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Lithium-ion battery modeling using equivalent circuit model

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ABSTRACT

With modern technologies, most devices such as electric vehicles are powered by lithium batteries. This kind of battery is advantageous to other types of batteries, such as higher energy density, reliability, etc. to work effectively, it is necessary to handle them using a battery management system BMS, which guarantees their safety and optimizes their performances in normal conditions. One of the things that a BMS must do is to estimate the state of charge SOC of the battery because it is the most critical indicator of battery state. This task is very challenging because the lithium-ion battery is a highly time-invariant, nonlinear, and complex electrochemical system. In this paper, we present a cell model that can be used in the state of the charge estimation process. This model is based on an electrical approach where we build an electrical circuit that has the same behavior as the real cell, this approach is called the Equivalent circuit model ECM. using a set of laboratory data, we will determine the model parameters using multiple techniques. Those parameters will be used in process of estimating the state of charge and other internal parameters.

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1. INTRODUCTION

The battery system is the most important energy storage source in electric vehicles (EVs) [1]. These days, the development trend in the field of electric vehicles is the use of high-capacity lithium-ion batteries as a battery energy storage system [2]. This kind of battery presents multiple benefits such as high-power density, lightweight, long life, and thermal stability.

To prolong the lifetime and increase the safety of these batteries, it is essential to monitor their state of charge in real-time. This task is performed by battery management systems that control, optimize and protect the battery. One of the main tasks of a battery management system is to estimate the number of fundamental quantities, such as the state of charge SOC of the cell, the state of health SOH of the cell battery, available power, and available energy. The best methods to produce these estimates require models that describe the dynamic behavior of the cell with precision.

Since the SOC cannot be measured directly, many approaches have been proposed to estimate the SOC of the battery [3–6]. One of those approaches is called model-based estimation of the state of charge, this approach is widely used in the application for its high accuracy and self-corrective ability [7–9]. One of the cell models that can be used to perform such an operation, is the equivalent circuit model ECM.

ECMs represent the operation of a lithium-ion cell by providing an electrical circuit, which behaves the same as cells. Data collected from cells via laboratory tests are used to optimize the parameter values of

the proposed circuit elements so that the current and voltage behaviors of the model match exactly those of the real cell. [10]
In the rest of this paper, we adopt the equivalent circuit model approach, where we build the model circuit element by element, starting with an explanation of the observed dominant behavior. Any difference between the model predictions and the observed behavior of the cells is therefore considered to be a modeling error. Each time, the reduction in the resulting error will be corrected by adding more elements to the circuit, until only a small level of error remains, where we are satisfied with the resulting model.

2. LITHIUM-ION CELL MODELLING

- **Open circuit voltage OCV**

We begin the cell modeling by explaining the most observed behavior of the battery cell. This model, figure (1), presents the cell as an ideal voltage source v(t). Indeed, the cell delivers a voltage to its terminals. This voltage is measured by a voltmeter, where we notice that it is constant, and is not a function of the current flowing in the load connected to the cell. This model is simple and it's very different from the reality where OCV depends on the cell state of charge.

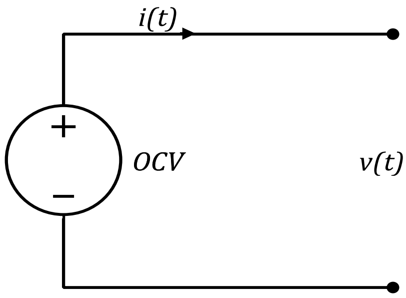

Figure 1. Cell ideal model diagram where open circuit voltage has a constant value.

- **State of charge effect on OCV**

The first improvement that we make to the simple cell model is due to the difference in voltages in a cell with different states of charge. Indeed, we notice that the cell voltage at equilibrium or the OCV of a fully charged cell is greater than the OCV of a fully discharged cell.

The improved cell model, Figure (2), includes OCV dependence on the state of charge of the cell. The ideal voltage source is replaced by a controlled voltage source, which has a value equal to OCV (z (t)), where z(t) is the state of charge of the cell. If we take into account the dependence of the OCV on temperature, we use the notation OCV (z (t), T (t)), where T (t) is the internal temperature of the cell as a function of time.

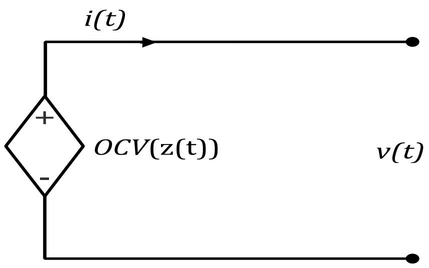

Figure 2. Cell model diagram including OCV dependence on the state of charge.

We can model the state of charge changes using the following differential equation:

$$\frac{dz(t)}{dt} = -\frac{\eta(t)i(t)}{Q}, \#(1)$$

where z (t) represents the state of charge, η (t) the Coulomb efficiency or the charging efficiency, Q the total capacity. When the cell is being discharged, the current i(t) is positive and η(t) takes the value of 1, which leads to the decrease of z (t). On the other hand, z (t) increases at the charge of the cell where the current is negative and the Coulomb efficiency is η (t) ≤1.

By integrating the equation (1) between time t0 and t and if we assume that the current is constant over the sampling interval, then we have:

$$z(t) = z(t0) - \frac{1}{Q}\int_{t0}^{t} \eta(t)i(t)dt \#(2)$$

This equation must be written in discrete-time so we can use it in numerical calculus. To do so, let t0 = kΔt et t = (k + 1) Δt. so:

$$z\big((k+1)\Delta t\big) = z(k\Delta t) - \frac{\Delta t}{Q}\eta(k\Delta t)i(k\Delta t)\#(3)$$

Finally:

$$\boldsymbol{z[k+1] = [z] - \frac{\Delta t}{Q}\eta[k]i[k]\#(4)}$$

- **Equivalent series resistance**

The first observation we notice is that when the cell powers an external load, the voltage across its terminals drops below the open-circuit voltage OCV (z(t)), and when the cell is being charged, the voltage at these terminals rises above the open circuit voltage OCV (z (t)). This phenomenon can be explained by placing a resistor in series with the voltage source. The new model is shown in the diagram in figure (3). The resistance added to the diagram represents what is called the equivalent series resistance (ESR) of the cell. The reason we choose this circuit over others is that the behavior observed in this case is similar to the response of the chosen circuit, where the voltage v(t) drops than OCV(z(t)) due to the presence of the resistor R0.

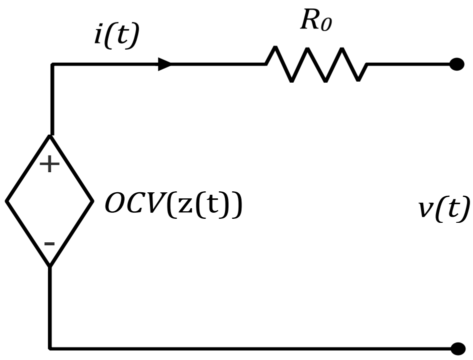

Figure 3. Cell model diagram including the equivalent series resistance.

In the new model, the state of charge equation remains unchanged. However, we add a second equation to the model which describes the voltage across the circuit.

In continuous time:

$$v(t) = OCV\big(z(t)\big) - i(t)R_0\#(5)$$

In discrete time

$$v[k] = OCV(z[k]) - i[k]R_0\#(6)$$

- **Polarization effect**

Polarization in the cell refers to any deviation between the voltage across the cell from the open-circuit voltage OCV(z(t)), due to current flow through the cell. In the equivalent circuit model that we have developed so far, we have modeled the instantaneous bias via the term i (t) × R0. Real cells have more complex behavior, where the voltage bias increases slowly over time when current is demanded from the cell, and then slowly decreases over time when the cell is allowed to rest.

This phenomenon is caused by the slow diffusion processes of lithium in a lithium-ion cell, this slowly changing voltage is called, the diffusion voltage. Its effect can be approximated in a circuit by using one or more resistor-capacitor sub-circuits in parallel. Figure (4).

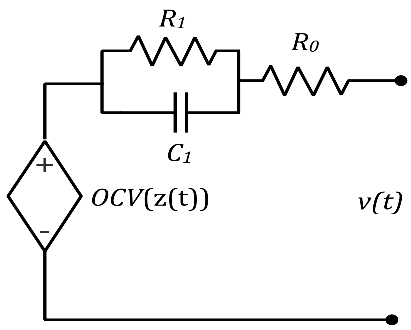

Figure 4. Cell model diagram including the polarization effect.

In this model, the state of charge equation remains the same as before, but the voltage equation changes:

In continuous time:

$$v(t) = OCV\big(z(t)\big) - R_0 i(t) - R_1 i_{R_1}(t)\#(7)$$

In discrete time:

$$v[k] = OCV(z[k]) - R_0 i[k] - R_1 i_{R_1}[k]\#(8)$$

To find the current flowing in resistor R1, we write the expression for the total current:

$$i(t) \;=\; R_1 i(t) + \; C_1 \dot{v_{C_1}}(t).\#(9)$$

We replace $\dot{v_{C_1}}(t)$ by $\frac{\mathrm{R_1 d(i_{R1}(t))}}{\mathrm{dt}}$, we get the following differential equation

$$\frac{di_{R1}(t)}{dt} = -\frac{1}{R_1 C_1} i_{R1}(t) + \frac{1}{R_1 C_1} i(t).\#(10)$$

By converting this equation from continuous-time to discrete-time, we get:

$$i_{R_1}[k+1] = exp\left(\frac{-\Delta t}{R_1 C_1}\right) i_{R_1}[k] + \left(1 - exp\left(\frac{-\Delta t}{R_1 C_1}\right)\right) i[k].\ \#(11)$$

- **Warburg impedance effect**

The Warburg impedance models the diffusion of lithium ions in the electrodes. It depends on the frequency, modeled as ZW = AW/j where the constant AW is called the Warburg coefficient, and ω is the applied frequency in radians per second.

There is no simple differential equation to model Warburg's impedance. However, its effect can be estimated via several resistor-capacitor networks in series, using two distinct structures which are, the Cauer structure and the Foster structure.

- Cauer's structure

Warburg impedance is represented by RC subcircuits as shown in figure (5)

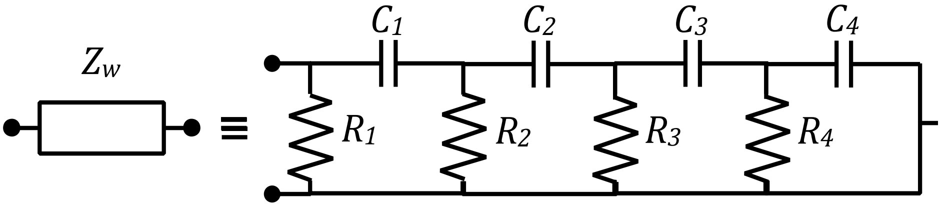

Figure 5. Cauer's structure diagram

- Foster structure

In this case the impedance is only a set of RC circuits parallel in series as in figure (6):

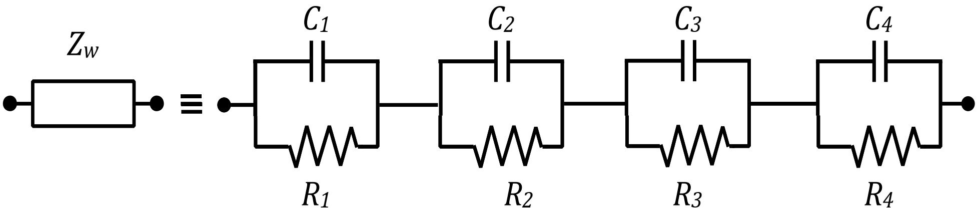

Figure 6. Foster's structure diagram

- **Hysteresis Effect**

The model we have developed so far, implies that the voltage drop across R0 will immediately drop to zero when the cell current is zero, and the voltage drop across capacitor C1, will decrease to zero over time by discharging to resistor R1. In other words, the voltage across the cell will converge to the open circuit voltage OCV (z (t)).

However, the reality is something else. The cell voltage decreases to a slightly different value from the OCV, and the difference depends on the previous use of the cell. For example, we notice that if we discharge a cell at 50% SOC, and we leave it at rest, then the equilibrium voltage is lower than the OCV. On the contrary, if we charge a cell with 50% SOC, and we leave it at rest, then the equilibrium voltage is higher than the OCV. These observations indicate that there is a voltage hysteresis across the cell.

The hysteresis voltages are different from the diffusion voltage, the diffusion voltages change over time, on the other hand, the hysteresis voltages only change when the SOC changes. In addition, the hysteresis voltages are not directly related to time. This is because if a cell is allowed to rest, the diffusion voltages will decrease to zero, but the hysteresis voltages will not change at all.

There are two types of hysteresis, the first is the dynamic hysteresis which depends on the state of charge SOC, the other is the instantaneous hysteresis which results when the sign of the current changes (for example, the current change from cell discharge mode to cell charge mode).

- **Dynamic hysteresis**

Let $h_D(z,t)$ be the dynamic hysteresis voltage as a function of SOC and time. The variation of this voltage as a function of the state of charge is described by the following differential equation:

$$\frac{dh_D\,(z,t)}{dz} = \gamma sgn(\dot{z})\big(M(z,\dot{z}) - h(z,t)\big). \#(12)$$

With:

$M(z,\dot{z})$: Is a function which gives the maximum polarization due to the hysteresis as a function of SOC (z) and of the rate of change of SOC($\dot{z}$).

The term $M(z,\dot{z}) - h(z,t)$: indicates that the rate of change of the hysteresis voltage is proportional to the distance of the current hysteresis value from the main hysteresis loop.

The term γ, is a positive constant that regulates the rate of decay.

The term $sgn(\dot{z})$ forces equation (12) to be stable for both charge and discharge of the cell.

To fit the differential equation of $h_D(z, t)$ in our model, it must be a differential equation with respect to time, and not with respect to SOC. And this is done by multiplying both sides of the equation by $\frac{dz}{dt}$:

$$\frac{dh_D(z,t)}{dz}\frac{dz}{dt} = \gamma sgn(\dot{z})\big(M(z,\dot{z}) - h_D(z,t)\big)\frac{dz}{dt} \#(13)$$

By replacing with:

$$\begin{cases} \frac{dz}{dt} = -\frac{\eta(t)i(t)}{Q} \\ \frac{dz}{dt}sgn(\dot{z}) = |\dot{z}| \end{cases},$$

then we get the equation in continuous time:

$$\frac{dh_D(t)}{dt} = -\left|\frac{\gamma\eta(t)i(t)}{Q}\right| h_D(t) + \left|\frac{\gamma\eta(t)i(t)}{Q}\right| M(z,\dot{z}). \#(14)$$

By converting this equation into discrete time:

$$h_D[k+1] = exp\left(-\left|\frac{\gamma\eta[k]i[k]\Delta t}{Q}\right|\right)h_D[k] + \left(1 - exp\left(-\left|\frac{\gamma\eta[k]i[k]\Delta t}{Q}\right|\right)\right). \#(15)$$

have $M(z,\dot{z}) = -Msgn(i[k])$, and since $h_D[k]$ it is in volts, and $-M \leq h_D[k] \leq M$. It is useful to rewrite the equation in an equivalent representation but slightly different, which has a unitless hysteresis state $-1 \leq h_D[k] \leq 1$

$$h_D[k+1] = exp\left(-\left|\frac{\gamma\eta[k]i[k]\Delta t}{Q}\right|\right)h_D[k] - \left(1 - exp\left(-\left|\frac{\gamma\eta[k]i[k]\Delta t}{Q}\right|\right)\right)Msgn(i[k]) \quad (16)$$

Finally, the dynamic hysteresis is modeled as:

Dynamic hysteresis voltage = $Mh_D[k]$

- **Instantaneous hysteresis**

In addition to dynamic hysteresis which changes when SOC changes, we will model the instantaneous hysteresis voltage which changes when the sign of the current changes.

$$h_I[k] = \begin{cases} sgn(i[k]), |i[k]| > 0; \\ h_I[k-1], \quad \text{otherwise} \end{cases} \#(17)$$

Finally, the instantaneous hysteresis is modeled as:

Instantaneous hysteresis voltage = $M_0 h_I[k]$

In total, the overall hysteresis is:

$$M_0 h_I[k] + Mh_D[k]$$

- **Enhanced self-correcting the cell model**

The Enhanced Self-Correcting (ESC) cell model combines all the elements already mentioned. The model is called Enhanced because it includes a description of the hysteresis, unlike some earlier models. The model is called self-correcting because the predicted terminal voltage of the model converges to the OCV plus the hysteresis when the cell is at rest, and converges to the OCV plus the hysteresis minus all resistive voltages at constant current. The final diagram of this model is shown in figure (7), which shows an example with a single resistor-capacitor pair in parallel. To compact the notation, we define a resistor-capacitor subcircuit speed factor $Fj = exp\left(-\frac{\Delta t}{R_j C_j}\right)$

$$i_R[k + 1] = \underbrace{\begin{bmatrix} F_1 & 0 & \cdots \\ 0 & F_2 & \\ \vdots & & \ddots \end{bmatrix}}_{A_{RC}} i_R[k] + \underbrace{\begin{bmatrix} 1 - F_1 \\ 1 - F_2 \\ \vdots \end{bmatrix}}_{B_{RC}} i[k] \#(18)$$

So, if we define

$$A_H[\mathrm{k}] = \exp\left(-\left|\frac{\gamma\eta[k]i[k]\Delta t}{Q}\right|\right) h_D,$$

therefore, we will have the dynamic aspects of the model described by the following relation:

$$\begin{bmatrix} z[k+1] \\ i_R[k+1] \\ h[k+1] \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & A_{RC} & 0 \\ 0 & 0 & A_H[\mathrm{k}] \end{bmatrix} \begin{bmatrix} z[k] \\ i_R[k] \\ h[k] \end{bmatrix} + \begin{bmatrix} -\frac{\eta[k]\Delta t}{Q} & 0 \\ B_{RC} & 0 \\ 0 & (A_H[k] - 1) \end{bmatrix} \begin{bmatrix} i[k] \\ sgn(i[k]) \end{bmatrix} \#(19)$$

This is the equation of state of the ESC model. The output equation of the model is:

$$v[k] = OCV(z[k], T[k]) + M_0 h_I[k] + M h_D[k] - \sum_j \mathrm{R_j i_{R_j}[k]} - \mathrm{R_0 i[k]} \ \#(20)$$

3. DETERMINING THE PARAMETERS OF THE CELL MODEL (ESC)

The model that we built describe two aspect of the cell, the first is static aspect of the cell, and the second is the dynamic aspect.

For the static aspect of the cell, this one is represented by open circuit voltage as a function of the state of charge, while another performance of the cell is dynamic. So, to determine the cell parameters. We do two kinds of experiments, the first one is where we determine the static aspect of the cell, here we charge and discharge the cell with a current almost equal to zero to minimize the excitation of the dynamic aspect of the cell. The second one is where we determine the dynamic aspect.

The data collected in the first experience are voltage values and ampere-hours charged and discharged in every step at different temperatures.

- **Determining the Coulombic efficiency**

The Coulombic efficiency at 25ºC :

$$\eta(25°\mathrm{C}) = \frac{\text{total Ampere Hours discharged in all steps at 25C}}{\text{total Ampere Hours charged in all steps at 25C}}$$

The coulombic efficiency at temperature different than 25oC:

$$\eta(T) = \frac{\text{total AH discharged}}{\text{total AH charged in all steps at T}} - \eta(25°\mathrm{C}) \times \frac{\text{total AH discharged in all steps at 25C}}{\text{total AH charged in all steps at 25C}}$$

*AH : Ampere-heurs

- **Determining of the relationship OCV versus SOC**

Using the data collected from the experience, we will determine the relationship between OCV and SOC. However, the relationship that we will obtain is an approximate relationship, and that because the charge voltage and discharge voltage are different. So, in the high state of charge, we are forced to base OCV estimate on the discharge voltage values because we don’t have any charge voltage information. While in the low states of charge we are forced to base the OCV estimate on the charge voltage values because we don’t have discharge voltage information. In the intermediate state of charge, we can base OCV estimate on both charge and discharge values.

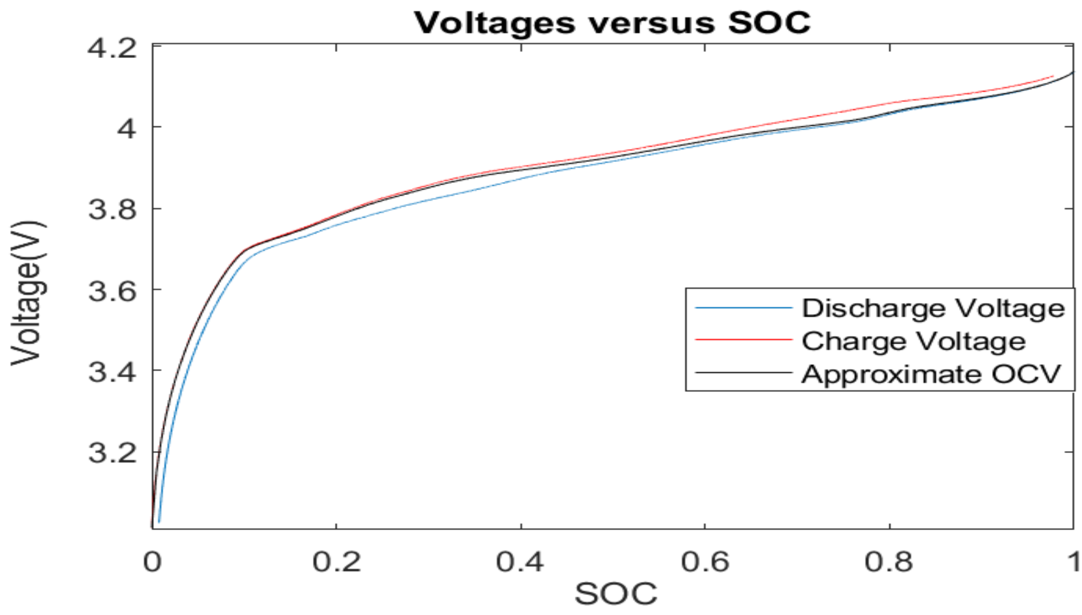

Figure 7. Open circuit voltage of the cell model based on data collected of discharge and charge OCV

This figure represents the approximate OCV/SOC relationship for a cell at room temperature. The black line is the approximate OCV, and the blue line is the discharge voltage curve, while the red line is the charge voltage curve. As we see, at high state of charge values, the OCV estimate is based on the discharge curve, while in the low state of charge, the OCV estimate is based on the charge voltage curve. In the intermediate states of charge, the OCV estimate is based on the two curves. The method used here to determine the OCV/SOC relationship at room temperature, is also used to determine it at all other temperatures of the experience.

- **Determining the dynamic parameters**

Once we find the cell’s OCV relationship, then we try to find the dynamic parameters of the cell model. This time, the cell must be exercised with profiles of current versus time that are representative of the final application of the resulting model.

Voltage values, current values, temperature values, ampere-hours charged, and ampere-hours discharged are recorded every second during the experience. These data are used to identify the cell model dynamic parameters. These parameters are; resistor value R_1 and capacitor value R_1 in the subcircuit, equivalent series resistor R_0 , hysteresis parameters M_0 *and* M , hysteresis rate constant γ. Some of these parameters cannot be computed directly from the measured data, instead, we have to use an optimization approach, which we call system identification.

The simple way to do this is to choose a set of parameter values, the second step is to simulate the ESC model using that set of parameter values with the same input current as was measured during the experience, the third step is to compare the ESC model voltage prediction with the measured voltages, the fourth step is to modify the parameter values to improve the model prediction and go back to the second step and start again from there until the optimization is considered complete.

One approach used to determine the parameters of the cell model is to use an optimization toolbox such as MathWorks Simulink Design Optimization Toolbox. To do so, we must create a block diagram to implement the cell model equations. Figure (8) shows the implementation of ESC model in Simulink. For implementation we assume a model circuit with two parallel resistor–capacitor circuits η = 1, γ = 3600, and $M_0 = 0$.

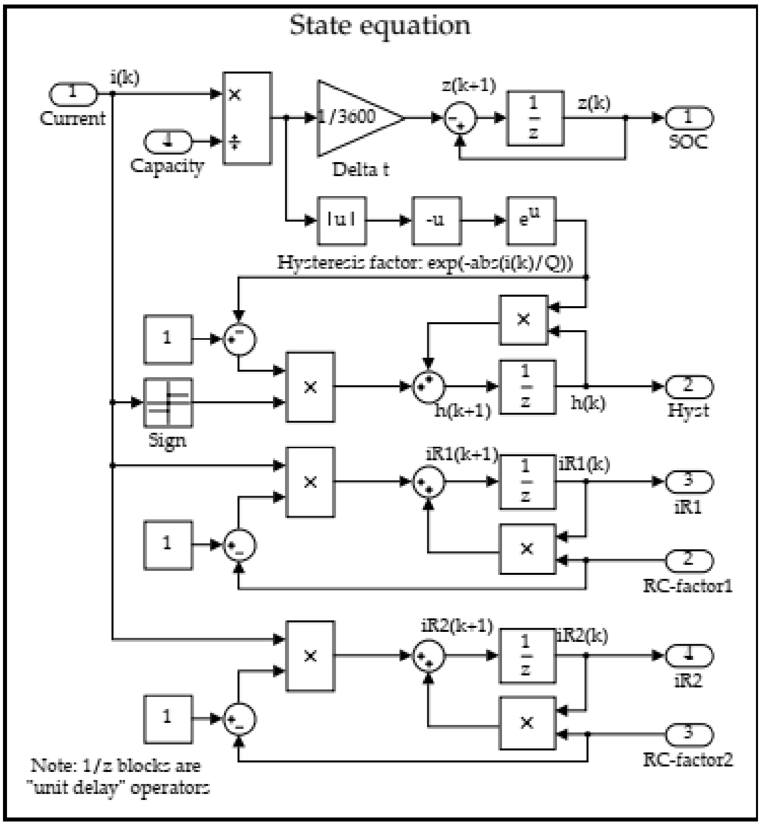

Figure 8. Block diagram of the Simulink Design Optimization Toolbox

This toolbox automatically generates values for cell capacitance, resistor-capacitor time constants, resistance values, and maximum hysteresis value, then runs the model to see how well the voltage predictions match the measured data. If there was a difference between the estimation and the measured data, we update parameter's estimates, and repeats until it converges to a solution.

This method gives good results quickly if we initiate the parameter's value with good guesses. To do so, we try to compute directly some parameters values.

- **Direct computation of *M, M_0, R_0, and R_j***

The first thing to do before we go through the computation of the parameters, is to find the time constant of the resistor-capacitor circuits. Actually, the way to this is simple by using a method called system identification.

If we take a look at the output equation of the model, we will see that there are known parts such the $OCV(z[k], T[k])$,and unknown parts which are the rest of the equation. We can rewrite equation 20 to distinguish known parts from unknown parts. $h_I[k]$ can be computed directly from the current profile. To compute $h_D[k]$ we require γ. For now, let's assume that we know its value. $i_{R_j}[k]$ can be computed once know the resistor-capacitor time constant.

$$\tilde{v}[k] = v[k] - OCV(z[k], T[k]) \qquad \#(21)$$

$$= M_0 h_I[k] + M h_D[k] - R_j i_{R_j}[k] - R_0 i[k]$$

The variables $h_I[k], h_D[k]$, $\mathrm{i}_{\mathrm{R_j}}[\mathrm{k}], \mathrm{i}[\mathrm{k}]$ are input variables to equation (21). And the parameter's values can be computed as follows:

$$\underbrace{\tilde{v}[k]}_{Y} = \underbrace{\begin{bmatrix} h_I[k] & h_D[k] & \mathrm{i}[\mathrm{k}] & \mathrm{i}_{\mathrm{R_j}}[\mathrm{k}] \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} M_0 \\ M \\ \mathrm{R_0} \\ \mathrm{R_j} \end{bmatrix}}_{X}$$

We can find the unknown parameters vector via the least-square solution.

- **Optimization of γ**

to find the parameters of the cell model, we assume that we know the value of γ in fact its value is unknown. So, we have to optimize it, to do that, we must bound it in some range, and then compute the quality of the fit for models optimized for each γ in this range, keeping only the model that offers the best quality of the fit.

4. CELL MODEL SIMULATION AND DISCUSSION

To give a better idea of the capabilities of our ESC model, we present some modeling results in this section. Data was collected from a 25 Ah automotive battery cell, and the open circuit voltage and dynamic modeling parameters were estimated from the data (using one sub-resistance-capacitor circuit in the model). Here, we focus on simulating the optimized model, where we compare its predictions with the voltage data measured for a test performed at 25 ◦C.

Figure 9 shows an overlay of the true voltage (blue line) and model predicted voltage (Orange line) over the entire 10-hour test. As we see in this figure there is fitness between measured voltage and predicted voltage. The root-mean-square difference between the actual results and the model results was 15.86 mV in this case. These results show more clearly that the circuit model captures cell performance quite well. As we see in figure 10, the error of the modeling is slightly small, the range of the error is between negative 0.1 and positve 0.1, this error depends on founded parameters values, but if somehow, we get a better value of those parameters this error will eventually decrease.

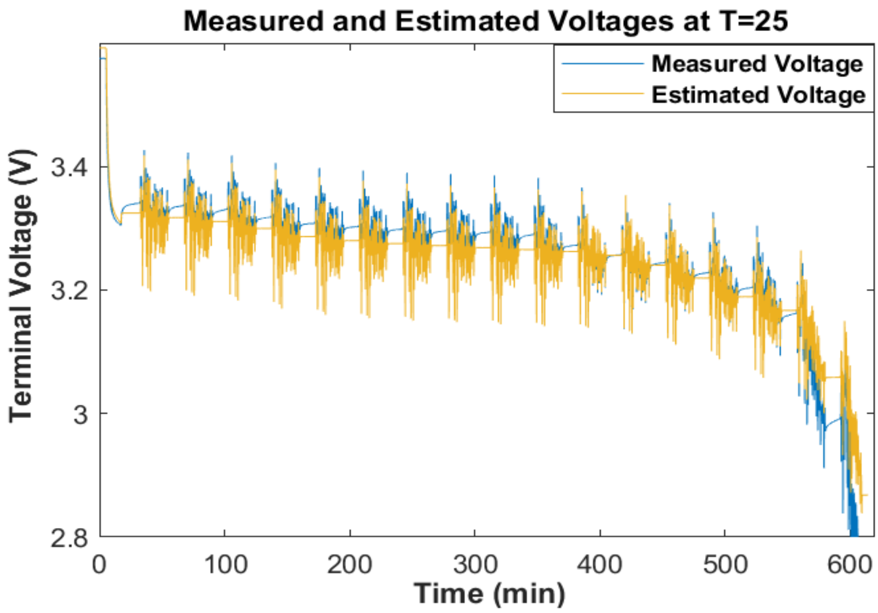

Figure 9. Cell measured voltage and cell model estimated voltage simulation versus time

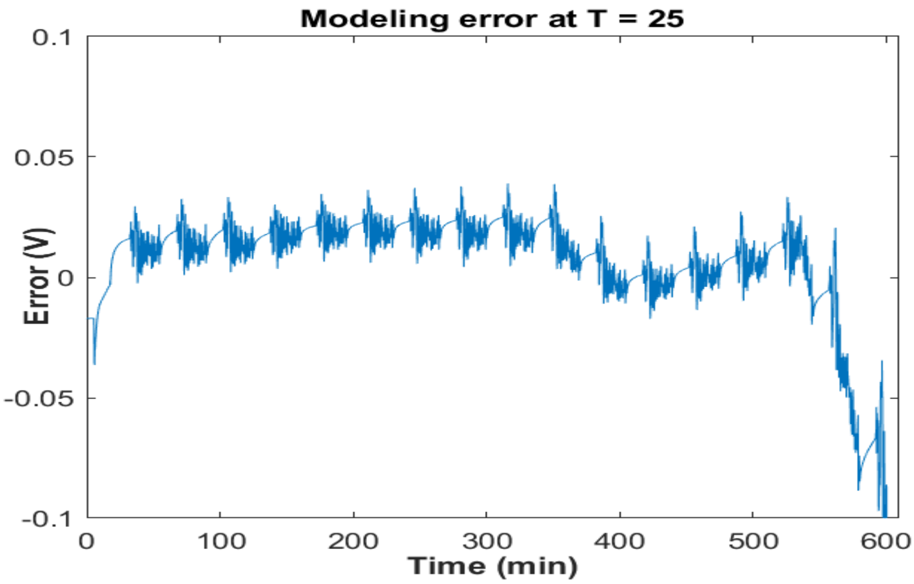

Figure 10. Error of the simulation versus time

Figures 11 show the optimized parameter values for this cell based on the test temperature (tests were performed from -25◦C to 45◦C in 10°C increments).

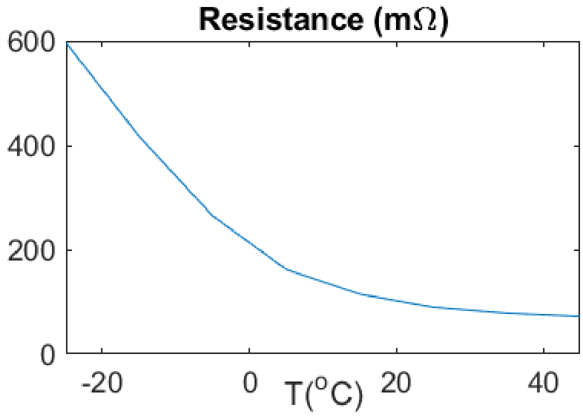

Figure 11-a

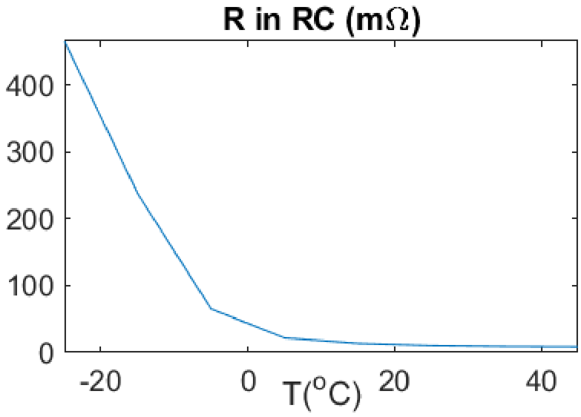

Figure 11-b:

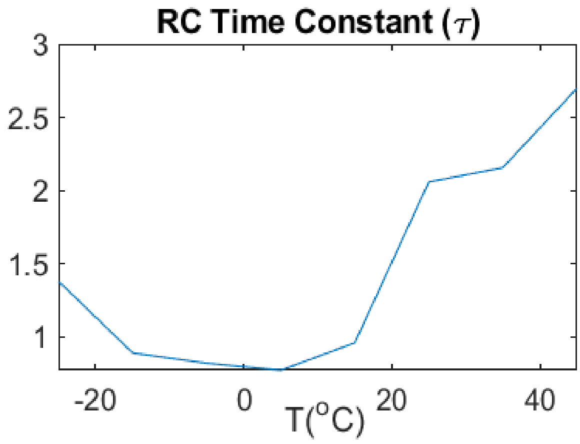

Figure 11-c

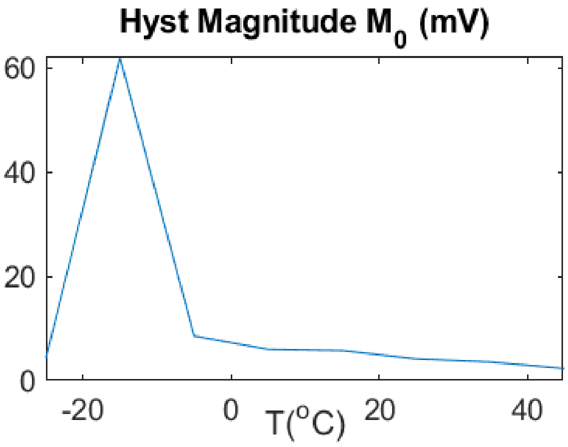

Figure 11-d

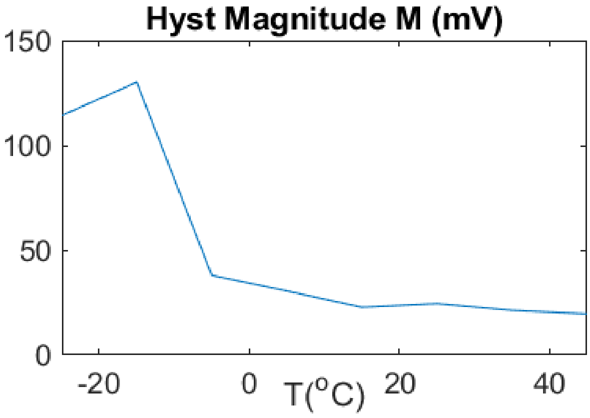

Figure 11-e

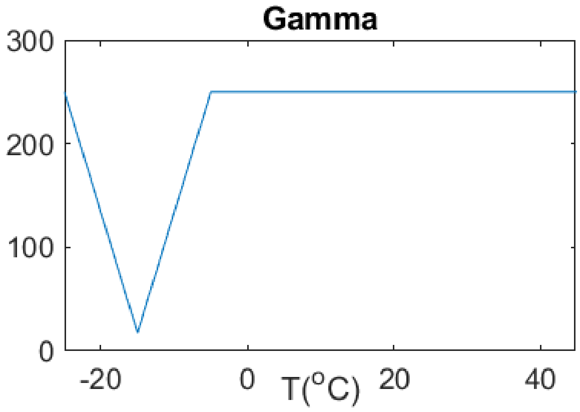

Figure 11-f

Figure 11-a shows serie resistance R_0 evolution as function of temperature. the equivalent series resistance R_0 decreases exponentially as the temperature increases. It is almost a universal result.

Figure 11-b shows the resistance (in resistance-capacitor subcircuit) evolution as a function of temperature. The resistor-capacitor resistances Rj tend to decrease exponentially as the temperature increases. This is also expected.

Figure 11-c shows the resistance-capacitor time constant evolution as a function of temperature. The resistor–capacitor time constants tend to increase with temperature increase. This might actually seem a surprising result, as we would expect the cell dynamics to speed up at warmer temperatures.

Figures (11-d, 11-e, 11-f) shows the hysteresis parameters evolution as a function of temperature and hysteresis time constant evolution as function of temperature. The Hysteresis is generally “speeding up” (i.e., a smaller change in SOC is required to effect a large change in the hysteresis state) and decreasing in magnitude as temperature increases. Hysteresis levels generally decrease as temperature increases.

In contrast to other cell models such as mathematical models, electrochemical models, thermal models, this model is intuitive and easy to impliment. This model uses only passive components such as resistors and capacitors and a voltage source, which they are suitable for use in circuit simulators. The accuracy of prediction and estimation achievable with this model is sufficient for many applications.

5. CONCLUSION

In this paper we built our model (ESC) using an electric analogy, our model can describe the behavior of the cell. Using a set of data collected from an application of the cell, we simulated our model and we compared the predicted voltage and measured voltage and we did find that our model predicts terminal voltage very well. The error of the modeling depends on the parameter’s values of the cell model and the measured data.

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