial x^2}(x, t) + p_{1,M} \tilde{u}_1 \quad (4.29)$$

which is equivalent to equation 4.26. So, the relationship between output injection gain of Bizeray's model and Moura's model can be easily seen, which is:

$$p_{1,B} = \frac{D_s^-}{(R_s^-)^2} p_{1,M} \quad (4.30)$$

If the same transformation is applied to the boundary conditions at surface of negative electrode, scaling factor of p_{10} can be found easily. Those conditions are respectively defined in Bizeray's and Moura's paper as follows:

$$\frac{\partial u}{\partial x}(1, t) - u(1, t) = -\frac{(R_s^-)^2}{D_s^-} j + p_{10,B} \tilde{u}_1 \quad (4.31)$$

where j is:

$$j = \frac{I(t)}{F a^- AL^-} \quad (4.32)$$

and:

$$\frac{\partial c}{\partial \bar{r}}(1, \bar{t}) - c(1, \bar{t}) = -\frac{R_s^-}{D_s^- F a^- AL^-} I(\bar{t}) + p_{10,M} \tilde{c} \quad (4.33)$$

After that, in Moura's model, time $\bar{t}$ and radial $\bar{r}$ are converted to their original coordinates t and r . And variable c is changed with u . Then, the equation is multiplied by R_s^- :

$$\frac{\partial u}{\partial x}(1, t) - u(1, t) = -\frac{(R_s^-)^2}{D_s^- F a^- AL^-} I(t) + p_{10,M} \tilde{u}_1 \quad (4.34)$$

Finally, by comparing equation 4.31 and equation 4.34, it can be seen that:

$$p_{10,B} = p_{10,M} \quad (4.35)$$

4.2.4 Implementation of Observer in Matlab

The spherical diffusion equation and surface boundary conditions are given in Bizeray's paper:

$$\frac{\partial u}{\partial t}(x, t) = \frac{D_s^-}{(R_s^-)^2} \frac{\partial^2 u}{\partial x^2}(x, t) \quad (4.36)$$

$$\frac{\partial u}{\partial x}(1, t) - u(1, t) = -\frac{(R_s^-)^2}{D_s^-} j(t) \quad (4.37)$$

The partial differential equation is discretized by using the Chebyshev orthogonal collocation:

$$\frac{\partial u_{1:N}}{\partial t} = \frac{D_s}{R_s^2} ([D_M^2]_{1:N,1:N} u_{1:N} + [D_M^2]_{1:N,N+2:M+1} u_{N+2:M+1}) \quad (4.38)$$

where D_M^2 is second derivative Chebyshev differentiation matrices with $M + 1$ Chebyshev nodes. M is equal to $2N$, where N is the number of Chebyshev nodes in half of the sphere including surface, not core. By symmetry:

$$u(r) = -u(-r) \Rightarrow u_{N+2:M+1} = -P u_{1:N} \quad (4.39)$$

where P is the permutation matrix which is the backward identity matrix ($P = P^{-1}$). By using this equality, solid phase diffusion equation can be written in terms of $u_{1:N}$:

$$\frac{\partial u_{1:N}}{\partial t} = \frac{D_s}{R_s^2} ([D_M^2]_{1:N,1:N} - [D_M^2]_{1:N,N+2:M+1} P) u_{1:N} \quad (4.40)$$

To simplify the equation, a new matrix $\tilde{D}_N^2$ is defined:

$$\tilde{D}_N^2 = ([D_M^2]_{1:N,1:N} - [D_M^2]_{1:N,N+2:M+1} P) \quad (4.41)$$

Also, $\tilde{D}_N^1$ matrix which is used for boundary condition is defined by applying same procedure as for $\tilde{D}_N^2$:

$$\tilde{D}_N^1 = ([D_M^1]_{1:N,1:N} - [D_M^1]_{1:N,N+2:M+1} P) \quad (4.42)$$

Finally, the discretized solid phase diffusion equation and boundary conditions are:

$$\frac{\partial u_{1:N}}{\partial t} = \frac{D_s}{R_s^2} [\tilde{D}_N^2]_{N,N} u_{1:N} \quad (4.43)$$

$$[\tilde{D}_N^1]_{1,1:N} u_{1:N} - u_1 = -\frac{R_s^2}{D_s} j \quad (4.44)$$

After discretized solid phase diffusion equation and boundary conditions are obtained, backstepping observer is implemented to the discretized model. Like explained in section 4.2.2, the observer is a copy of the plant with boundary state error injection:

$$\frac{\partial u_{1:N}}{\partial t} = \frac{D_s}{R_s^2} [\tilde{D}_N^2]_{N,N} u_{1:N} + [p_{1,B}]_{1:N} (u_1 - \hat{u}_1) \quad (4.45)$$

$$[\tilde{D}_N^1]_{1,1:N} \hat{u}_{1:N} - \hat{u}_1 = -\frac{R_s^2}{D_s} j + p_{10,B} (u_1 - \hat{u}_1) \quad (4.46)$$

The boundary condition at the particle surface is equivalent to:

$$[\tilde{D}_N^1]_{1,2:N} \hat{u}_{2:N} + ([\tilde{D}_N^1]_{1,1} - 1) \hat{u}_1 = -\frac{R_s^2}{D_s} j + p_{10,B} (u_1 - \hat{u}_1) \quad (4.47)$$

It allows $\hat{u}_1$ to be defined as a function of the other nodes:

$$\hat{u}_1 = \frac{[\tilde{D}_N^1]_{1,2:N}}{1 - p_{10,B} - [\tilde{D}_N^1]_{1,1}} \hat{u}_{2:N} + \frac{R_s^2}{D_s} \frac{1}{1 - p_{10,B} - [\tilde{D}_N^1]_{1,1}} j - \frac{p_{10,B}}{1 - p_{10,B} - [\tilde{D}_N^1]_{1,1}} u_1 \quad (4.48)$$

Then, since $\hat{u}_1$ is known, the diffusion equation is written for the inner nodes only $\hat{u}_{2:N}$:

$$\frac{\partial \hat{u}_{2:N}}{\partial t} = \frac{D_s}{R_s^2} \left([\tilde{D}_N^2]_{2:N,2:N} \hat{u}_{2:N} + [\tilde{D}_N^2]_{2:N,1} \hat{u}_1 \right) + [p_{1,B}]_{2:N} (u_1 - \hat{u}_1) \quad (4.49)$$

And by replacing $\hat{u}_1$ in the equation above:

$$\begin{aligned} \frac{\partial \hat{u}_{2:N}}{\partial t} = \frac{D_s}{R_s^2} & \left([\tilde{D}_N^2]_{2:N,2:N} \hat{u}_{2:N} \right. \\ & + \left([\tilde{D}_N^2]_{2:N,1} - \frac{R_s^2}{D_s} [p_{1,B}]_{2:N} \right) \left(\frac{[\tilde{D}_N^1]_{1,2:N}}{1 - p_{10,B} - [\tilde{D}_N^1]_{1,1}} \hat{u}_{2:N} \right. \\ & + \left. \frac{R_s^2}{D_s} \frac{1}{1 - p_{10,B} - [\tilde{D}_N^1]_{1,1}} j - \frac{p_{10,B}}{1 - p_{10,B} - [\tilde{D}_N^1]_{1,1}} u_1 \right) \\ & + [p_{1,B}]_{2:N} u_1 \end{aligned} \quad (4.50)$$

The diffusion equation can be written in the following state space form:

$$\frac{\partial \hat{u}_{2:N}}{\partial t} = D_s A \hat{u}_{2:N} + B j + \frac{D_s}{R_s^2} G_1 u_1 \quad (4.51)$$

where the matrices A , B and G_1 defined as follows:

$$\begin{aligned} A &= \frac{1}{R_s^2} \left([\tilde{D}_N^2]_{2:N,2:N} + \frac{\left([\tilde{D}_N^2]_{2:N,1} - \frac{R_s^2}{D_s} [p_{1,B}]_{2:N} \right) [\tilde{D}_N^1]_{1,2:N}}{1 - p_{10,B} - [\tilde{D}_N^1]_{1,1}} \right) \\ B &= \frac{[\tilde{D}_N^2]_{2:N,1} - \frac{R_s^2}{D_s} [p_{1,B}]_{2:N}}{1 - p_{10,B} - [\tilde{D}_N^1]_{1,1}} \\ G_1 &= - \frac{[\tilde{D}_N^2]_{2:N,1} - \frac{R_s^2}{D_s} [p_{1,B}]_{2:N}}{1 - p_{10,B} - [\tilde{D}_N^1]_{1,1}} p_{10,B} + \frac{R_s^2}{D_s} [p_{1,B}]_{2:N} \end{aligned} \quad (4.52)$$

By recalling the value of $p_{1,B}$ and $p_{10,B}$ as in equations 4.30 and 4.35, the matrices A , B and G_1 can be eventually obtained as follows:

$$\begin{aligned}
 A &= \frac{1}{R_s^2} \left([\tilde{D}_N^2]_{2:N,2:N} + \frac{([\tilde{D}_N^2]_{2:N,1} - [p_{1,M}]_{2:N}) [\tilde{D}_N^1]_{1,2:N}}{1 - p_{10,M} - [\tilde{D}_N^1]_{1,1}} \right) \\
 B &= \frac{[\tilde{D}_N^2]_{2:N,1} - [p_{1,M}]_{2:N}}{1 - p_{10,M} - [\tilde{D}_N^1]_{1,1}} \\
 G_1 &= - \frac{[\tilde{D}_N^2]_{2:N,1} - [p_{1,M}]_{2:N}}{1 - p_{10,M} - [\tilde{D}_N^1]_{1,1}} p_{10,M} + [p_{1,M}]_{2:N}
 \end{aligned} \tag{4.53}$$

Finally, output c which is the vector containing the Lithium concentration values at the nodes is given by:

$$\hat{c}_{1:N} = \frac{\hat{u}_{1:N}}{r_{1:N}} = C \hat{u}_{2:N} + \frac{D}{D_s} j - G_2 u_1 \tag{4.54}$$

where the matrices C , D and G_2 can be obtained as follows:

$$\begin{aligned}
 C &= \begin{bmatrix} \frac{1}{R_s} \frac{[\tilde{D}_N^1]_{1,2:N}}{1 - p_{10,M} - [\tilde{D}_N^1]_{1,1}} \\ \frac{1}{r_2} \\ \vdots \\ \frac{1}{r_n} \end{bmatrix}_{N \times N-1} \\
 D &= \begin{bmatrix} \frac{R_s}{1 - p_{10,M} - [\tilde{D}_N^1]_{1,1}} \\ 0 \\ \vdots \\ 0 \end{bmatrix}_{N \times 1} \\
 G_2 &= \begin{bmatrix} \frac{p_{10,M}}{R_s (1 - p_{10,M} - [\tilde{D}_N^1]_{1,1})} \\ 0 \\ \vdots \\ 0 \end{bmatrix}_{N \times 1}
 \end{aligned} \tag{4.55}$$

The diffusion equations above is solved for the states $\hat{u}_{1:N}$, because core dynamics is not considered by Bizeray, so:

$$u(r = 0) = 0 \tag{4.56}$$

which means:

$$u_{N+1} = 0 \tag{4.57}$$

To compute the value of concentration at the core of the particle c_{N+1} , the Neuman boundary condition at the surface of particle is recalled:

$$\left. \frac{\partial c(r, t)}{\partial x} \right|_{x=1} = -\frac{R_s^-}{D_s^-} j \quad (4.58)$$

by recalling symmetry $c(x) = c(-x)$, this equation can be written in discrete form as follows:

$$([D_M^1]_{1,1:N} + [D_M^1]_{1,N+2:M+1}P)c_{1:N} + [D_M^1]_{1,N+1}c_{N+1} = -\frac{R_s^-}{D_s^-} j \quad (4.59)$$

which gives the equation of concentration at the core of the particle:

$$c_{N+1} = -\frac{[D_M^1]_{1,1:N} + [D_M^1]_{1,N+2:M+1}P}{[D_M^1]_{1,N+1}}c_{1:N} - \frac{1}{[D_M^1]_{1,N+1}}\frac{R_s^-}{D_s^-} j \quad (4.60)$$

After that, A , B , C , D , G_1 and G_2 matrices are implemented in Matlab and the performance of backstepping observer are evaluated by performing several simulations as explained in the next chapter.

5 Observer Results

In this chapter, simulation results and experimental results that illustrate the performance of the proposed observer are presented. While investigating the performance of the observer, both constant current discharge and pulses sequence at 0-2C are considered. Firstly, the observer is initialized at different initial error on SoC and robustness of the estimator is tested for both tests with different λ (tunable reaction coefficient which appears directly in the observer gains). Secondly, the observer is validated in the presence of noisy voltage measurements for two scenarios explained above. Thirdly, uncertainty in the model parameters D_s , R_f , k_p and k_n which are found by using automatic optimization as shown in the previous chapter is investigated for a chosen λ value. Lastly, the designed observer's capability is examined for SOC estimation as compared to the actual SoC results derived from experimental results.

5.1 Observer Simulation Results

In this section, simulation results are demonstrated to show the performance of the proposed observer. As shown in the previous chapter, in the design of observer, the error between the measured and estimated surface concentration is given in feedback, so that estimated surface concentration closes to the measured one. For this purpose, the comparison of SoC estimation are shown first for 2C constant current discharge test and 2C pulse discharge test, and then voltage responses are depicted to illustrate that backstepping observer also has the capability to estimate the correct voltage results. Results for inner concentrations are shown only for the first test as an example, for the sake of brevity. However, correct convergence of state estimations for all elements along r is obtained for all proposed situations; bulk SoC is thus taken as a synthetic value describing the average state convergence rate.

5.1.1 Simulation Results

In the constant current discharge test, the simulator starts at SoC = 100% and an input current of 2C is provided. The observer is initialized at SoC = 50%, and SoC error (e_{SoC}) is defined as follow:

$$e_{SoC} = SoC - \hat{SoC} \quad (5.1)$$

where $\hat{SoC}$ is the estimated SoC from the observer. The results are shown for $\lambda = -20, -10, -5, -1$. As it can be seen from Figure 5.1 and Figure 5.2, SoC error converges fast to zero even with a large initialization error (for example 50%). SoC estimation error at steady-state is less than 0.6% for all λ . e_{SoC} converges to values below 1% in 10s, 140s, 220s, 375s and 460s for $\lambda = -20, -10, -5, -1$ and -0.1 respectively. The observer states converges to the model states quicker for high λ .

Figure 5.3 and Figure 5.4 show the surface stoichiometry and the distribution of stoichiometry along r for different λ . As shown in Figure 5.4, at time instant 0, the observer results have 50% error and stoichiometry are far from the model. In steady-state, at $t=1001s$ and $t=1551s$ where SoC

is 45% and 15% respectively, stoichiometry results of the observer have a good match with the model for all λ . Hence, it can be stated that the backstepping observer can successfully estimate Lithium-ion concentrations along r and SoC. Figure 5.5 demonstrates voltage response, and even if the surface concentration is given in feedback only, the observer still can converge to the true voltage response.

Secondly, pulse current test at 2C is carried out. Simulator starts at SoC = 100% and runs until the simulator reaches the cut-off voltage. Like in the constant current discharge test, the observer is launched with an initial SoC error of 50%.

Figure 5.6 presents that even with a large initial error 50%, SoC estimation errors converge to zero. Furthermore, the steady-state errors are less than 0.5% for the SoC and convergence time at 0.5% is roughly 70s, 160s, 300s, 530s, and 675s, respectively for $\lambda = -20, -10, -5, -1$ and -0.1 as shown in Figure 5.7. Figure 5.8 shows voltage response for the first 50s of the test, which is far from the model as expected. Figure 5.9 presents the voltage response at towards the end of the test, when the observer converges to the actual voltage.

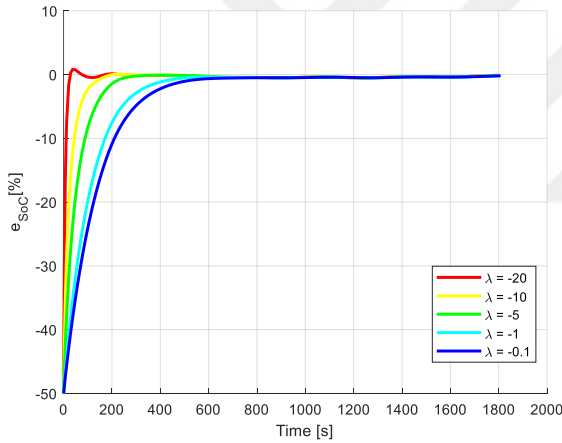
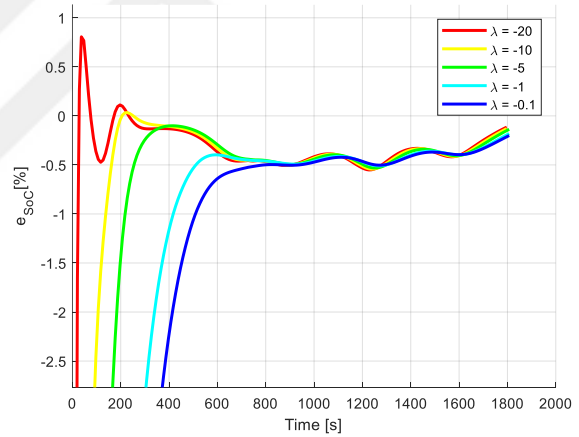
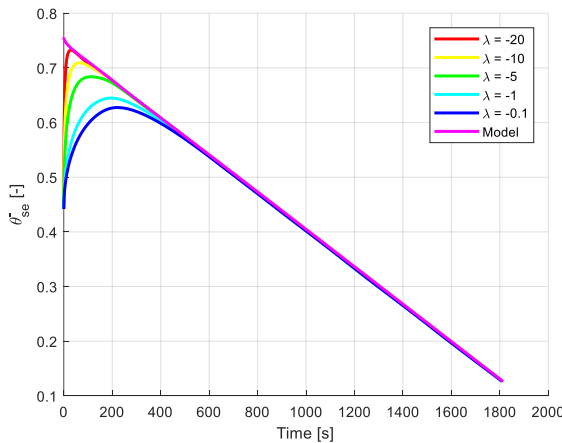
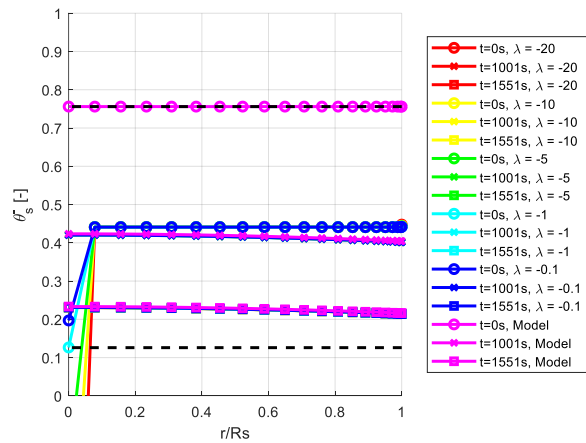

 Figure 5.1 SoC error estimation for different λ


Figure 5.2 A zoom to SoC error


 Figure 5.3 Surface concentration for different λ

 Figure 5.4 Stoichiometry results along r for different λ at 3 different time instant.

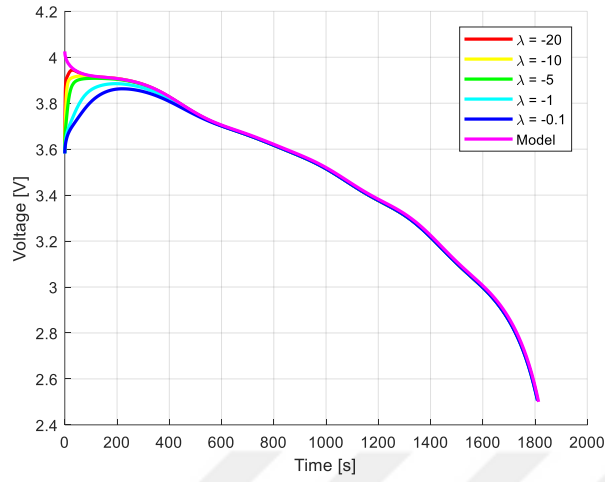


Figure 5.5 Voltage responses of the observer for different λ

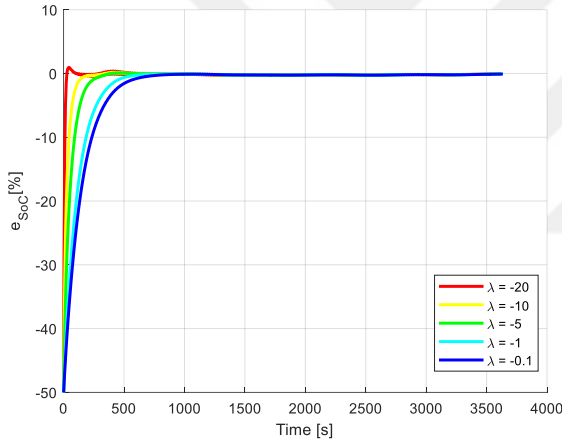


Figure 5.6 SoC error estimation for different λ

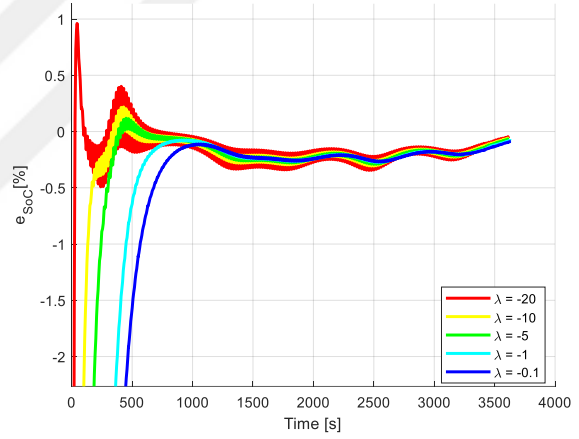


Figure 5.7 A zoom to SoC error

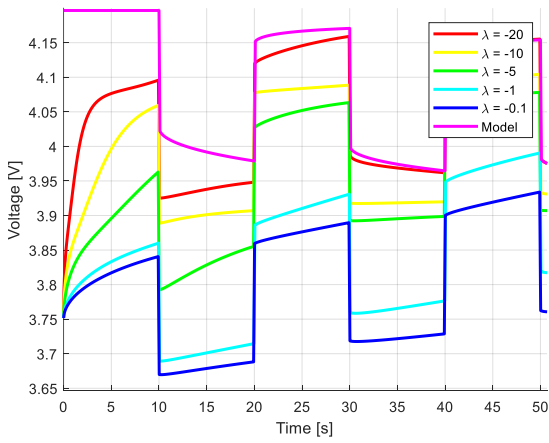


Figure 5.8 Voltage response for the first 50s of the pulse test

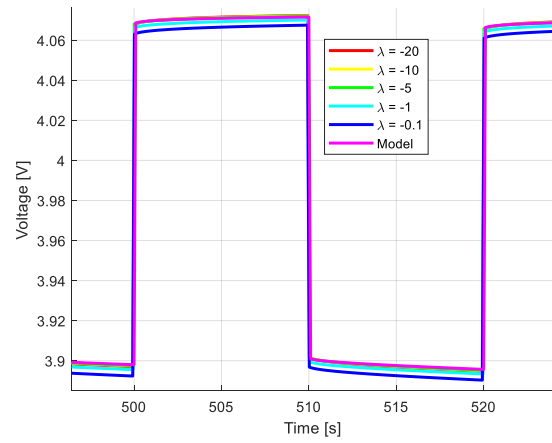


Figure 5.9 Voltage response towards the end of the pulse test

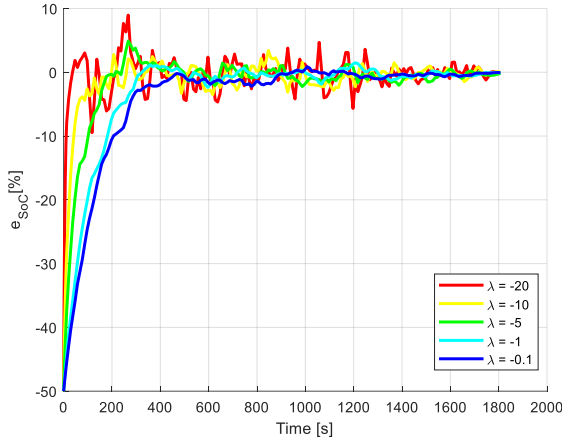


Figure 5.10 SoC error estimation for different λ with noise on Voltage

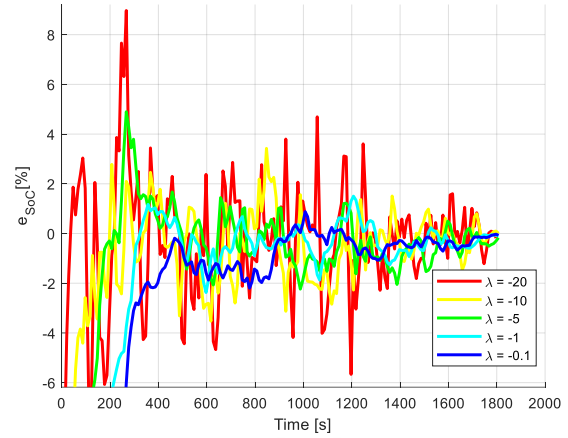


Figure 5.11 A zoom to SoC error estimation for different λ with noise on Voltage

5.1.2 Simulation Results with Noisy Measurements

In this section, the robustness and performance of backstepping observer are investigated in the presence of measurement noise to emulate a realistic voltage sensor. Additive white noise is added to the voltage measurements and the two tests presented above are carried out again. This noise translates to an equivalent noise acting on the measured surface concentration, through the inversion of output function as shown in Figure 4.3.

The first test is 2C discharge test with additive white noise. The variance (σ^2) of white noise is chosen as $1mV$.

From a general point of view, it can be said that the observer close to the true value of SoC as illustrated in Figure 5.10 and Figure 5.11; however, for high λ values, in particular $\lambda = -20$ there is strong oscillation (about $\pm 5\%$) around the true value. On the other hand, the oscillations can be filtered with low values of λ , as expected. (see also Figure 5.12)

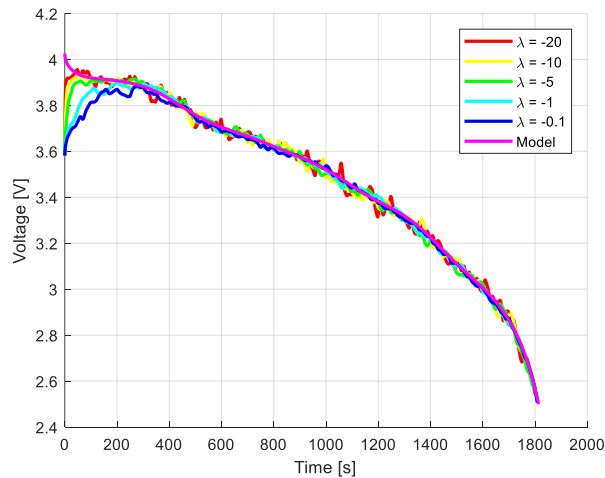


Figure 5.12 Voltage responses of the observer for different λ with noise on Voltage measurements

In the second test, the performance of the observer is investigated for a pulses sequences input current at 0-2C. The observer starts with an initial error of 50%, and tunable reaction coefficient λ is selected in the same as for the previous test. SoC estimation error cannot be driven exactly to zero for high (for example $\lambda = -20$) as demonstrated in Figure 5.13 and Figure 5.14. There is an oscillation on SoC estimation due to the effect of measurement noise, even though SoC estimation error enters the band less than 2% for all the values of λ . For low λ , the results of SoC estimation can successfully converge to a true value of SoC that is much closer to true one.

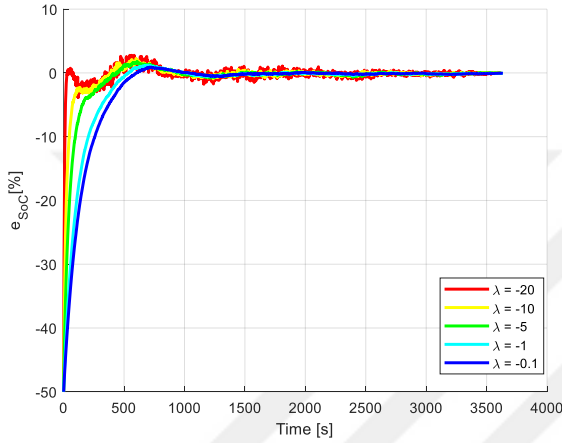


Figure 5.13 SoC error estimation for different λ with noise on voltage measurements

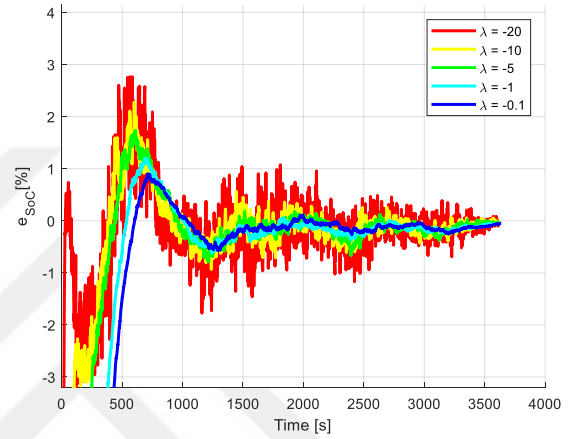


Figure 5.14 A zoom to SoC error estimation for different λ with noise on Voltage

As it can be seen from the Figure 5.15 and Figure 5.16, the observer can also follow the measured voltage for all λ values.

As a consequence of both the tests, it can be stated that the observer is robust with respect to noise on the voltage. There is a trade-off between convergence time and noise rejection, and by considering the effects of λ on convergence time and noise rejection, the selected value is $\lambda = -5$ for the simulations shown in the following.

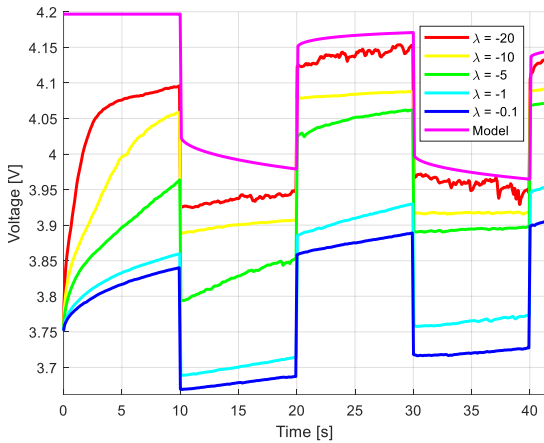


Figure 5.15 Voltage response for the first 40s of the pulse test with noise on voltage measurements

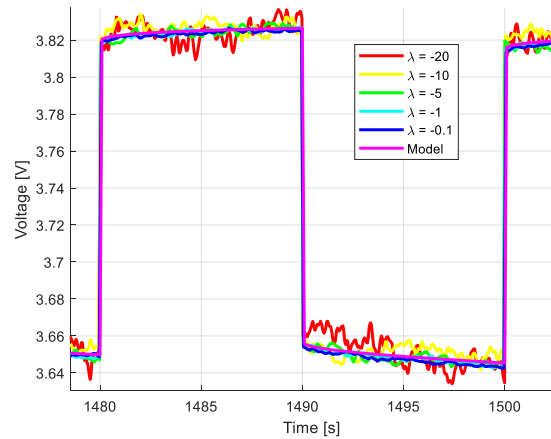


Figure 5.16 Voltage response towards the end of the pulse test with noise on voltage measurements

5.1.3 Simulation Results with Parameter Uncertainty

Like most observers, the performance of backstepping observer depends on the knowledge of model parameters. Because of that, the robustness of backstepping observer with respect to model parametric uncertainty is evaluated by changing several parameters (D_s , k_p , k_n and R_f). The observer starts with a different initial state like previous tests and simulation results are shown for the chosen λ value which is -5.

5.1.3.1 Parameter Uncertainty in D_s

D_s is decreased by 50%, and constant current discharge test at 2C is carried out.

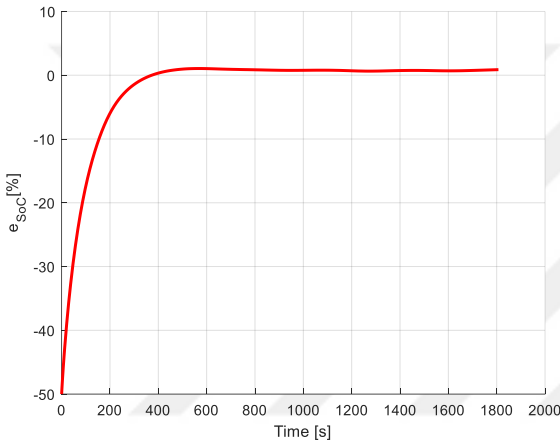


Figure 5.17 SoC error estimation for parameter uncertainty in D_s ($\lambda = -5$)

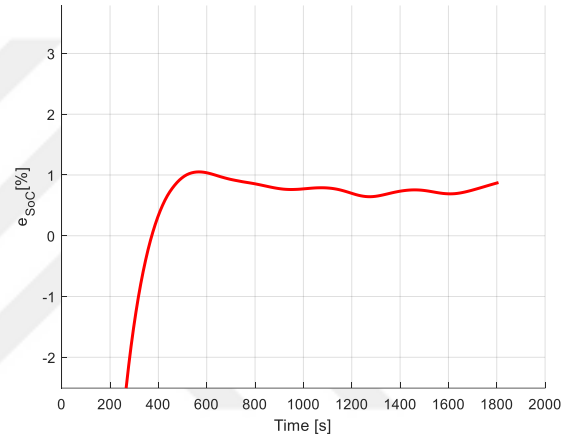


Figure 5.18 A zoom to SoC error estimation for parameter uncertainty in D_s ($\lambda = -5$)

Figure 5.17 and Figure 5.18 present simulation results of SoC error estimation. As shown in those figures, SoC can be still correctly estimated, even in the presence of uncertainties in parameter D_s . SoC estimation error is driven to values less than 1.1% in 314s. The RMS error is only 0.78% after SoC estimation error enters the error band 1.1%. Moreover, as shown in Figure 5.19, the voltage can still be corrected even in the presence of parameter uncertainty in the model.

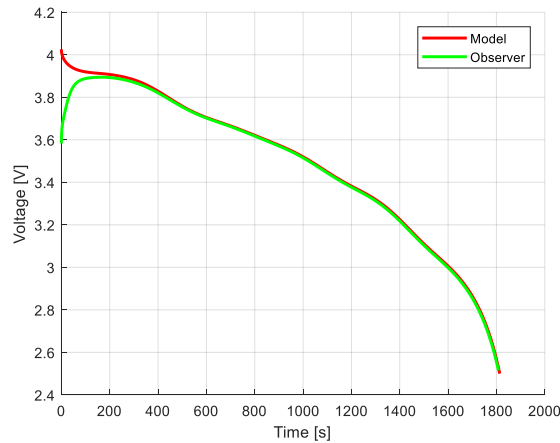


Figure 5.19 Voltage response for parameter uncertainty in D_s ($\lambda = -5$)

After that, pulse test is carried out by introducing 50% error in the D_s parameter. Also, in the pulse test, the observer still can converge to the actual value of SoC as depicted in Figure 5.20 and Figure 5.21. SoC estimation enters the 1% error band in approximately 380s. The RMS error of estimated SoC is found as 0.58% after SoC estimation error enters the band 1%. Despite uncertainty in D_s parameter, after a certain time, the observer can follow the actual voltage with 2 mV error as shown in Figure 5.23.

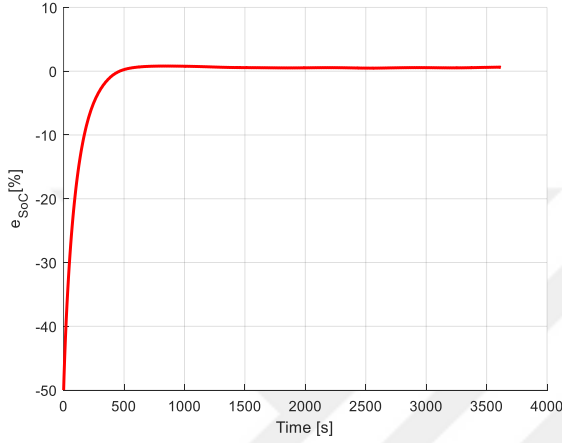


Figure 5.20 SoC error estimation for pulse test

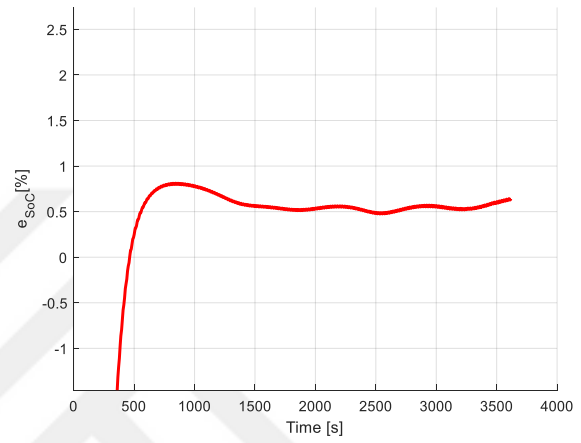


Figure 5.21 A zoom to SoC error estimation for pulse test

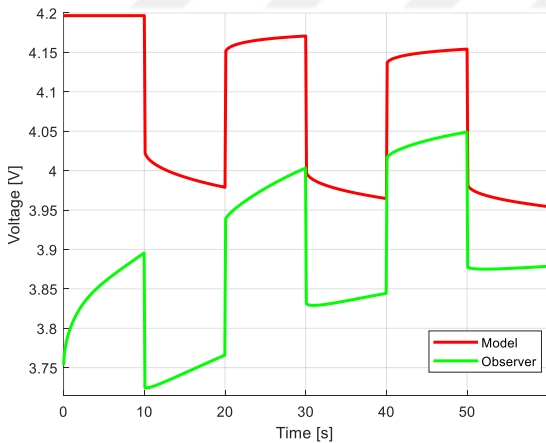


Figure 5.22 Voltage response for the first 50s of the pulse test

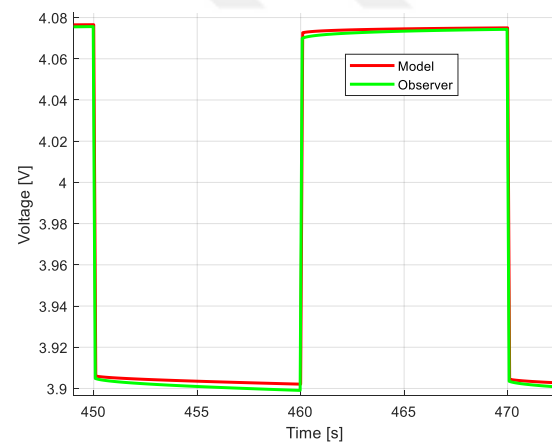


Figure 5.23 Voltage response towards the end of the pulse test

5.1.3.2 Parameter Uncertainty in k_p and k_n

Secondly, the parameters k_p and k_n are varied at the same time to study the robustness of backstepping observer. $k_{p,n}$ parameters are reduced by 98%, and simulations are performed.

As depicted in the following Figure 5.24 and Figure 5.25, the observer can estimate SoC successfully despite a very large error in $k_{p,n}$ parameters for 2C constant current discharge test. SoC estimation error is less than 1% after 212s, and the RMS error after the convergence is only 0.52%. However, in voltage response in Figure 5.26, there is almost 70 mV difference between the

model and the observer in the steady-state due to the uncertainty in the model. The reason of this error is that backstepping observer just corrects surface concentration and inner states along r , not voltage. As shown in previous chapters, the output voltage equation is:

$$V = U_p(\theta_p, T) - U_n(\theta_n, T) + \eta_p - \eta_n - R_f I \quad (5.2)$$

When $k_{p,n}$ are changed, the overpotential $\eta_{p,n}$ is changed since it is mainly related to $k_{p,n}$, and voltage output equation will be different. Therefore, it is evident that even if the observer estimates the true value of surface concentration and the other states, the voltage response might not converge to actual voltage response if a parameter related to voltage output equation changes.

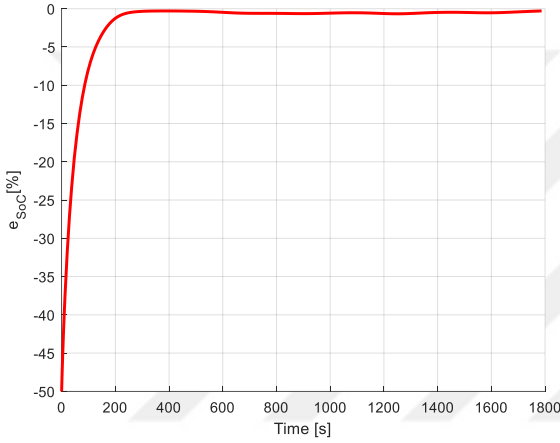


Figure 5.24 SoC error estimation for parameter uncertainty in $k_{p,n}$ ($\lambda = -5$)

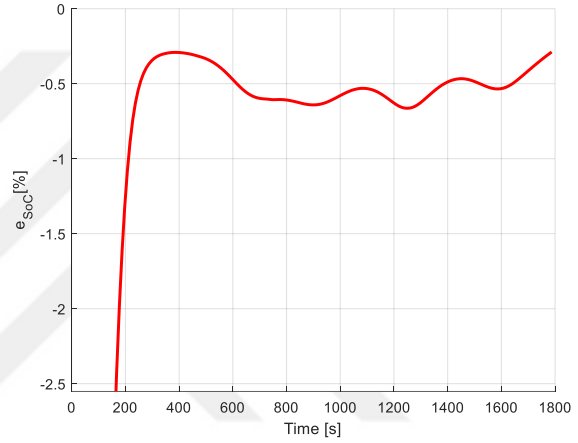


Figure 5.25 A zoom to SoC error estimation for parameter uncertainty in $k_{p,n}$ ($\lambda = -5$)

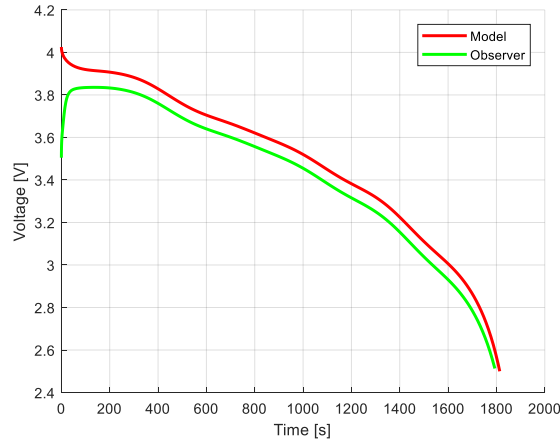


Figure 5.26 Voltage response for parameter uncertainty in $k_{p,n}$ ($\lambda = -5$)

Secondly, the same test is repeated for pulse current test. The results are similar to the ones obtained from constant current discharge test. As it can be seen from Figure 5.27 and Figure 5.28, the SoC estimation error is less than 0.5%, and the RMS error is 0.26%. On voltage response, the observer can estimate the actual value of the voltage at rest after a while (for example, between 340s and 350s, as shown in Figure 5.30). However, as depicted in Figure 5.30, after step input is applied,

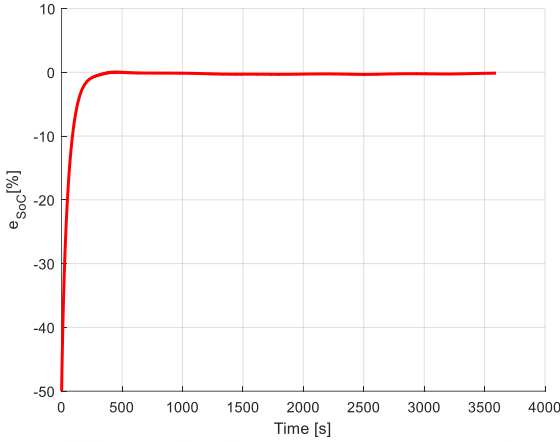


Figure 5.27 SoC error estimation for parameter uncertainty in $k_{p,n}$ ($\lambda = -5$)

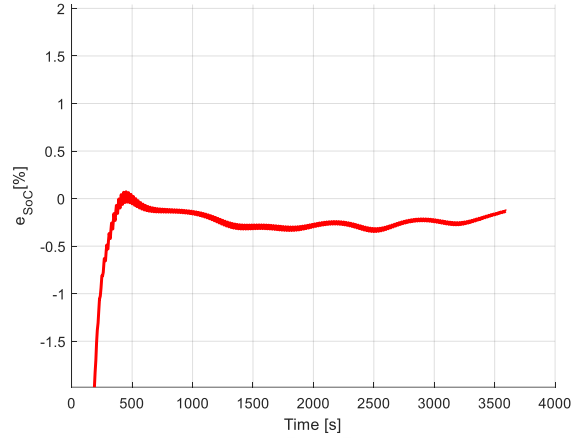


Figure 5.28 A zoom to SoC error estimation for parameter uncertainty in $k_{p,n}$ ($\lambda = -5$)

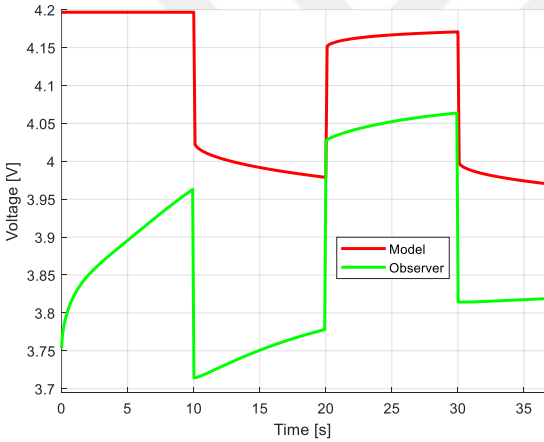


Figure 5.29 Voltage response for first 35s of the pulse test for parameter uncertainty in $k_{p,n}$ ($\lambda = -5$)

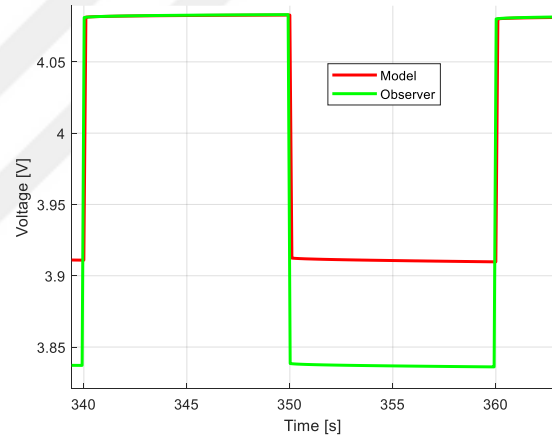


Figure 5.30 Voltage response towards the end of the pulse test for parameter uncertainty in $k_{p,n}$ ($\lambda = -5$)

there is approximately 70 mV error because of the reason explained above (for example, between 350s and 360s).

5.1.3.3 Parameter Uncertainty in R_f

R_f is increased by 50%, and 2C constant current and 2C pulse discharge tests are performed. Since the simulation results are similar to the ones obtained with parameter uncertainty in $k_{p,n}$, simulations results are not shown here for those tests. State estimation is correctly done by the backstepping observer, and there is a voltage difference between model and the observer for constant current test and pulse current test.

For 2C constant current test, the SoC error estimation converges to the true value of SoC in 210s roughly. The SoC error is less than 1%, and the RMS error of estimated SoC is 0.57%. Also, voltage response is very similar to the obtained with parameter uncertainty in $k_{p,n}$ test. There is 70 mV difference between the model and the observer in the steady-state.

For the pulse current test, the SoC estimation error remains within 0.5% error band, and the RMS error is only 0.27%. Voltage response at the beginning of the test are far from the model, but it is close to the model towards the end of the test. Although voltage response is close to the model towards the end of simulation, the observer can track the actual value of the voltage only at rest. When step input is applied after the rest, there is roughly 90 mV error due to a similar reason to that explained in section 5.1.3.2. In fact, R_f appears linearly in the last term of voltage equation, and its effect is directly visible on estimated voltage, despite the states are very close to their true value.

5.2 Experimental Results

In this section, the performance of the backstepping observer is demonstrated for the commercial Li-ion cell produced by Samsung presented in Chapter 3. The two tests shown for simulation studies in the previous sections are also performed for experimental studies, and SoC response and Voltage response are monitored.

Firstly, 2C constant current test is carried on. Like the previous simulations, the observer is launched with a 50% initial SoC error and λ is chosen to be -5. The true SoC in the experiment is obtained by initializing the cell at SoC=100% through a standard CC-CV charge protocol, and then taking the integral of current in time, according to the equation 5.3:

$$SoC(t) = SoC_0 - \int_0^t \frac{i(t)}{3600 C_{nom}} dt \quad (5.3)$$

In contrast to the simulation study, SoC estimation error is larger on the experimental test as shown in Figure 5.31 and Figure 5.32. The main reason of this estimation error is due to some modelling accuracy problems. However, through the end of the simulation, estimation error is less than 1%, and the RMS error is 2.91% in the last 800s of the test.

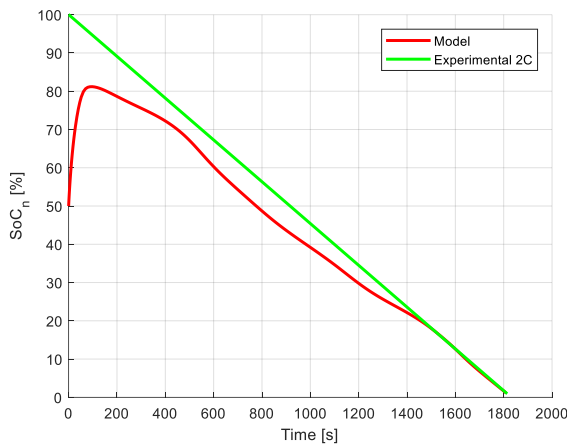


Figure 5.31 SoC estimation for 2C experimental test

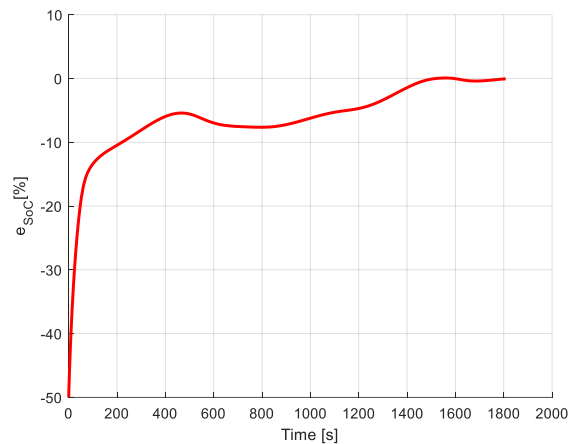


Figure 5.32 SoC estimation error for 2C experimental test

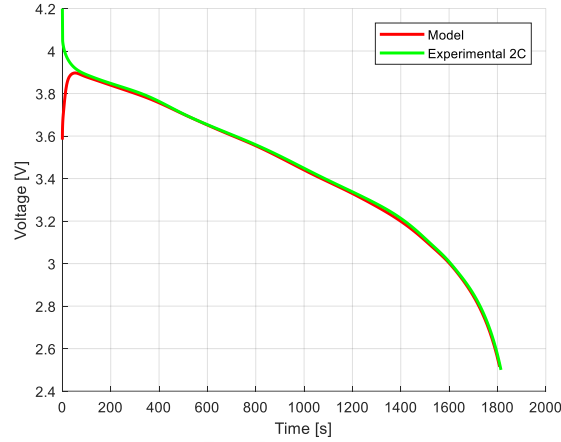


Figure 5.33 Voltage response for 2C experimental test

Secondly, 2C pulse current discharge test is performed on Li-ion cell. As it can be seen from Figure 5.34 and Figure 5.35, SoC estimation error is less than 5% after 680s, and the RMS error is 3.3% after that time.

Figure 5.36 and Figure 5.37 present the voltage response for the first 50s of the test and towards the end of the test, respectively. As shown in Figure 5.37, the experimental voltage has more curvature, and initial voltage drop when step input is applied is less than the model. This is expected behavior, because of the trade-off that needs to be faced when dealing with parameters identification, as explained in Chapter 3.

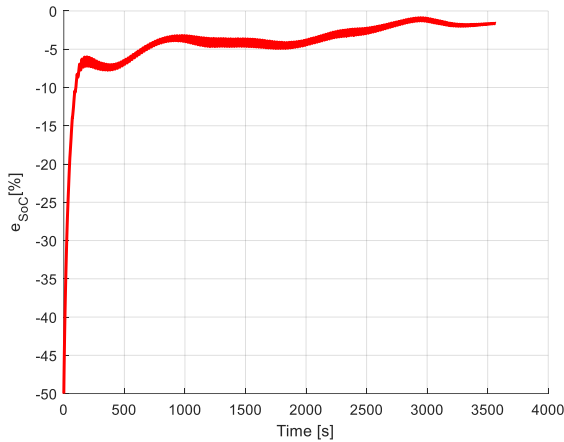


Figure 5.34 SoC estimation error for pulse current test

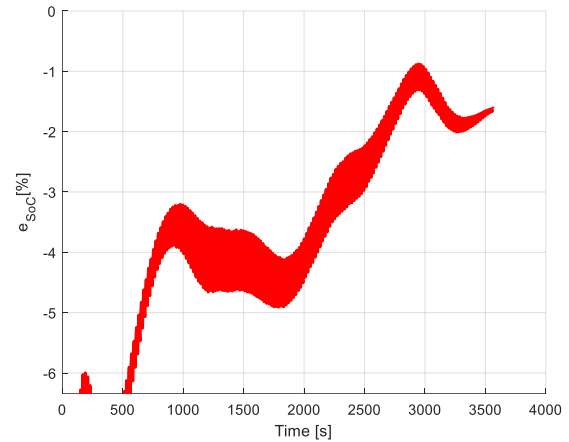


Figure 5.35 A zoom to SoC estimation error

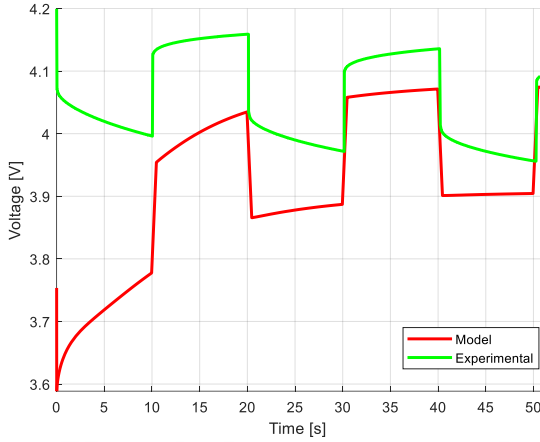


Figure 5.36 Voltage response for the first 50s of the experimental pulse test

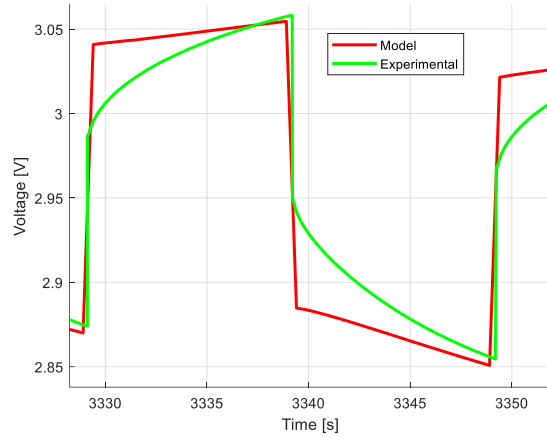


Figure 5.37 Voltage response towards the end of the experimental pulse current test

5.3 Conclusions

As a result, the backstepping observer is able to track the surface concentration and inner gradients along r successfully despite parameter uncertainty in the model and noisy measurements on voltage. With parameters uncertainty, voltage can not accurately be estimated by the observer, but this is not the primary scope of the backstepping observer. On the other hand, SoC estimation can converge to the actual one for experimental studies, although experimental results are somehow less good than simulation results.

6 Conclusions

In this thesis, design and experimental validation of a backstepping observer for a Li-ion battery are presented. Firstly, a comparison between complete P2D model and SPM are performed by using *Lionsimba* and *Spectral li-ion SPM* simulators. Then, parameters of electrochemical SPM are estimated to match the model response with experimental data obtained by a production of Samsung Li-ion cell. Next, a PDE backstepping observer for the Lithium-ion battery based on a reduced SPM including a bulk thermal model is designed, which allows to estimate not only SoC but also Lithium concentration along the radius of the particle. Then, the performance of the backstepping observer is investigated in both simulations for constant current and pulse current test to demonstrate that the backstepping observer successfully estimates SoC and Lithium concentration along the particle radius. Moreover, the robustness of the observer in the presence of uncertainty in model parameters and noise on voltage measurements are tested, and it is confirmed that proposed observer is robust with respect to uncertain parameters in model and noise on voltage measurements. Finally, the performance of the backstepping observer is validated in the experimental setup.

As a future work, parameter identification techniques can be improved since the model parameters usually change over time due to the aging effects. Moreover, instead of using SPM, SPM_e can be used that allows higher predictive accuracy than SPM [15].



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Appendix A

Parameters of thermodynamic equilibrium potential function of positive electrode	
a_0	$= -0.383840840559902$
a_1	$= 7.16162217143929$
b_1	$= -3.55802625413598$
a_2	$= -4.47189961453598$
b_2	$= 4.77981362602821$
a_3	$= 1.85221574725051$
b_3	$= -4.39829518202000$
a_4	$= -0.176010485365790$
b_4	$= 3.02661559779257$
a_5	$= -0.412433522670212$
b_5	$= -1.57592101606874$
a_6	$= 0.371839980308341$
b_6	$= 0.598775891915542$
a_7	$= -0.181468081439295$
b_7	$= -0.154835129769539$
a_8	$= 0.0484154073885265$
b_8	$= 0.0175497279116792$
w	$= 8.86410460535222$