

DYNAMIC BATTERY MODEL AND STATE OF CHARGE ESTIMATION

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ABSTRACT

Mathematical modeling and the dynamic simulation of battery storage systems can be challenging and demanding due to the nonlinear nature of the battery chemistry. This paper introduces a new dynamic battery model, with application to state of charge estimation, considering all possible aspects of environmental conditions and variables. The aim of this paper is to present a suitable convenient, generic dynamic representation of rechargeable battery dynamics that can be used to model any Lithium-ion rechargeable battery. The proposed representation is used to develop a dynamic model considering the thermal balance of heat generation mechanism of the battery cell and the ambient temperature effect including other variables such as storage effects, cyclic charging, battery internal resistance, state of charge etc. The results of the simulations have been used to study the characteristics of a Lithium-ion battery and the proposed battery model is shown to produce responses within 98% of known experimental measurements.

Keywords: Unscented Kalman Filter, Dynamic modeling, Temperature effect, Hybrid vehicles, Simulation, Lithium-ion.

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I.INTRODUCTION

Efficiency, novelty and the latest technology in hybrid cars pose the greatest attraction among commuters in the automotive world. More than just the fuel economy, hybrid vehicles offer many green advantages. A small increase in fuel economy makes a large difference in emissions over many years. Battery designs play an important role in these vehicles, and the price per kilowatt-hour varies according to battery type as mentioned in Smith [1].

The Lithium-ion (Li-ion) batteries have attracted the popularity among many battery types to be used in hybrid electric vehicles. Dynamic modeling that accounts for all aspects of the battery life cycle such as self-discharging, gassing effect, diffusion processes, acid stratification, state of charge, over voltage stabilization etc. is quite an involved process as outlined by Zoroofi [2].

Broadly, battery models may be classified as circuit based models and electro-chemical models. However the distinction is only superficial, as all electro-chemical models can be represented by equivalent circuits, if one permits the circuit elements to be active or regenerative elements rather than just passive circuit elements. Furthermore the circuit elements may be non-linear functions of the internal state of the battery. The basic circuit model is the Thevenin equivalent circuit of the battery and its extensions as discussed in Vepa [3]. In these approaches one establishes a linear model of the relationship between the terminal voltage and the current available to the application. The polarization losses are expressed as nonlinear voltage losses. An alternate approach is to assume a linear relationship between the rate of change of the terminal voltage and the rate of change of the state of charge (*SOC*), which is usually the key metric of interest. The proportionality constant could be assumed to be locally linear or nonlinear. The *SOC* is defined as the percentage of the completely

extractable charge capacity remaining in the battery. The SOC indicates the amount of electrical energy remaining in a battery. A key performance parameter is an accurate estimate of the SOC as and when it is being used and is important both for the battery application designers as well as for the battery users. An accurate indication of the battery SOC during the runtime allows the user to ensure that the battery is neither over-charged or under-discharged, resulting not only in the optimum use of the power available but also in a longer battery life. The methods of estimating the batter *SOC* can be broadly classified as:

- i) Discharge test under controlled conditions to determine the capacity remaining at any instant after a specific loss of capacity;
- ii) Ampere hour counting or charge counting (initial *SOC* must be known and involves estimation of the current loss);
- iii) Based on the relation between the open circuit voltage and *SOC*;
- iv) Model based estimation;
- v) Heuristic interpretation of measured data (electrolyte properties and other).

Several of the above methods rely on test data and the usual tests carried out on a battery are:

- i) Open Circuit Voltage Test to determine the relationship between the terminal voltage, the terminal current and the state of charge;
- ii) Hybrid Pulse Test: Hybrid Pulse Power Characterisation (HPPC) profiles with constant current discharge and charge pulses with rest periods or pauses with no charging or discharging are used to measure battery performance characteristics;
- iii) Federal Urban Driving Schedules Tests (FUDS): FUDS is a typical dynamic driving cycle and is usually used in the USA to verify the usefulness and the accuracy of the battery models.

Most measured data is characterised by uncertainties and there are usually five classes of uncertainties to consider: i) measurement uncertainty, ii) algorithmic uncertainty, iii) environmental uncertainty, iv) model parameter uncertainty and v) model dynamics uncertainty or un-modelled dynamics. Thus the first step is usually to extract the model parameters by applying suitable model identification and parameter estimation methods to the measured data as discussed by Birkl and Howey [4]. One can adopt either a time domain approach, such as the method of Alavi, Birkl and Howey [5] which can then be used directly to simulate the battery dynamics (see for example Thanagasundram et al [6]) or a circuit based approach as in Howey et al [7]. One could also adopt a direct approach and identify the *SOC* characteristic from the measured data as was done by Li, Chattopadhyay and Ray [8].

A novel approach to battery modeling can be found in Sepasi, Ghorbani and Liaw [9] and in Xia et al [10]. Here, we investigate to present a cell level battery model which incorporates the most significant parameters that have been mentioned previously. As mentioned earlier, circuit based electrical models are very useful and complex enough to represent the electrochemical behaviour within the cells that describe the dynamics of the electron transfer and energy dissipation. Zhang et al [11], Thanagasundram et al [6] and MathWorks [12] used the open circuit voltage to estimate the state of charge of the battery. Erdinc, Vural, Uzunoglu [13] employed the battery internal resistance as a function of *SOC* when modeling discharging/charging characteristics. Storage and cyclic effects also were added to the internal resistance. The dynamics of the *SOC*, is given by Erdinc, Vural, Uzunoglu [13] and is,

$$\frac{d SOC(T)}{dn} = k_1 n + k_2 . \quad (1)$$

The temperature effect on the battery system was modeled along with the rate of change of *SOC*. In equation (1), n is the cycle number, k_1 and k_2 are constants. The

variable T identifies the operating temperature of the battery. The equation (1) was based on a semi empirical formulation for variation of SOC at the negative electrode with the cycling effect confined to two specific temperatures of 25°C and 50°C.

When modeling the effect of battery temperature, experiments by Tan, Mao and Tseng [14] demonstrate that it is essential to consider both the change in the ambient temperature T_{amb} due to environmental conditions and the rise in internal battery cell temperature T_{Cell} due to chemical reactions in the electrolyte and the electron transfer effect. Although most experiments are conducted at a constant temperature (see for example Chen and Rincon-Mora [15]), for electric vehicles (EV) especially, the rise in the ambient temperature due to a hot external environment as well as the heat emission from an automobile engine can affect the battery performance severely as mentioned by Kroeze and Krein [16]. To account for all the performance characteristics, the effects of both the ambient and internal battery cell temperature have to be explicitly considered. Though, the change is not substantial, temperatures above a critical temperature can affect the battery performance. Simulation results show that this critical temperature for a lithium-ion battery T_{Cell} is about 42°C.

In this paper a new dynamic Li-ion battery model is proposed and validated. One of the key features of this paper is that, it presents a dynamic battery model that is accurate and consistent not only at a constant cell temperature but also at varying ambient and internal cell temperatures. The other contributions made in this paper are categorized as follows a) a new table of coefficients for the variable model parameters of R_{intS} , R_{TS} , R_{TL} , C_{TS} , C_{TL} (which will be described in section- IV). b) The implementation of thermal energy balance model that can be described as a reduced order thermal model. c) The introduction of two new variable voltage sources $\Delta E(T)$

and $\Delta V_{Che}(T)$ that depend on the temperature. The change of $\Delta E(T)$ represents the equilibrium potential correction of the battery open-circuit voltage, that depends on the temperature and the amount of active material available in the electrodes, that can be specified in terms of state of discharge (*SOD*) (Panday and Bansal [17]). $\Delta V_{Che}(T)$ represents the voltage increase due to temperature effect on the electrolyte chemistry (film formation, non-uniform ions distribution, non-uniform heat generation rate, conductivity difference in the electrolyte due to hot regions, diffusion and over-voltage stabilization). d) Due to temperature and *SOC* change during simulation time (see for example [12, 18]) the variable discharge/charge current has been included in the model to get the accurate battery terminal voltage. e) A new formulation representing the *SOC* variation due to varying temperature.

The paper is organized as follows. Section II briefly describes the existing dynamic battery models. The new dynamic battery model is described in section III. The thermal energy balance equation, with our contributions to the new dynamic battery model is given in section IV. The final non-linear state equations of the model are summarised in section V. The comparison of the model with the experimental results at 25⁰C is presented in section VI. The effect of the variable temperature on the model is discussed in section VII. The application to *SOC* estimation is reviewed and discussed in section VIII. The conclusion is given in section IX.

II. EXISTING DYNAMIC BATTERY MODELS

Li-ion batteries have been considered for modeling as they have been getting greater attention from the researchers than NiMH and Lead-acid batteries due to their higher specific energy, specific density, durability and lower self-discharge rate (See for example Panday and Bansal [17]). In addition, Li-ion batteries have earned a good

reputation for their excellent life cycle with no memory effects. These physical characteristics make the Li-ion batteries preferable for next generation of hybrid electric vehicles [13]. The parameters required for these models have been defined in the nomenclature.

Various classes of mathematical models of battery performance based on the chemistry of the electrolyte, the SOC, the electro-chemical behaviour and the thermal effects have been presented by Zoroofi [2], MathWorks Inc. [12], Tremblay and Dessaint [18], Gallo et al [19], Huria [20], Tan, Mao and Tseng [14], Chen and Rincon-Mora [15], Bhide and Shim [21]. All of these models could be used, in part, although none of the above models have ventured to include all of the effects that are of importance for representing the battery dynamics for electric vehicle and hybrid energy system applications. In this paper we have integrated the battery chemistry, the evolution of the SOC, the electro-chemical dynamics and the thermal effects into one single model.

III. NEW DYNAMIC BATTERY MODEL

A dynamic battery model that can accommodate both electrical and thermal properties which is suitable to apply for any hybrid energy systems is sought. The equivalent electrical circuit for such a model is shown in fig.1(a) which has the following five parts from left to right:

a) Source voltage V_{OC} , in parallel with the $R_{self}(T, n, SOC)$ which is identified as R_{self} representing the battery self-discharge feature due to storage effects which is a function of temperature T , SOC and the cycle number n . The cycle number n signifies the number of cycles the battery is charged or discharged.

- b) Battery internal resistance which is modelled by two resistances in series R_{intS} and R_{CYC} representing the electrolyte resistance and the resistance change due to the number of charging and discharging cycles the battery has undergone.
- c) Two RC circuit loops with RC elements given by, R_{TS}, C_{TS} and R_{TL}, C_{TL} which represents the short and long transient effects of the battery. The transient effects arise due to double-layer formation at the electrode/solution interface (Thanagasundram et al [6]). The capacitances C_{TS} and C_{TL} represent the electrical polarization capacitance and the diffusion capacitances. Transient response of the battery is influenced by double layer diffusion capacitance when the rates of reactions are high.
- d) The parameters $R_{intS}, R_{TS}, R_{TL}, C_{TS}, C_{TL}$ and SOC/SOD usually depend on temperature. Their dependence is included separately in the model by using mathematical relationships that will be discussed later in this section.
- e) Finally, the other temperature dependent characteristics are included into the model by the addition of two variable voltage sources $\Delta E(T)$ and $\Delta V_{Che}(T)$.

A selection of batteries with different electrolytes which are associated with different chemistries and temperature effects and are dissimilar, have been considered for the electro-chemical modelling. Due to the gassing effect and film formation at the electrodes the electron transfer rates will be changed. Temperature change can influence these effects and alter the equilibrium potential or open circuit voltage (Thanagasundram et al [16]). These effects have been included in this study.

IV. THERMAL MODEL

The thermal model presented here is based on the general energy balance equations used in Bernardi, Pawlikowski and Newman [22]. Heat is produced in batteries from three fundamental sources: activation (interfacial kinetics), concentration (species

transport), and Ohmic (Joule heating from the movement of charged particles) losses. The proposed thermal model assumes the natural convection conditions and the heat generation and heat dissipation throughout the electrolyte as uniform, although models of uneven heat generation of the type discussed by Wu et al [23] could be incorporated into the analysis. The model parameters and the chemistry between anode, cathode and the separator have not considered separately but taken as average values. The generation rates of reversible and irreversible heat during charge and discharge are taken as equal with the same *SOC* and current rate. The temperature distribution is taken as symmetrical with respect to centre line in the battery cell. Initial battery cell temperature is assumed to be equal to the ambient temperature. Detailed description in this context can also be found in Wu, Li and Zhang [24]. The equation for the total heat generation rate given by equation (7) in [24] is used to model the thermal model. Hence the energy balance equation according to [22] can be written as given below (2):

$$\Delta T = (T_{Cell} - T_{amb}) \quad (2)$$

$$\frac{dT_{Cell}}{dt} = \frac{1}{mC_p} \left[i \{V_{bat} - V_{OC}\} + \frac{T_{Cell}}{F} \Delta S \Phi - A \alpha \Delta T \right] - A \lambda \Delta T - A \sigma \varepsilon (T_{Cell}^4 - T_{amb}^4) \quad (3)$$

The parameter α is normally identified as the heat transfer coefficient for forced cooling or in literature sometimes it is defined as the convective heat exchange coefficient. The symbol Φ is the current density (A/cm^2). The parameter F is defined as the Faraday constant. The parameter σ is the Stefan- Boltzmann constant. The effect of other two parameters, λ which is identified as the conductive heat coefficient and ε which is defined as the radiation coefficient are neglected due to minimal effects. The combined entropy change ΔS , can also be taken as zero as in Viswanathan et al [25].

Hence the equation (3) can be simplified to equation (4) as given below ([2, 21]):

$$\frac{dT_{Cell}}{dt} = \frac{1}{mC_p} [i\{V_{bat} - V_{OC}\} - A\alpha\Delta T], \quad (4)$$

where m is the unit mass. The temperature effect on activation, diffusion polarization and due to different electrolyte chemistries is modelled by the parameter $\Delta V_{Che}(T)$ which is a function of the temperature.

The parameter $\Delta V_{Che}(T)$ is modeled by the polynomial as given by the equation (5):

$$\Delta V_{Che} = \beta w \exp^{(1/i)} \Delta T + \left. \frac{dV_{che}}{dT} \right|_{T=T_{Cell}} (C_{Che} + C_{Che1}\Delta T)(1 + \beta)\Delta T \quad (5)$$

where T_{Cell} is the battery internal temperature. Though it is not uniform here we assumed the T_{Cell} to be uniform within the cell and T_{amb} is the operating temperature of the battery. The parameters β , w , C_{Che} and C_{Che1} are all constants that depend on the properties of the electrolyte, the anode and the cathode materials. The first derivative dV_{che}/dT is defined as the effective voltage gradient. $\Delta E(T)$ can be modelled by the equation as given in (6), as,

$$\Delta E(T) = (1 + C_{E1}\Delta T) \left. \frac{dV_r}{dT} \right|_{T=T_{Cell}} \Delta T \quad (6)$$

The first derivative dV_r/dT is defined as the voltage gradient and is assumed to be constant for the temperature range. Table-I gives the parameters and constants derived from simulation results [indicated in the table as ‘sim’] and directly from the literature or estimated from the literature [indicated in the table as ‘Lit’].

By considering the two RC parallel loops the following mathematical relationships can be deduced by using Kirchoff’s law ((7), (8) and (9)).

$$\frac{dV_j}{dt} = \frac{i}{C_{Tj}} - \frac{V_j}{R_{Tj}C_{Tj}}, \quad j = 1, 2. \quad (7)$$

In (7),

$$C_{Tj} = C_{TL}, R_{Tj} = R_{TL}, \text{ for } j = 1,$$

and:

$$C_{Tj} = C_{TS}, R_{Tj} = R_{TS}, \text{ for } j = 2.$$

$$V_{OC0} = V_{bat} + i(R_{int.s} + R_{cyc}) + V_1 + V_2 \quad (8)$$

The parameters V_1 and V_2 represents the voltages across the two capacitors C_{TS} and C_{TL} . The open circuit voltage V_{OC} is then expressed as,

$$V_{OC} = V_{OC0} + \Delta E(T) + \Delta V_{che}(T). \quad (9)$$

The battery terminal current is related to the battery voltage by the relation,

$$i = C_{bat} \dot{V}_{bat}. \quad (10)$$

If the battery voltage is assumed to be related to the state of charge by the relation,

$$V_{bat} = k * SOC + d, \quad (11a)$$

we obtain the model equation in differential form,

$$\dot{V}_{bat} = k * \dot{SOC} \quad (11b).$$

In the non-linear case we begin with a locally linear model of the form given by equation (11b) which can then be integrated to give a nonlinear model of the battery voltage and SOC relationship. Using equations (11a) and (11b) in equations (8) and (10) respectively gives,

$$V_{OC0} = k * SOC + d + i(R_{int.s} + R_{cyc}) + V_1 + V_2 \quad (12)$$

$$\dot{SOC} = i/kC_{bat} \quad (13)$$

Where $V_{OC0} = V_{OC0}(SOC, n, T)$ is the open circuit voltage under standard conditions or at the room temperature and the state of charge is given by the charge counting equation,

$$SOC = SOC_{ini} - \int (i / C_{usable}) dt \quad (14)$$

Using equation (13) we can write:

$$SOC = SOC_{ini} / (1 + kC_{bat} / C_{usable}) \quad (15)$$

Hence the constant k is defined by,

$$k = C_{usable} (SOC_{ini} - SOC) / C_{bat} SOC \quad (16)$$

The complete set of equations defining the battery dynamics above, do not include a noise model. We will include two noise sources: The first with the current in the form of a process noise and modify the current equation to,

$$\dot{i} = w_1 . \quad (17)$$

The second noise source is in the measured open circuit voltage, V_{OC} ,

$$V_{OC} = V_{OC0} + \Delta E(T) + \Delta V_{Che}(T) + v_n . \quad (18)$$

The usable battery capacity C_{usable} changes depending on the storage time and temperature. When the temperature increases the usable capacity decreases. An excellent detailed description on C_{usable} with the effect of temperature can be found in Spotnitz [26] and in Planklang and Pornharuthai [27]. From Valerie, Johnson and Pesaran [28] it was noted that from 0°C to 60°C the usable capacity decreases roughly about 4% for a simulation time of one hour. Hence, the change of this parameter is included in the model by using a capacity correction factor (CCF) which is reasonable, instead of representing the variation with a polynomial equation that fits into manufacturers' data. The CCF is generally calculated by using the operating temperature and the time of storage which is normally measured in months as it gives

an indication of the per cent loss in the capacity fading. The capacity fading can also be calculated using the equations given in Nasar and Unnewehr [29]. From the Lithium-ion Rechargeable Batteries technical data handbook [30], discharge capacity remains constant from 22⁰C to 45⁰C. The discharge capacity decreases linearly from 22⁰C to 0⁰C. This can be taken as a negative gradient of 2 mAh per degree Celsius. For Li-ion though the discharging temperature range is permissible between -20⁰C to 60⁰C, the charging temperature range is only recommended from 0⁰C to 45⁰C and not below freezing temperature as also given in BU-Charging [31].

The battery equivalent internal impedance ($R_{intS} + R_{cyc}$) contributes to the instantaneous drop in the battery terminal voltage as given by Zoroofi [2]. As discussed earlier, the passive circuit elements R_{TS} and the C_{TS} represent the fast dynamics associated with the reaction kinetics between the electrical charges at the electrode's surface barrier and the charges in the electrolyte. The R_{TS} is the charge transfer resistance and the capacitance C_{TS} models the electrochemical double layer capacitance. The R_{TL} and the C_{TL} circuit elements represent the slower dynamics of the cell in the order of hours. They are more representative of the battery chemistry related to the diffusion processes in the electrolyte and active electrode material. All of these parameters are functions of the ambient temperature, electrolyte temperature T_{Cell} , SOC , and the battery current. The components of RC networks R_{TS} , C_{TS} , R_{TL} and C_{TL} are responsible for the short and the long-term transients in the battery internal impedance. Ideally this equivalent circuit should include two additional parallel loops to account for hysteresis phenomena of the battery. When the additional loops are included, both the short hysteresis and the long hysteresis behaviour of the battery can be predicted. These temperature effects were included in the mathematical model

presented by the equations (4) and (5) defined earlier. The parasitic behaviour of the capacitors which is considered to be minimal and hence it is being ignored in this model but could be included if and where necessary. Models of the hysteresis of the type discussed by Huria, Ludovici and Lutzemberger [32] and Windarko and Choi [33] could be easily included if and when necessary.

The self- discharging effect which is modeled by a loop containing V_{OC} source parallel with $R_{self}(T, n, SOC)$ as given by fig.1(a). Panday and Bansal [17] have presented a method and a formula for simulating the self-discharge current through the $R_{self}(T, n, SOC)$ in terms of the self-discharging current i_{s_D} through $R_{self}(T, n, SOC)$. There the parameter C_p is the initial battery capacity before storage. The symbol T signifies the variable temperature, R_{gas} is the gas constant and K_o is a reaction rate constant. The reaction rate is given by the Arrhenius equation in terms of T, R_{gas}, K_o and the activation energy, E_A and was used by Panday and Bansal [17].

However, as the resistance of $R_{self}(T, n, SOC)$ which is identified as R_{self} , is very high compared to $(R_{intS} + R_{CYC})$, and therefore the current passes through R_{self} can be taken as zero. Hence, we can neglect the voltage drop across the R_{self} resistor.

The effect of R_{intS}, B, C_{TS} , and C_{TL} due to the battery SOC can be calculated as given in [13] and expressed by the generic equation, (19):

$$R_{cg}(SOC) = C_{g1} \exp(-C_{g2}SOC) + C_{g3} \exp(C_{g4}SOC). \quad (19)$$

The capacitances are limited to small positive values when the SOC is zero. The constants C_{g1}, C_{g2}, C_{g3} and C_{g4} are presented in the Table II. The effect of the temperature on $R_{intS}(SOC, T)$ can be given by the polynomial and is defined as,

$$R_{intS}(SOC, T) = -1.399 \times 10^{-5} T^2 - 0.0002768 \times T + R_{intS-ref}(SOC). \quad (20)$$

In (20) the parameter $R_{intS-ref}(SOC)$ is the battery internal resistance at 0°C , $R_{intS-ref}(SOC) = 0.146$ for the Panasonic 17500 Li-Ion-battery with a nominal voltage of 3.7V for a discharge current of 830mAh , at 25°C and $SOC = 1$)

The SOC change due to temperature has been proposed by many researchers using Arrhenius equation, [17, 29]. According to experimental data available from Valerie, Johnson and Pesaran [28] and from He et al [34] it was noted that the SOC decreases with the increase of temperature and the simulation time. The SOC can decrease up to 50% from 100%, with the increase of temperature from 15°C to 60°C . It was also noted from the literature that SOC change can be taken as linear within the above temperature range. Experimental/simulation data shows that the temperature increase due to one hour discharge at (1C rate) is less than 0.2°C (Spotnitz [26]) and hence the variation due to simulation time can sometimes be neglected in modeling if the simulation time is one hour or less. Using experimental data from Zhu et al [35] and considering the SOC to be a maximum when the temperature is nearly ambient, a polynomial equation is proposed in this paper to calculate initial SOC due to temperature effect and is given by the polynomial equation (21):

$$SOC_{ini} = 1 - 0.000442(\Delta T + 0.714932)^2, \Delta T = T_{Cell} - T_{amb}. \quad (21)$$

From equation (3), assuming the inputs are slowly varying, it follows that the battery cell temperature T_{Cell} is related to the time by the equation:

$$T_{cell} = \frac{[i\{V_{bat} - V_{oc}\} + A\alpha T_{amb}]}{A\alpha} \left(1 - \exp\left(-\frac{A\alpha}{mC_p}t\right) \right). \quad (22)$$

Equation (13) was verified by fitting the simulation data with two exponential functions and it was found that one of them was indeed very slowly varying and

almost constant. The battery open circuit voltage, which is dependent on battery SOC can be calculated by using equation (23) as given in [13].

$$V_{OC0} = -1.031 \times \exp(-35 \times SOC) + 3.685 + 0.2156 \times SOC - 0.1178 \times SOC^2 + 0.321 \times SOC^3. \quad (23)$$

Battery internal resistance change due to cyclic effect is assumed to be given by the empirical equation, (24), as in [13]:

$$R_{cyc} = \zeta \times n^\lambda \quad (24)$$

In equation (24), n is the discharge/charge cycle number and ζ is a constant ($\zeta = 0.0015$). The constant λ is normally taken to be equal to $\frac{1}{2}$ according to [13]. The SIMULINK simulation diagram of the system shown in fig. 1(a), is shown in fig. 1(b) and includes all of the equations represented by (1)-(16) and (19)-(24).

V. FINAL NONLINEAR STATE SPACE 5-STATE MODEL EQUATIONS

The final nonlinear, 5-state, state space equations defining the dynamic battery model are summarized below.

i) Battery Current:

$$\dot{i} = w_1; \quad (17)$$

ii) State of Charge (SOC):

$$\dot{SOC} = i/kC_{bat} \quad (13)$$

iii) Fast & Slow Polarization Over-potential:

$$\frac{dV_j}{dt} = \frac{i}{C_{Tj}} - \frac{V_j}{R_{Tj}C_{Tj}}, j=1, 2. \quad (7)$$

iv) Cell Temperature:

$$\frac{dT_{Cell}}{dt} = \frac{1}{mC_p} [i\{V_{bat} - V_{OC}\} - A\alpha\Delta T], \quad (4)$$

v) Open Circuit Output Voltage:

$$V_{OC} = V_{OC0} + \Delta E(T) + \Delta V_{Che}(T) + v_n; \quad (18)$$

vi) Open Circuit Output Voltage without film & chemistry:

$$V_{OC0} = i(R_{ints} + R_{cyc}) + k * SOC + V_1 + V_2 + d; \quad (12)$$

vii) Voltage due to electrode film formation:

$$\Delta E(T) = (1 + C_{E1}\Delta T) \left. \frac{dVr}{dT} \right|_{T=T_{Cell}} \Delta T; \quad (6)$$

viii) Voltage due to electrolyte electron transfer chemistry:

$$\Delta V_{Che} = \beta K \exp^{(-1/t)} \Delta T + \left. \frac{dV_{che}}{dT} \right|_{T=T_{Cell}} (C_{Che} + C_{Che1}\Delta T)(1 + \beta)\Delta T. \quad (5)$$

VI. THERMAL MODEL COMPARISON WITH EXPERIMENTAL RESULTS

AT 25 °C

The experimental results published by Tan, Mao and Tseng [14] and Thanagasundaram et al [6] have been used in this paper to test and validate the model. The Li-ion TCL PL-383562, which has the capacity of 850 mAh is used to validate the model and the parametric constants generated by using the Panasonic 17500 Li-ion-battery is also used (as the nominal voltages are same).

The current pulse tests at discharging currents of 80, 160, 320 and 640 mA had been used. The nominal capacity (the average capacity) of the battery is 800 mAh \pm 5% at a discharge rate of 0.2A in 0.2C (5 hour discharge) and it was discharging at a temperature of 25⁰C with more than 300 cycles. The battery can be charged at a charge rate of 0.8A in 1C (1 hour charge). When discharging at 1.6A it will last 2

hours (0.5C). The manufacturers specify the charge cut off voltage as 4.2 V and the discharge cut off voltage as 2.75V. The results from the simulation of the proposed model are compared with the experimental results published by Chen and Rincon-Mora [15]. Fig. 2, 3 and 4 illustrate open-circuit voltage and the error variations of the battery parameters with the *SOC* at 750mA battery current. Percentage error was calculated for each graph by using the formula given by equation (25) which is embedded into MATLAB code and finally calculating the mean percentage error, which can be simply calculated by using MATLAB command.

$$Err(\%) = 100 \frac{(1 - (abs(V_{OC_sim} - V_{OC_Exp}))}{V_{OC_sim}} \quad (25)$$

The parameters V_{OC_sim} , and V_{OC_Exp} represents the data arrays of simulation results and the experimental results respectively. These comparisons confirm the validity of the new model and the responses within 98% of known experimental measurements.

From fig.3, the simulation and experimental data the percentage accuracy was 98.215%. Selected battery data is stated for reference: CC/CV charge at 4.2V, 1C +25⁰C and CC discharge at .2C to 2.75V; Nom. Volt.: 3.75, Nom. Capacity: 190mAh to 1800mAh, Max^m current: 1C; Max^m voltage: 4.2V.

The new model was tested for known experimental data, published by Thanagasundaram et al [6] and the the response calculated by using Matlab (and equation(25)) happened be within 98.7% accuracy (fig.4). The battery data used in [6] is as follows: Lithium Manganese Oxide Battery; nominal voltage 3.6CC: 750mA, nominal capacity 2200mAh.

VII. THE VARIABLE TEMPERATURE EFFECT: MODEL COMPARISON WITH EXPERIMENTAL RESULTS

Simulation and battery data results so far presented assumed that the temperature was constant during the time of simulation and the operating temperature was 25°C during the time of battery charging/discharging. The parameter values $R_{\text{int},S}$, R_{TS} , R_{TL} , C_{TS} , C_{TL} and SOC changes according to charging or discharging. They are assumed to be invariant with respect to charging or discharging Plangklong [27].

The Panasonic Lithium-ion batteries, CGR18650 and CGR17500 were chosen for this part of the simulations with temperature effect and the manufacturer's specifications are recorded for reference. The charge and discharge conditions of the batteries are also provided by Tan, Mao and Tseng [14], Chen and Rincon-Mora [15], and the handbooks [36] and [37]. For CGR18650: Charge Conditions: constant voltage/constant current, 4.2V, 910 mA (max), 2 hours, at 20°C as specified by the manufacturers. Discharge conditions: Constant current (CC) 260 mA. For CGR17500: Charge conditions: CV/CC, 4.2V, 550 mA (max), 2 hours, 20°C . Discharge Conditions: Constant current 780 mA. The specifications and experimental data from Tan et al [14] for Li-ion battery CGR17500 have been used in this model to validate the thermal and electrical model.

At high temperatures chemical reactions require less activation energy as the atoms can move faster. This will result in a higher cell voltage. However, optimum rate of reaction occurs between 38°C to 42°C . Increase in temperature beyond the optimum limit along with the ambient temperature can be detrimental to the battery life. Conversely, at low temperatures, intercalation and de-intercalation requires higher activation energy for the chemical reactions. In Li-ion batteries, this occurrence can cause less lithium ion participation in the cell mechanism resulting in temporary loss

of capacity. Fig. 5 shows the manufacturers' data and the new model simulation results with varying temperatures. Fig. 5(b) shows the battery discharge capacity versus the cell voltage with different constant ambient temperatures during the time of simulation and also with varying temperatures from -20°C to 60°C during the time of simulation which confirms the model as correct.

As it can be seen from fig.6, the simulation curves coincide with the experimental data plots and hence, the model can be validated as an accurate model which has both electrical and thermal properties. In addition, the experimental data reported in a NREL report which was presented by Valerie et al [28] where it was confirmed that at 40°C , the *OCV* is nearly the same as its value at the ambient temperature in addition to the information given in BU-Charging/discharging [31]. The reported data also conforms to the new simulations and the data plots as given by fig.6.

VIII. APPLICATION TO SOC ESTIMATION

It may be observed first the equations (17), (13), (7), (4) and (18) may be expressed as two decoupled sets of equations. Introducing the variable, $\Delta V_{OC} = V_{OC} - V_{bat}$, and using equation (12), equation (18) is expressed as,

$$\Delta V_{OC} = i(R_{ints} + R_{cyc}) + V_1 + V_2 + \Delta E + \Delta V_{Che} . \quad (28)$$

Equation (13) is now completely decoupled from equations (17), (7), (4) and (18).

To demonstrate a typical, novel application of the model, we describe briefly a typical application of the battery model to *SOC* estimation. Our aim is to use a simple extended Kalman filter and yet obtain results similar to those obtained with adaptive filtering or by using the unscented Kalman filter as has been done by He et al [34], Plett [38] and Tian et al [39]. Early reviews of *SOC* estimation based on measured

impedance data was presented by Rodrigues, Munichandraiah and Shukla [40] and by Piller, Perrin and Jossen [41]. A comparative study of various state estimation algorithms is presented by Barillas et al [42], Li et al [43] and Zou et al [44]. While an enhanced Coulomb counting method has been proposed by Ng et al [45], the current focus is on model based estimation as demonstrated by He et al [46] and Sun et al [47]. Xing et al [48] have included temperature effects in their model although it does not include temperature dynamics. Both real time (He, Xiong and Guo [49]) and adaptive estimation (Waag and Sauer [50]) have been pursued. To deal with the specific issues that arise with *SOC* estimation, a multi-model approach is proposed by Wang, Zhang and Chen[51], a dual time scale approach by Dai et al [52] as well as multi-scale approaches by Hu, Youn and Chung [53] and by Xiong et al [54] to Kalman filtering, have been proposed. Because, the model equations naturally decouple into two sets, a dual Kalman filtering approach has been proposed by Walder et al [55] based on the use of two decoupled Kalman filters which has since been improved by Campestrini et al [56] and Lee et al [57]. There have also been some novel applications of estimation to original battery configurations presented by Zhong et al [58], Pérez et al [59] and Fares, Meyers and Webber [60].

The estimation of SOC in this paper also exploits the decoupled nature of the model equations. It is based on the extended Kalman filter and is done by writing the model equations, (17), (7), (4) and (28) in the form:

$$\dot{i} = w_1; \tag{29a}$$

$$\dot{V}_{TS} = \frac{1}{C_{TS}} \left(i - \frac{V_{TS}}{R_{TS}} \right), \dot{V}_{TL} = \frac{1}{C_{TL}} \left(i - \frac{V_{TL}}{R_{TL}} \right), \tag{29b}$$

$$\frac{dT_{Cell}}{dt} = \frac{-1}{mC_p} [i\Delta V_{OC} + A\alpha\Delta T], \tag{29c}$$

$$\dot{R}_{TS} = w_2, \quad (29d)$$

$$\dot{R}_{TL} = w_3, \quad (29e)$$

$$\dot{C}_{TS} = w_4, \quad (29f)$$

$$\dot{C}_{TL} = w_5, \quad (29g)$$

where w_n , $n = 1, 2 \dots 5$ are Gaussian White noise disturbances of known intensity and ΔV_{OC} is given by equation (28). The measurement is given by, $\Delta V_{OCm} = \Delta V_{OC} + v_n$, where v_n is a Gaussian White noise disturbance of known intensity. Equations (29) and the measurement are used to estimate the current i and ΔV_{OC} initially. The estimated SOC is then obtained by integrating equation (13), which is expressed as,

$$\hat{SOC} = \hat{i} / kC_{bat}. \quad (30)$$

The equations are linearized so the methodology of the extended Kalman filter is applied at every step of the simulation. The extended Kalman filter has the predictor-corrector structure and corrects the estimate based on the innovation or new information in the measurement. It must be added that the estimation could be extended to the case when k and d are nonlinear functions of the state and need to be updated in real time.

The estimate of the SOC at the room temperature of 30°C is compared in the first of subplot of fig. 7 to the simulation over a time frame of 600 seconds and the error is less than 2%. Also shown in the second subplot of fig. 7, is a comparison of the estimated and measured V_{OC} . The estimate of the current \hat{i} based on an initial constant current input (discharging) of $i = -5$ amps is shown in fig. 8. All of the battery parameters necessary for the simulations were first calculated from the

manufactures data sheets. The estimate error is less than 0.02%. In this simulation the temperature was assumed to be a constant. Similar curves may also be obtained when the temperature is dynamically measured and filtered.

IX. CONCLUSIONS

In DC power source applications such as hybrid electric vehicles (*HEVs*), monitoring algorithms use current and voltage measurements to estimate the battery's *SOC* and available power. The literature says that the *SOC* change has no effect on the generation rate of the ohmic heat contributed by the contact resistance between electrode and current collector. The open circuit voltage and electrode surface concentration nonlinearities, film formation at electrodes, side reactions and the temperature effect cause dynamic modeling difficulties for real time applications. The new battery model presented here could provide satisfactory results and offer good solutions for many questions that simulation engineers face with. The decoupled approach to *SOC* estimation presented in the preceding section is a novel and unique feature of this paper and such a decoupled approach has not been used previously. It is currently being used in developing a real time *SOC* estimation methods based on both nonlinear unscented and extended Kalman filtering in order to explicitly demonstrate that the extended Kalman filter gives comparable results to the unscented Kalman filter in a real-time scenario. Thus the models developed in this paper are proving to be extremely useful both for simulation and estimation studies.

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