Mathematical modeling of Li-ion battery for charge/discharge rate and capacity fading characteristics using genetic algorithm approach

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Kannan Thirugnanam
Khalifa University

Parvind Kumar
National Institute of Technology, Kurukshetra

Mathematical Modeling of Li-Ion Battery for Charge/Discharge Rate and Capacity Fading Characteristics using Genetic Algorithm Approach

Kannan Thirugnanam, Himanshu Saini and Praveen Kumar
Indian Institute of Technology Guwahati/Electronics and Electrical Engineering, Guwahati-781039, India,
e-mail: kannan@iitg.ernet.in, h.saini@iitg.ernet.in and praveen_kumar@iitg.ernet.in.

***Abstract* – The objective of this work is to develop an accurate Battery Model (BM) and Capacity Model (CM) to study the performance of vehicle-to-grid interaction. Using BM and CM, the amount of capacity fading is analyzed while the power is stored in the battery or transferred to the grid. The BM is developed for Li-ion battery based on the Electrical Equivalent Circuit (EEC) and the CM is proposed based on processed energy for different charging/discharging rate. The proposed model is simulated using MATLAB Simulink environment and the parameters are optimized using Genetic Algorithm (GA) approach to compare the results with manufacturer's catalogue data. The obtained battery characteristics are in close agreement with the measured (manufacturer catalogue) characteristics.**

Keywords - Battery model, battery, capacity fading, capacity model, electrical equivalent circuit, genetic algorithm, Li-ion, state-of-charge, vehicle-to-grid.

NOMENCLATURE

$a_1 - a_{31}$	Polynomial coefficients.
A, B	Pre-exponential factor.
C_1	Capacitance (F).
C, D, z	Adjustable factor.
C_r, D_r	Charge rate and discharge rate
E_c, E_d	Processed energy for charging and discharging (Wh).
$F_{optimum}$	Optimum value for fitness function
I_c, I_d	Charge and discharge current (A).
Q	Battery nominal capacity (Ah).
$Q_{L,i}^{M}$	Measured capacity losses for ith cycle as given in the catalogue by the manufacturer
$Q_{L,i}^{C}$	Calculated capacity losses for ith cycle
R	Universal gas constant (J/mol K).
R_1, R_2	Battery internal resistance (Ω).
T	Temperature (K).
V_o	Open-circuit voltage (V).
$V_{bc/db}$	Battery voltage for charging/discharging scenario (V).
V_{batt,C_i}^{M}	ith measured voltage for charging scenario (V) as given in the catalogue by the manufacturer.
V_{batt,C_i}^{C}	ith calculated voltage for charging scenario (V).
V_{batt,D_j}^{M}	jth measured voltage for discharging scenario (V) as given in the catalogue by the manufacturer.
V_{batt,D_j}^{C}	jth calculated voltage for discharging scenario (V).

I. INTRODUCTION

In order to understand the performance, charge/discharge rate and Capacity Fading (CF) of the battery, a dynamic model for the battery of an electric vehicle is required. In general, the dynamic models for the battery are developed using various modelling tools such as SPICE, MATLAB Simulink and LABVIEW. Several types of battery models are reported in the literature: (a) experimental, (b) electrochemical, (c) mathematical and (d) Electrical Equivalent Circuit (EEC) based models [1]. Experimental and electrochemical models are not well suited to representing dynamics of the battery because these models are computationally expensive and require extensive experimentation in order to determine the parameters of the model [2]. The mathematical model of the battery is based on the empirical equations and they are used to predict the charge/discharge time, efficiency and capacity loss of the battery [3]. However, the mathematical model has limited use in circuit simulators since it is not sufficiently related to the model parameters and the I-V characteristics of the battery [4-6]. The EEC based models are used to efficiently represent the performance characteristics of the batteries. The simplest EEC model consists of an open-circuit voltage in series with a resistance and a parallel combination of resistance and capacitance [1, 3-4]. The EEC parameters are represented in terms of polynomial equation, as a function of State-of-Charge (SOC), Depth-of-Discharge (DOD) and charge/discharge rate.

In order to use the EEC model effectively in Vehicle to Grid (V2G) system, it is important to determine the EEC parameters accurately. Generally, these parameters are derived from experiments which are resource intensive and time consuming. It is not feasible to perform such expensive and extensive experiments and evaluate the performance characteristics for different types of batteries. Moreover, the existing EEC models [1] do not take the capacity losses into consideration. Hence, a mathematical model has been proposed for Li-Ion battery which takes into account of the capacity losses. The prediction of capacity fading is based on the battery nominal capacity, processed energy for charging/discharging and charge/discharge rate. These characteristics are determined using polynomial representation since EEC parameters are directly proportional to charge/discharge rate [3-4]. The coefficients of polynomial equations are optimized using Genetic Algorithm (GA). Fig. 1 represents the block diagram of the battery with capacity model.

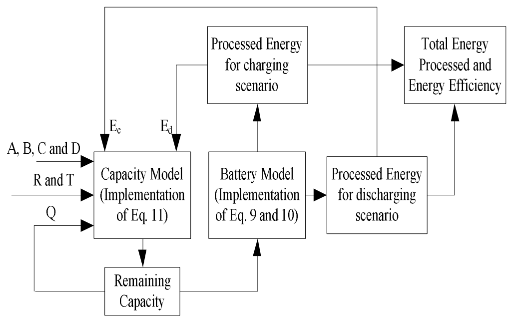

Fig. 1. A simple block diagram of the proposed battery model

This paper is organized as follows: Section II presents the mathematical model for Li-ion batteries charge/discharge rate characteristics. In section III, the concept of capacity fading at different charge/discharge rate for a Li-ion battery is explained. In the IV section, the polynomial representation of the battery model and the estimation of the polynomial coefficients based on genetic algorithm are discussed. The results are discussed in section V. Section VI concludes this paper.

II. BATTERY MODEL

In this section, the simple electric EEC for Li-ion battery is discussed. It describes the charge and discharge characteristics at different charge/discharge rate (discharge current as well as the charge current of a battery). The most common, simple EEC for Li-ion battery is shown in Fig. 2 [1, 3-4].

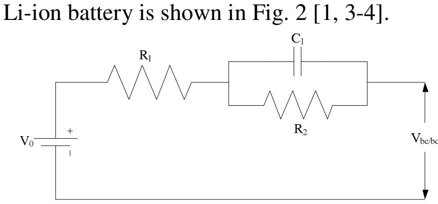

Fig. 2. Electric equivalent circuit for Li-ion battery.

The EEC model has three parameters: an open circuit voltage (V_0), an internal resistance (R_{int}) having two parameters R_1 and R_2 and the effective capacitance (C_1). This model is used to extract the circuit parameters for different charge/discharge rate. The accuracy of this model is verified by comparing the calculated terminal voltage values with the measured battery terminal voltage values provided by battery manufacturers. The mathematical representations for R_1, R_2, C_1 and V_0 under constant current charging conditions are given in Eq.1-4 [1]. The battery parameters are represented as polynomial equations as a function of charge/discharge rate, SOC for charging scenario and DOD for discharging scenario.

$$R_1 = (a_1 + a_2 \times C_r + a_3 \times C_r^2) \times e^{-a_4 \times SOC} + (a_5 + a_6 \times C_r + a_7 \times C_r^2) \quad (1)$$

$$R_2 = (a_8 + a_9 \times C_r + a_{10} \times C_r^2) \times e^{-a_{11} \times SOC} + (a_{12} + a_{13} \times C_r + a_{14} \times C_r^2) \quad (2)$$

$$C_1 = -(a_{15} + a_{16} \times C_r + a_{17} \times C_r^2) \times e^{-a_{18} \times SOC} + (a_{19} + a_{20} \times C_r + a_{21} \times C_r^2) \quad (3)$$

$$\begin{aligned} V_0 = {} & (a_{22} + a_{23} \times C_r + a_{24} \times C_r^2) \times e^{-a_{25} \times SOC} + \\ & (a_{26} + a_{27} \times SOC + a_{28} \times SOC^2 + a_{29} \times SOC^3) - a_{30} \times C_r + a_{31} \times C_r^2 \end{aligned} \quad (4)$$

The polynomial equations for discharging conditions are given in Eq. 5-8 [1].

$$R_1 = (a_1 + a_2 \times D_r + a_3 \times D_r^2) \times e^{-a_4 \times DOD} + (a_5 + a_6 \times D_r + a_7 \times D_r^2) \quad (5)$$

$$R_2 = (a_8 + a_9 \times D_r + a_{10} \times D_r^2) \times e^{-a_{11} \times DOD} + (a_{12} + a_{13} \times D_r + a_{14} \times D_r^2) \quad (6)$$

$$C_1 = -(a_{15} + a_{16} \times D_r + a_{17} \times D_r^2) \times e^{-a_{18} \times DOD} + (a_{19} + a_{20} \times D_r + a_{21} \times D_r^2) \quad (7)$$

$$\begin{aligned} V_0 = {} & (a_{22} + a_{23} \times D_r + a_{24} \times D_r^2) \times e^{-a_{25} \times DOD} + \\ & (a_{26} + a_{27} \times DOD + a_{28} \times DOD^2 + a_{29} \times DOD^3) - a_{30} \times D_r + a_{31} \times D_r^2 \end{aligned} \quad (8)$$

Once the polynomial coefficients are found using GA at specified charge/discharge rate, it is used for calculating battery terminal voltage for charging/discharging with various charge/discharge rates. Under the constant current, the battery terminal voltage for charging scenario with respect to time is given in Eq.9 [1].

$$V_{bc}(t_c) = \left(\left(\frac{Q}{C} + I_c \times R_2 \right) \times \exp\left(-\frac{t_c}{R_2 \times C_1} \right) \right) + V_0 - \left(I_c \times (R_1 + R_2) \right) \quad (9)$$

Similarly, the battery terminal voltage for discharging scenario is given in Eq. 10.

$$V_{bd}(t_d) = \left(\left(\frac{Q}{C} + I_d \times R_2 \right) \times \exp\left(-\frac{t_d}{R_2 \times C_1} \right) \right) + V_0 - \left(I_d \times (R_1 + R_2) \right) \quad (10)$$

In the next section, mathematical model for capacity fading as a function of processed energy for charging/discharging, nominal capacity of the battery, charge/discharge rate, pre-exponential and adjustable factor is presented.

III. CAPACITY MODEL

The battery capacity represents the maximum amount of energy that can be extracted from the battery under certain specified conditions such as charge/discharge rate, SOC and temperature [6]. The capacity fade of Li-ion batteries can be related to the unwanted side reactions that occur during the overcharge and high charge/discharge conditions, which reduce the battery life time. Thus, capacity fading is directly proportional to the charge and discharge rate [7-8]. Generally, the capacity fading is estimated through experimentation. In real life scenarios the battery will be subjected to different charge and discharge rates and this has to be included in the modelling of Electric Vehicle Drive Train Simulations or G2V simulations. Performing experiments to determine the capacity fading for different charge and discharge rates and their combinations is a tedious and time consuming process. Hence, mathematical models come in handy. The mathematical modelling techniques are comparatively simple and are sufficient to calculate battery capacity fading at different charge/discharge rate. The mathematical model for capacity fading is developed based on the Arrhenius equation and is given as [9-10].

$$Q_{loss} = A \times \exp\left(-\frac{E_a}{R \times T} \right) \times t^z \quad (11)$$

This equation is used for calculating capacity fading under fixed charge/discharge rate. Conversely, in the practical case, the charge and discharge rate varies with respect to the grid condition. As a result, the capacity fading increases with respect to the increasing charge/discharge rate, SOC and temperature [11-14].

Fig.3 shows the battery performance characteristics for a cycle. The number of charge/discharge cycles the battery can experience before it fails to meet performance criteria is called battery life [15]. Considering these variations, an accurate mathematical model is required to predict the capacity fading at different charge/discharge rate. In this work the capacity fading model as given by Arrhenius equation has been extended to include rate of charge and discharge. The proposed capacity fading equation depends on nominal capacity, charge (C Rate) /discharge (D Rate) rate, processed energy for charging (E_c)/discharging (E_d), pre-exponential and adjustable factors, gas constant and temperature.

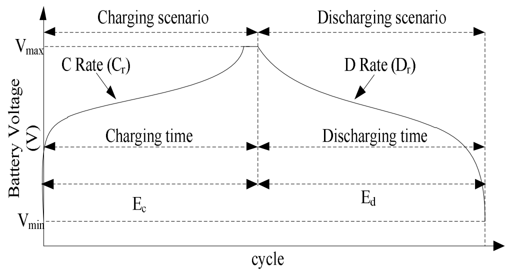

Fig. 3. Battery performance characteristics for a cycle

The proposed mathematical model for capacity fading at different charge and discharge rate is given in Eq.12.

$$Q_L^C = \left(A \times \exp\left(-\frac{C \times E_c \times Q \times C_r}{R \times T} \right) \right) + \left(B \times \exp\left(-\frac{D \times E_d \times Q \times D_r}{R \times T} \right) \right) \tag{12}$$

The advantage of this model is that it is capable of determining the capacity loss of the battery when it is subjected to charge and discharge cycles at different C-rates. For example this model can predict the capacity loss of a battery when it is charged at 1C and discharged at 2C. The parameters of the eq.12 can be determined from the capacity loss data given by the battery manufacturers.

The next section presents in detail the computation of the optimal values for polynomial coefficients at different charge/discharge rate using the genetic algorithm (GA).

IV. GENETIC ALGORITHM

Genetic Algorithm (GA) is computerized search and optimization algorithm inspired by the mechanics of genetics and natural selection. GA is a best and robust kind of optimization algorithm. The battery polynomial coefficients are calculated by using GA and it gives most accurate "solution sets" [1].

The process starts by generating a random set of solutions to the problem. Where the solutions are represented in a form to closely mimic the gene behaviour, for example the binary representation used in this work. Next requirement is some measure of quality of solutions. For that we need to establish a fitness function, so that we can rate each solution according to its fitness. This step is followed by the checking for optimality condition i.e. whether any of the solution has reached an optimum fitness level or not. If not, the present generation would be taken as parent for next generation step. This reproduction step is the most crucial part of the GA, because here to exhibit the process of natural selection which will ensure a non-decreasing average fitness with every progeny. There are several methods to imitate natural selection. In this work, Roulette Wheel (RW) method is used for finding optimal solution. In which the probability of a solution sets are selected for reproduction. It is directly proportional to the fitness function. Two units are selected and their genetic material is mixed in a way to create a new unit which is not an identical copy of either parent. Now the new solution set is again checked for fitness and optimality condition. As the fit individuals were selected for parenting the next generation, the newly formed individuals are supposed to have an increased or at least non decreased fitness level. Since the algorithm proceeds gradually from lower to higher average fitness. It becomes a guided search for optimal solution. The optimum solutions are checked with charge/discharge equations as represented in Eq. 1-9 for charging and discharging scenario. The resultant characteristics are checked with manufacturer data. The flow chart of the GA is shown in Fig 4.

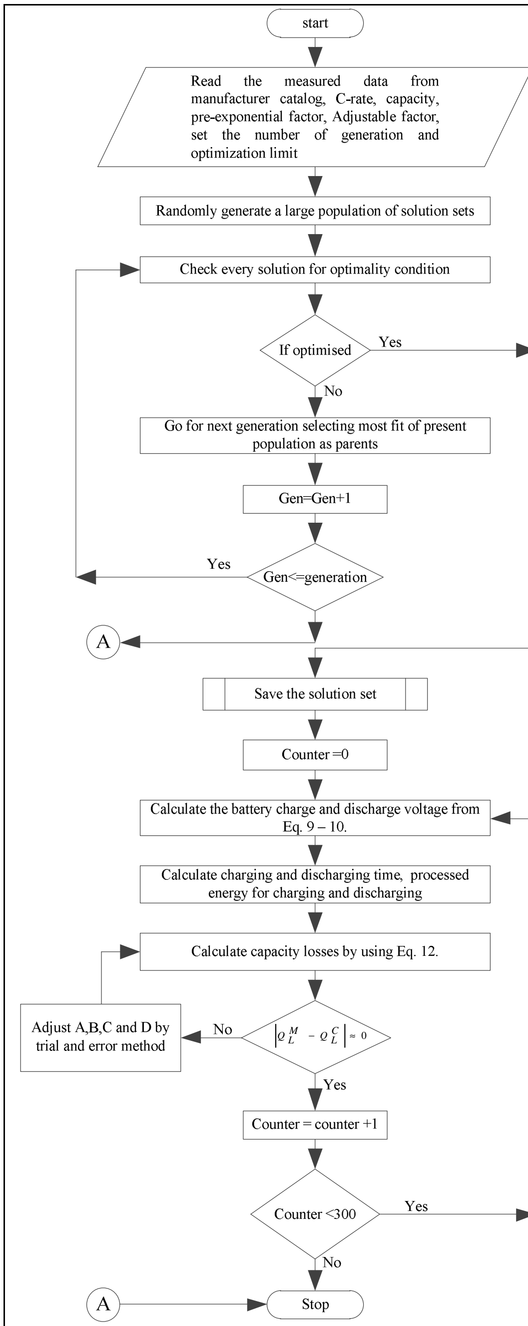

Fig. 4. Flow chart for parameter extraction using genetic algorithm approach and capacity fading at different charge/discharge rate.

The Li-ion batteries manufactured by different manufacturers are considered for parameter extraction problem [1, 3-4]. For Li-ion battery SOC verses battery terminal voltage for charging, SOC verses battery terminal voltage for discharging and cycle verses capacity losses at different charge/discharge rates, as given in the manufacturer catalogue. To obtain the parameters (a_1-a_{31}), measure the charging voltage, discharging voltage and capacity loss at different charge/discharge rate. The parameters for charging and discharging characteristics are calculated from GA and the capacity fading parameters are calculated from trial and error method. The mathematical formulation of fitness function for obtaining one set of the parameters for charging and discharging scenario is given by Eq.13-14.

$$F_{optimum} = \sum_{i=0}^{n}\left(V^{M}_{bc,C_i} - V^{C}_{bc,C_i}\right) \tag{13}$$

$$F_{optimum} = \sum_{j=0}^{m}\left(V^{M}_{bd,D_j} - V^{C}_{bd,D_j}\right) \tag{14}$$

Similarly, the mathematical formulation of fitness function for obtaining one set of the pre-exponential and adjustable factors are given by Eq. 15.

$$F_{optimum} = \sum_{i=0}^{n}\left(Q^{M}_{L,i} - Q^{C}_{L,i}\right) \tag{15}$$

One set of parameters for charging and one set of parameters for discharging are shown in Table I.

TABLE I

Polynomial coefficients for charging and discharging scenario

Polynomial coefficients for charging scenario		Polynomial coefficients for discharging scenario	
Coefficients	Values	Coefficients	Values
a_1	0.02109	a_1	0.05256
a_2	0.000579	a_2	0.002547
a_3	0.000064	a_3	0.000587
a_4	42.76495	a_4	30.3548
a_5	0.01246	a_5	0.05215
a_6	0.000396	a_6	0.003147
a_7	0.000033	a_7	0.00032
a_8	0.009526	a_8	0.022546
a_9	0.000238	a_9	0.012547
a_{10}	0.0000031	a_{10}	0.022657
a_{11}	29.38634	a_{11}	18.26547
a_{12}	0.00687	a_{12}	0.010001
a_{13}	0.000324	a_{13}	0.00088
a_{14}	2.20E-05	a_{14}	0.000023
a_{15}	8.635732	a_{15}	1.222364
a_{16}	0.369508	a_{16}	0.010693
a_{17}	0.028163	a_{17}	0.004548
a_{18}	0.668211	a_{18}	15.90916
a_{19}	5.235634	a_{19}	134.2356
a_{20}	0.110554	a_{20}	0.012207
a_{21}	0.063747	a_{21}	0.002661
a_{22}	0.012559	a_{22}	1.01254
a_{23}	42.780107	a_{23}	20.2145
a_{24}	2.146841	a_{24}	2.5423
a_{25}	0.188108	a_{25}	0.22547
a_{26}	0.024947	a_{26}	0.1101
a_{27}	0.002864	a_{27}	0.02103
a_{28}	0.162724	a_{28}	0.00151
a_{29}	0.015353	a_{29}	0.0009
a_{30}	0.011420	a_{30}	1.42546
a_{31}	0.00642	a_{31}	0.00032

Table II show the optimal values for the pre-exponential and adjustable factors for Sony US 18650 batteries.

TABLE II

Pre-exponential and adjustable factor for Sony 18650 battery

Pre-exponential factor		Adjustable factor	
A	B	C	D
0.09051	0.003873	1.295	1.442e-5

The results of established mathematical model for battery and capacity fading at different charge/discharge rate are given in the next section.

V. RESULTS AND DISCUSSION

Three types of battery charge/discharge rate characteristics were obtained and compared with the measured (manufacturer catalogue) data. The first battery is EIG Li-ion battery having a rated capacity of 8Ah. The second battery is Sony US 18650 Li-ion battery with a rated capacity of 1.4Ah. The third battery is Sony 1700 Li-ion battery having a rated capacity of 0.83 Ah. The Sony and EIG battery percentage of capacity fading and processed energy for charge/discharge rates after 300 cycles are shown in Table III.

TABLE III

Battery performance for different types of manufacturer

Sl. No	Battery Manufacturer	Q (Ah)	C_r -D_r	$E_c + E_d$ (kWh)	Q_l after 300 cycle (%)
1	EIG	8	1-1	5.6687	15.5687
2	Sony US 18650	1.4	1-2	2.8958	13.578
3	Sony 1700	0.83	0.66-0.94	0.9874	9.4587

A. *Charge rate characteristics for EIG battery*

Fig. 5 gives the plots of charge curves obtained for various charge rates (0.5C, 1C and 2C) calculated using Eq. (9). The experimental data's are measured from the battery manufacturer's catalogue. It is evident from the plots that the simulated curves are in close agreement with the measured data. If the battery is charged at low charge/discharge rate, the charging time of the battery and total energy extracted from the battery is high. The charging energy of the battery at 1C rate is 2.9344 kWh. The total processed energy is given in Table III.

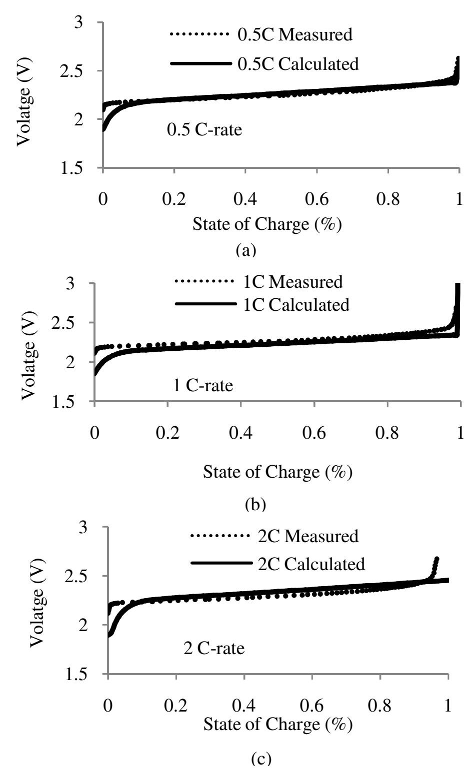

Fig. 5. Measured and Calculated EIG battery charge rate characteristics at different charge rate (a) 0.5 (b) 1 and (c) 2

B. Discharge rate characteristics for EIG battery

The plots of discharge curves obtained for various rates (0.5C, 1C and 2C) using Eq. (10) is shown in Fig.6. Accordingly, the discharge current is assumed as 4A, 8A and 16A. During the discharging condition, the output terminal voltage is equal to the difference between initial open circuit voltage and the voltage drop inside the battery. It is observed that the basic shape of these discharge curves remain very similar to the manufacturer's data. The energy extracted from the battery is inversely proportional to the discharge rate and is directly proportional to voltage and current. If the charge/discharge rate is increased, the discharge current increases and discharge voltage decreases. Therefore, it is concluded that the processed energy decreases at high current. The average energy extracted from the battery for different charge/discharge rate is given in Table IV.

TABLE IV

Energy extracted from the battery at different rate (1 cycle)

	0.5C	1C	2C
Measured for catalogue (Wh)	17.2	16.68	16.67
Calculated (Wh)	17.8	17.5	17.26

From the Fig.6, we infer that the battery provides energy continuously up to two hours if the battery discharges at 0.5C rate. Similarly, the battery provides the energy up to one hour if the battery discharges at 1C rate. At low rates (0.5C and 1C), the battery provided an average voltage of 2.22V and 2.17V, respectively. At high charge/discharge rate (2C) the battery provides the average voltage of 2.16V.

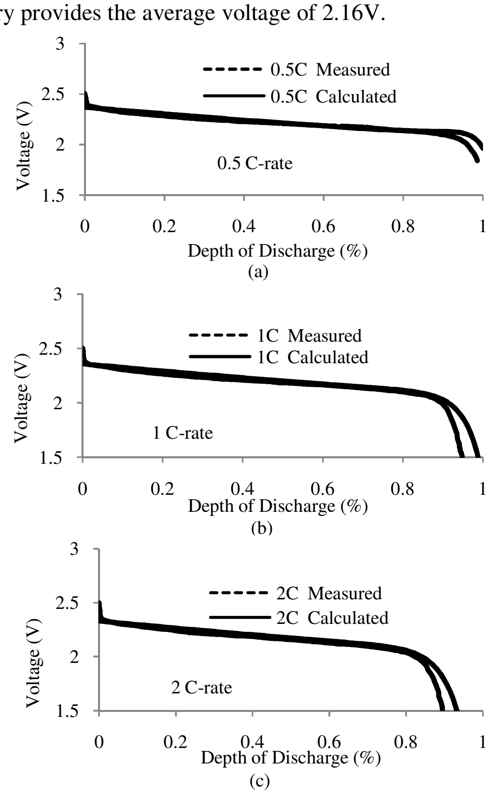

Fig. 6. Measured and calculated EIG battery discharge rate characteristics at different discharge rate. (a) 0.5 (b) 1 and (c) 2

C. Charge rate characteristics for Sony 1700 battery

Charge rate characteristic for Sony 1700 Li-ion (0.830mAh) battery at 0.66C is calculated. Comparison between the measured and simulated charge rate characteristic at 0.66C is shown in Fig. 7. Charging is performed for constant-current. The voltage window for Sony 1700 Li-ion battery is set as 3.5V to 4.2 V. From Fig.7, it is clearly evident that the measured data and the calculated data are similar.

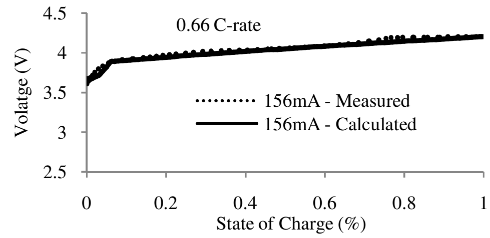

Fig. 7. Sony 1700 battery charge rate characteristics at 066C-rate

D. Discharge rate characteristics for Sony 1700 battery

Discharge rate characteristic for Sony 1700 Li-ion battery discharge at 0.94C is shown in Fig. 8. The discharge rate is defined as the ratio between the current extracted from the battery and nominal capacity of the battery. The discharge characteristic of the Sony 1700 battery is obtained for the voltage range of 4.2V to 2.5 V.

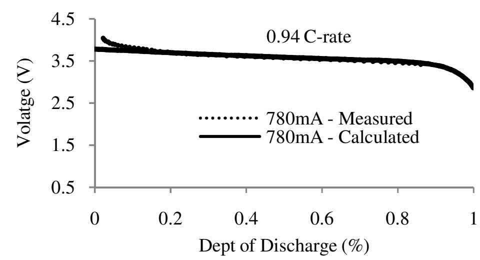

Fig. 8. Sony 1700 battery discharge rate characteristics at 0.94D-rate

E. Capacity fading characteristics for Sony US 18650 battery

Fig. 9 shows the comparison between the measured and calculated capacity fading and the processed energy for Sony US 18650 Li-ion battery at different charge/discharge rate. The batteries are cycled at high discharge rate (3C). It is observed that the internal resistance of the battery increased relative to the resistance of the fresh batteries [6]. The rate capability losses were proportional to the increase in discharge rate and the number of cycles. Similarly, the major causes for the capacity loss were identified as a function of cycle number and temperature [7]. From Fig.9, it is also concluded that if the battery is charged/discharged at high charge/discharge rate (2C and 3C) the capacity fade is high. Similarly, at low charge/discharge rate, the capacity fade is low. Therefore, it is verified that the capacity losses estimated using the proposed mathematical model confirms to the manufacturer's data. The measured and the calculated capacity losses for Sony US 18650 Li-ion battery at different charge/discharge rate is shown in Table V.

TABLE V

Measured and calculated capacity fading for Sony US 18650 Li-ion battery at different charge/discharge rate.

C-rate	Measured (Ah)	Calculated (Ah)	Measured (%)	Calculated (%)
1C	1.27	1.27	9.5	9.54
2C	1.21	1.23	13.2	12.68
3C	1.16	1.14	16.9	17.28

From Table V, it is observed that the battery cycled at 1C discharge rate losses almost 9.5% of its initial capacity after 300 cycles. The calculated capacity fades almost 9.54 % of its initial capacity after 300 cycles.

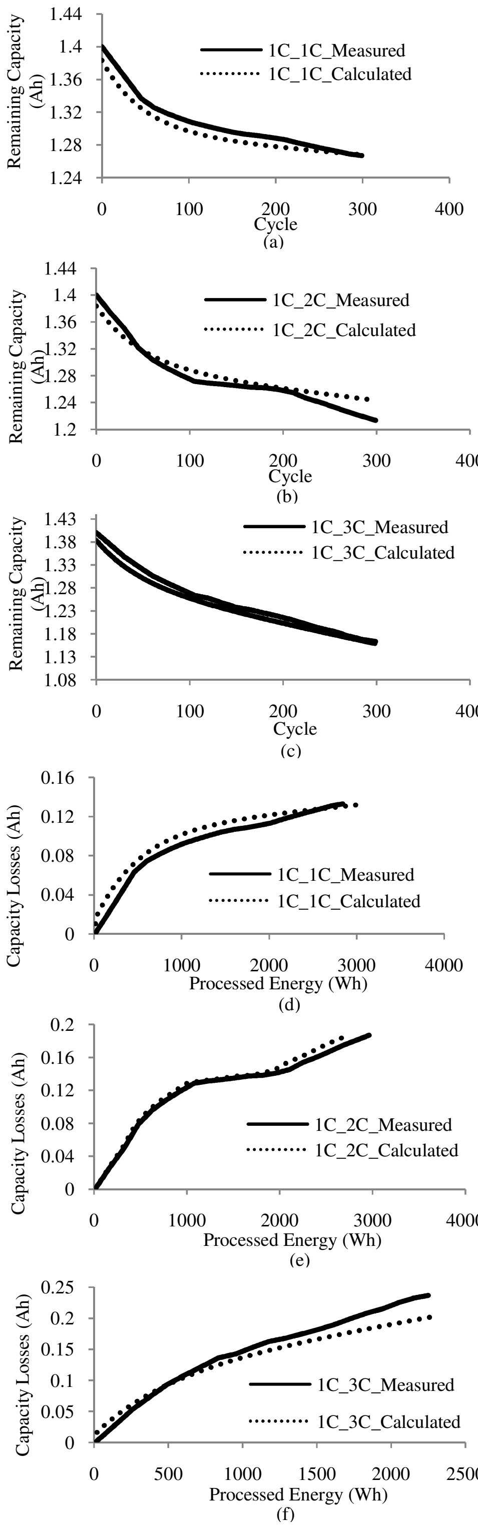

Fig. 9. (a), (b) and (c) Measured and calculated capacity fading characteristics at different charge/discharge rate and (d), (e) and (f) Measured and calculated processed energy characteristics at different charge/discharge rate (Sony US 18650).

VI. CONCLUSION

A comprehensive battery model was discussed for Li-ion battery to understand its performance characteristics at different charge/discharge rates. The time, charge/discharge rate, and SOC dependent EEC parameters were calculated using the polynomial equation. The polynomial coefficients are optimized using GA. The simulated battery characteristics are in close agreement with the measured characteristics. The proposed battery model and capacity model used to study the performance of V2G configurations and to analyse the amount of capacity losses while the power stored in the battery or transferred to the grid.

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