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Characterisation and Modelling Lithium Titanate Oxide Battery Cell by Equivalent Circuit Modelling Technique

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Abstract— Lithium Titanate Oxide (LTO) battery cells have immense potential as energy storage systems in large-scale stationary grid applications due to their better cycling performance, lower self-discharge and higher safety margins compared to other Lithium based battery chemistries. Hence, accurate LTO performance models at various operating conditions are required for different purposes like determination of their dynamic behaviour, modelling LTO's suitability to an application as well as to the development of battery and energy management systems (BMS and EMS). LTO battery cell performance is mainly affected by parameters such as, state of charge (SOC) and temperature. Hence, in this paper, second order equivalent circuit model (ECM) of an LTO cell will be developed based on their experimental characterisation at different SoC's (every 10% intervals) and temperatures (15 °C, 25 °C, 35 °C and 45 °C). Modified version of the Hybrid pulse power characterisation (HPPC) test method will be utilised for parametrisation of the ECM of 2.9 Ah LTO cell. The simulation model will be developed in Matlab/Simulink platform and compared with the laboratory measurements for ECM validation.

Keywords—Lithium-ion battery; cell characterization; equivalent circuit models;

I. INTRODUCTION

Battery energy storage systems (BESSs) have established their credibility for various applications, especially in land-based grid-scale energy storage and electro-mobility [1]. Lithium-ion (Li-ion) batteries have been the forefront electrochemical energy storage technology in the recent times for increased deployment of BESSs for grid applications due to their current economic viability and technological superiority [2–4].

Li-ion battery working mechanism is based on subsequent redox reactions in closed state, where its voltage and current values are measurable parameters [5]. These measurements are used to monitor the battery performance and estimate other parameters such as State-of-Charge (SOC) and state-of-health (SOH). Hence, Li-ion batteries should be characterised in different conditions that affects its performance and develop their working models in detail. Development of accurate Li-ion battery models are important and used multiple reasons (simulation studies to hardware controller development) such as,

- Development of state-of charge (SOC) and SOH algorithms [6–8]
- Development of effective battery management system which manages the overall operations of any battery system (i.e. from electric vehicles to grid storage applications) [5], [9]
- Design and development of BESS grid-side controllers (i.e. their DC/DC and DC/AC voltage source converters' control optimisation) [10], [11]
- Optimal utilization of Li-ion ESSs in power system planning studies including their techno-economic analysis [3], [12]

Nickel-Manganese-Cobalt (NMC) and Lithium-Ferrous-Phosphate (LFP) cathode type Lithium-ion batteries have been widely used for energy storage applications due to their superior performance characteristics in terms of lower rate self-discharge, higher energy and power densities[13]. However, their peak power capability for short bursts of load currents, typically seen in land-based grid applications such as mitigating frequency fluctuations in active network management (ANM) solution are limited (due to maximum their maximum discharge capability of less than 5C discharge rate).

Lithium-Titanate-Oxide (LTO) anode type Li-ion battery has been gaining prominence in recent times for various energy storage applications in power grids, mainly due to their formidable power density [14]. Table 1 provides short comparison on performances of different Li-ion battery chemistries. LTO battery cells are capable of providing continuous higher charging and discharge rates, which are close to ten times their nominal discharge rate (i.e. 10C), in comparison with other chemistries, where it can support upto 5C rates at short pulse intervals. Therefore, the power capability horizon of the LTO battery packs are suitable for utilisation in land based grid application whose requirement poses higher ramp rates and short burst of higher power needs.

Hence, in this paper LTO battery cell has been characterized to evaluate its performance at different temperatures and SOC by developing an equivalent circuit model (ECM) battery model in the process. Developed ECM model will be used for studying the capability of LTO battery cells for land-based grid applications. Proposed ECM and their methodology are explained in detail in section II.

Table I. Comparison of Li-ion cell characteristics [15]

Cell Chemistry	Nominal Voltage (V)	C-rate capability	Energy Density (Wh/Kg)	Cycle Life
NMC	3,60	~ 5C (short burst)	110-170	2000-3000 at 80% DoD
LFP	3,3	~ 5C (Continuous)	90-115	more than 3000 at 80% DoD
LTO	2,2	>10C (Continuous)	60-75	more than 5000 at 100% DoD

Section III explains the parameterisation method to obtain ECM parameters and section IV provides details on the experimental setup. Performance of the developed simulation model and their validation is explained in section V and the conclusion for this work is presented in section VI.

II. LTO ECM - PROPOSED METHODOLOGY

Modelling dynamic behavior of Li-ion battery cell (including LTO type cell) is complex considering their highly non-linear performance, which further is affected by various parameters such as temperature, current rate, SOC and aging.

Li-ion batteries when utilised for power system studies are modelled as an ideal DC [16] or by using empirical/math-based models [17],[18]. Another common technique used is kinetic battery models (KBM) [19], which was first used to represent lead acid batteries. Most of the recent literature uses modified KBMs [20–22] for stationary grid applications. KBMs perform well at certain defined conditions, but cannot address the non-linear performance characteristics of Li-ion batteries, that are influenced by various SOC, temperature, current rate and age. Most accurate battery models are provided by physics based model solved by Finite element model based simulation methods [23]. However, they require enormous computing power to simulate, making it practically impossible to be used for grid integration studies. Different approaches have varying ranges of computational complexity and accuracy with mathematical models providing least of both. Equivalent circuit models (ECM) represent operation of a battery cell in terms of variable resistors and capacitors, whose circuit parameters are determined by means of characterization tests [24]. ECMs are considered as a trade-off between mathematical and electrochemical models due to their performance metrics.

ECMs provide good accuracy and low computational effort, making them suitable for studies pertaining to stationary grid applications. Second order equivalent circuit model (SOEC) technique, based on Thevenin's circuit model represents Li-ion battery in form of resistances and capacitances[6], there by portraying battery operation comprising of processes such as diffusion, solid electrolyte interface and charge transfer [11]. However, it needs to be developed in detail testing the battery cells at different operating conditions, details of which are discussed below and forms the scope of this paper.

Fig. 1 shows the proposed dynamic SOEC for the LTO cell. The SOEC parameter values will be calculated by means of hybrid pulse power characterization (HPPC) tests performed different operating conditions (i.e. SOC and temperatures). Next step is to parameterize the ECM elements described in the following section.

III. PARAMETERISATION PROCESS

Open Circuit Voltage (OCV) is the voltage seen between the battery cell terminals at no-load conditions in equilibrium state. OCV has been modelled as an ideal voltage source in

this paper, where its values are variable at different SOCs and temperatures. OCV is captured from the HPPC test profile at the end of each rest phase after the high current charge/discharge pulse, i.e. when the voltage has attained a steady state value. Other parameters of the SOEC model are evaluated by analysing the voltage response of HPPC pulse discharge and charge.

The internal resistance was modelled as R_i . Two RC combinations will be used in this for study for LTO battery cell, so the dynamic behavior is modelled as R_1 , C_1 , R_2 and C_2 . The hysteresis effect and polarization effect in the Li-ion cells can be simulated accurately enough with the two RC combinations and the model structure is simpler than with more RC combinations. As the actual behavior of the LTO cells are significantly non-linear, all the parameters vary with SOC and temperature of the cell. Therefore, the ECM parameters (i.e. OCV, R_i , R_1 , C_1 , R_2 and C_2) are evaluated from HPPC tests of LTO battery cell at various SOC's (0% to 100% with a step change of 10%) and temperatures (15°C, 25°C, 25°C and 45°C), details of which are explained below.

The experimental testbed for battery characterisation testing is shown in Fig 2. Fig 3 shows the HPPC current profile used to characterize the LTO cells. Its corresponding voltage response is shown in Fig 4. Equivalent circuit parameters are calculated from the voltage response of the high current discharge pulse at every defined SOC and temperature. A closer view of the voltage response from the HPPC profile at discharge pulse is applied. R_i is calculated as a function of ΔV_0 by (1), which is contributed by resistance of active 80% SOC and 25 °C can be seen in same figure. It shows voltage drop (ΔV_0) at the instant when the high current material, electrolyte, and current collector. It can be also observed that there are time varying voltages (ΔV_1 and ΔV_2). Therefore, the equivalent circuit parallel branch resistances, R_1 and R_2 are calculated as a function of ΔV_1 and ΔV_2 , respectively by means of (2) and (3). The two RC branches are divided on the basis of short (t_1) and long (t_2) time transients, which is helpful in calculating C_1 and C_2 by (4) and (5) respectively. (6) represents the terminal voltage of the battery cell, which is a function of all the equivalent circuit parameters.

The HPPC parameterization process has to be repeated at every step of temperature to obtain the variable values of SOEC parameters. Hence, a Matlab script is developed to extract the measurements of HPPC tests, particularly the voltage response of high current charge/discharge pulses at every step of SOC and repeated for all the HPPC curves (i.e

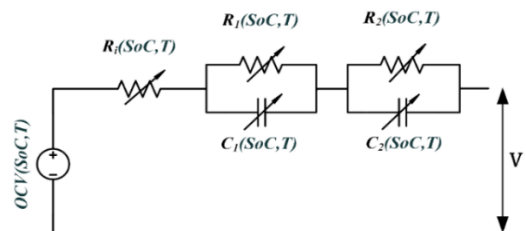


Fig 1. Proposed equivalent circuit model.

$$R_i = \frac{\Delta V_0}{I} \quad (1)$$

$$R_1 = \frac{\Delta V_1}{I} \quad (2)$$

$$R_2 = \frac{\Delta V_2}{I} \quad (3)$$

$$C_1 = \frac{t_1}{R_1} \quad (4)$$

$$C_2 = \frac{t_2}{R_2} \quad (5)$$

$$V(t) = OCV + I(t)R_i + I(t)R_1 \left(1 - e^{-\frac{t}{t_1}}\right) + I(t)R_2(1 - e^{-\frac{t}{t_2}}) \quad (6)$$

15°C – 45°C experiments). In order to obtain parameters for the two RC parallel branches in the SOEC, the 10 second pulse response is divided into two more time points, where t_1 represents the short-transient and t_2 represents the long transient responses. Therefore, knowing the values of t_1 and t_2 , the SOEC parameters are calculated from (1)-(5) to get the initial estimates. Initially calculated values at different SOC's and temperature are then normalized by using *lsqfit* in Matlab, which provides least squares fitting methodology for non-linear data.

3-dimensional response showing the evolution of SOEC parameters with respect to SOC and temperature shall be observed in Fig. 5. Values of R_i , the internal resistance of the cell calculated by the voltage response ΔV_0 is shown in 4(a), where it increases with SOC and decreases with temperature. Parameter evolution of R_1 and C_1 denoting the fast transient response of the SOEC model, which is derived from the voltage response, ΔV_1 and t_1 , is shown in Figs 4(b)-(c). Charge transfer process in the Li-ion battery has a fast transient response. Hence, the first RC in the SOEC is assumed to portray the charge transfer process. Parameter evolution of R_2 and C_2 denoting the slow transient response of the SOEC model is shown in Figs 4(e)-(f). The second RC branch whose values are obtained from ΔV_2 and t_2 , is assumed to depict the diffusion process of the battery cell. OCV-SOC evolution at different temperature is depicted in Fig 4(f).

SOC is estimated by using coulomb counting method (CC) [25]. CC method provided the best accuracy with minimal computational effort in an environment where the measurement noise was minimal [26], such as measurements from battery cyclers. Hence, the SOC calculation from the CC method has been considered as the reference value in this study. The experimental setup used to conduct various characterization tests and the details of the HPPC test to obtain the SOEC parameters are described in Section 3.

IV. EXPERIMENTAL SETUP

The test setup (Fig.2) consist of Neware BTS8000 battery cell tester with 4 testing channels rated at 5V and 300A (detailed specs in Table II). The cell-under-test (CUT) will be placed in the thermal chamber which is capable of operating at temperatures from -10 °C to +90 °C. Experiments are developed and controlled by the control station and the data will be saved in the data server.

HPPC test, a modified version of the standard test defined in PNGV manual, will be induced to the CUT (2.9 Ah LTO cell) at different temperature (15°C – 45°C) and at different SOC levels (10% intervals), Before the HPPC test, the battery cell is fully charged in constant-current-constant-voltage (CCCV) mode at 1C followed by resting the battery to obtain equilibrium. Then followed by high current charge and discharge pulses in the below order,

1. It is then discharged for 10s at 3C rate
2. Rest for 40s Charged for 10s at 3C rate
3. Charged for 10s at 3C rate
4. Discharge at 1C until next SOC step
5. Steps 1-4 are then followed until 0 % SOC

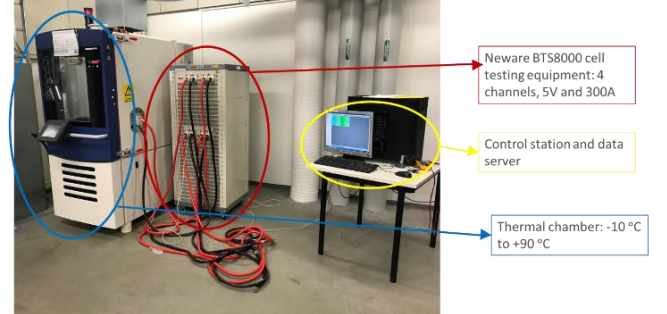


Fig 2. Experimental test setup for battery characterization

Table II. Neware BTS 8000 specifications

Number of Channels	4
Voltage and current measurement	Yes
Charging current (A)	1 to 300
Discharging current (A)	-1 to -300
Operating Voltage (V)	+5 to 0
Data acquisition rate (Hz)	10

V. MODEL VALIDATION AND RESULTS

The proposed SOEC cell model has been developed in Simscape platform of Matlab/Simulink. SOEC simulation model was developed by using the ECM parameters generated by the Matlab script at different SOC and temperature points. LTO battery cell model was simulated with same current profile used to run perform HPPC tests.

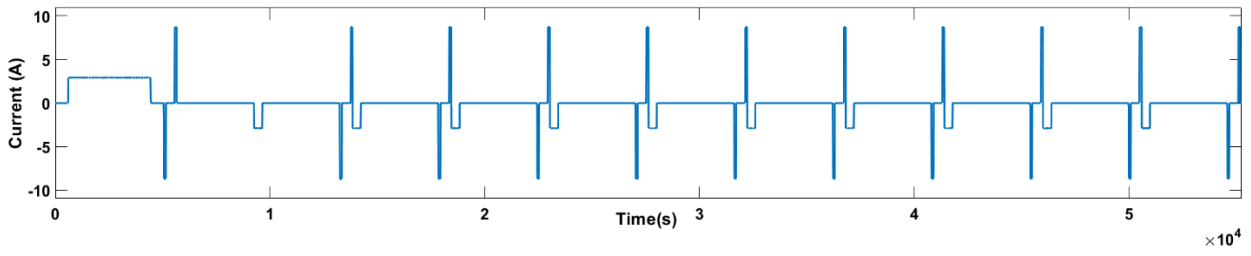


Fig 3. HPPC Current Profile

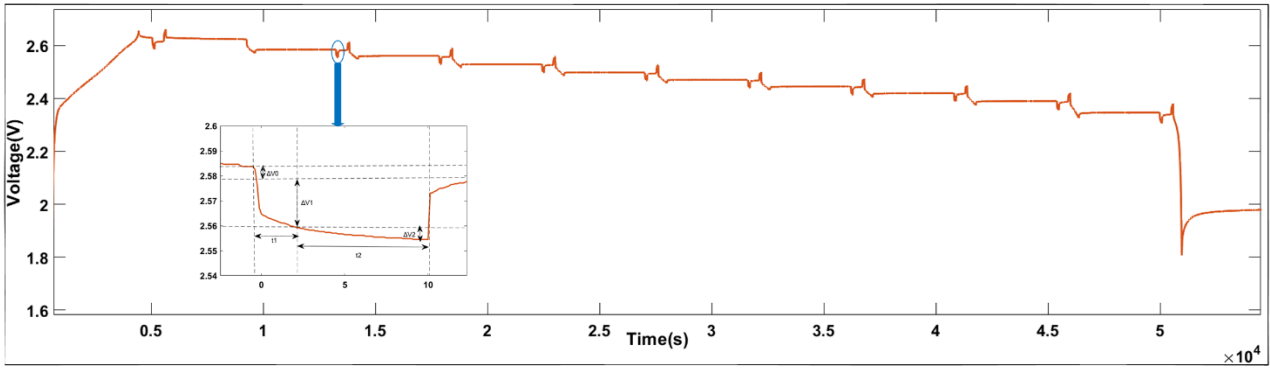


Fig 4. HPPC Voltage response

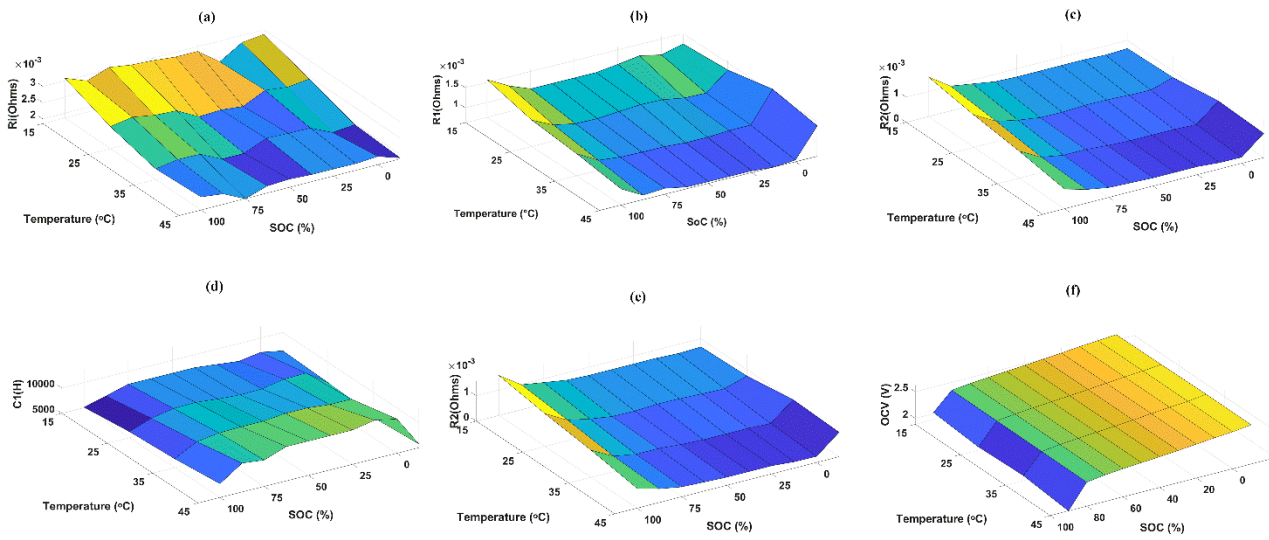


Fig 5. ECM parameters at different temperature and SOC

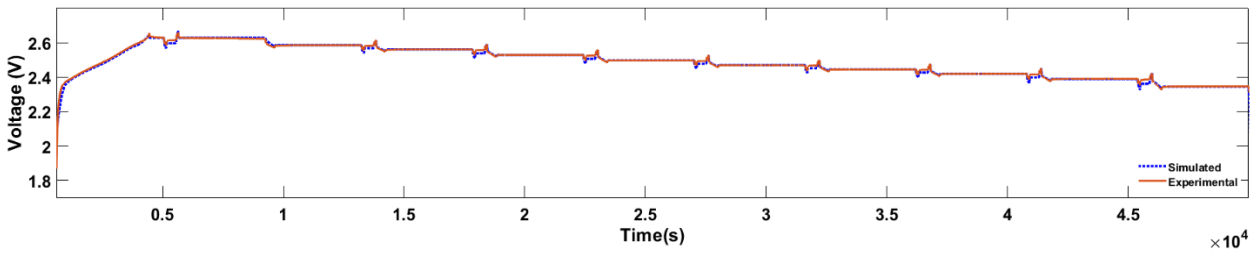


Fig 6. SOEC model performance in comparison with experimental curve at 35 °C

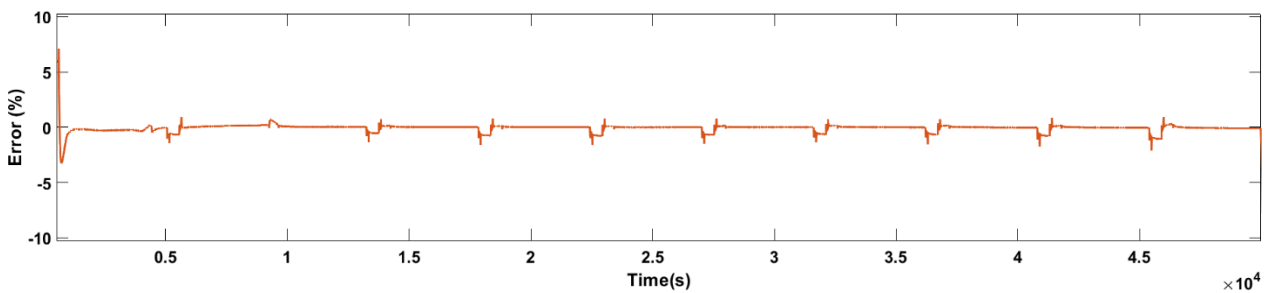


Fig 7. Comparison of error percentages at 35 °C

Fig. 6 shows the comparison between simulated voltage curve and measured voltage measurement at 35°C. It can be observed that the simulated voltage curve almost superimposes the experimental curve, there by validating the efficiency of the developed method. Fig. 7 shows the modelling error for 35 °C simulation results. The key observation from this result is that the SOEC model captures the dynamic non-linear voltage response of the cell very well with an error of almost 0% during steady state charge/discharge operations and approximately less than 2% error for the high current pulse profiles from 10% SOC to 100% SOC.

Nevertheless, the model accuracy is reduced at SOC's less than 10% which gives about 5% error. At very low SOC's, the cell seems to behave in a different way. It can also be observed that the accuracy error is about 5% when the voltage changes occurs during changeover from discharge/charge current. The results for different temperatures, i.e 15°C, 25°C and 45°C are similar in nature, i.e. their accuracy is slightly reduced nearer to the lower SOC region.

VI. CONCLUSION

This work aims to establish an extensive SOEC model for the LTO type lithium-ion battery cell considering SOC (0 to 100%) and temperature (15°C, 25°C, 35°C and 45°C) as the parameters affecting its performance. The simulation model has been developed with the objective of utilising it for multiple purposes for land-based grid applications mentioned earlier. The developed simulation model was validated by comparing its performance with the experimental curves. It was found that the developed model worked exceptionally well (error less than 2%) except for its reduced accuracy at lower SOC (i.e. last 10% of SOC). The possible solutions to mitigate this error could be by changing the structure of the SOEC model at very low SOC's or the improvising the method of obtaining the ECM parameters. Another probable issue may be due to be CC method to calculate the SOC. Better SOC estimation methods such as Kalman filtering techniques may improve the SOC prediction accuracy and hence the overall model performance. Therefore, detailed investigation on improving the current LTO battery cell model forms the basis for future studies.

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