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Battery digital twin: State of Charge and State of health estimation of LTO battery storage

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ABSTRACT

Battery storage is one of the key technologies in the transition toward net zero. Technology is quickly developing toward making energy grids digital. It is important to observe the condition of the battery in real time. A digital twin of battery storage is a virtual replica of a physical battery, which estimates and analyses battery operation and its state in real time. A battery digital twin consists of data collection, pre-processing, parameter estimation, modelling, and forecasting of the state of charge and state of health of the battery. This paper presents the concept and development of a digital twin for a lithium titanium oxide battery using a physics-based and data-driven model. A physics based Thevenin equivalent circuit model was developed. Experimental data from a lithium titanium oxide battery was collected from a robot application to analyze. Experimental data was used in a model-based state estimation approach of the Kalman filter for the state of charge estimation of battery storage. The state of health of the battery was estimated by the estimation of a decrease in total cell capacity and an increase in equivalent series resistance. The least square method was used to estimate total cell capacity. Equivalent series resistance was estimated using experimental voltage and current data. The output terminal voltage of the model is found to be well compared with experimental data.

Keywords: Lithium titanium oxide battery, Kalman filter, cell capacity, terminal voltage, cell current

NOMENCLATURE

Abbreviations	
DT	Digital twin
LTO	Lithium titanium oxide
OCV	Open circuit voltage
SOC	State of charge
SOH	State of health
WLS	Weighted least square method
Symbols	
A, B, C, D	State space model parameters respectively
i, v	Current and voltage respectively
L	Kalman gain
R, C	Resistance and capacitance
Q	Cell capacity
z_p, z_e	Predicted and estimated SOC respectively
$v_{T,p}$, v_T	Predicted and true terminal voltage respectively
$\sum z$, $\sum z_e$	Predicted and estimated error covariance respectively
$\sum_p$, $\sum_s$	process and sensor noise covariance respectively
τ	Time constant
η	Coulombic efficiency
α	Forgetting factor

1. INTRODUCTION

Battery technology has a crucial role in the development of the energy sector. Battery technology assists the transition towards net zero using various renewable energy technologies such as wind and solar. The current state of battery storage for grid applications exhibits significant progress, offering grid operators valuable tools to manage electricity supply and demand effectively. These systems are increasingly adept at storing renewable energy, improving grid stability, and providing backup power during outages. Nonetheless, several limitations persist. There is considerable research addressing the limited energy density and relatively high costs of advanced battery technologies, along with challenges associated with the recycling and disposal of battery materials. Additionally, grid integration is

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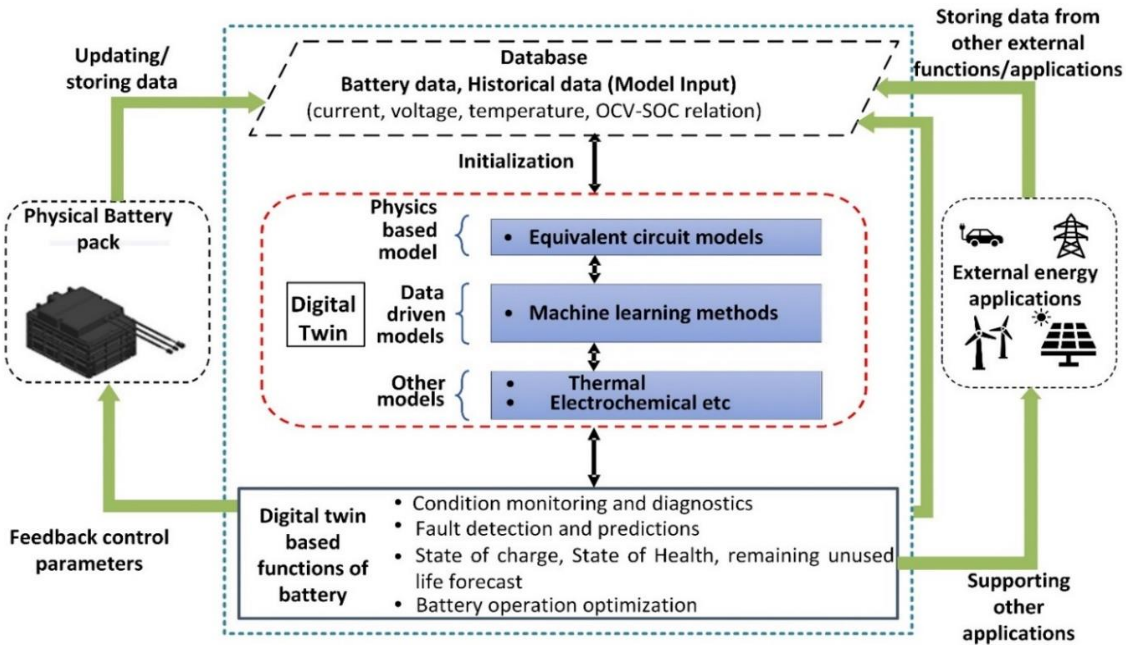

Fig. 1. Architecture of Battery digital twin

necessary to ensure maximize the advantages of grid-connected batteries. Ongoing research and development efforts are essential to address these shortcomings and optimize battery storage for grid applications [1–4]. The key challenge to using battery technology is to provide energy efficiently to various grid applications such as frequency response[3–6].

A Digital twin (DT) is a virtual replica of a physical object or system that replicates its dynamic behaviour in real-time using physics-based and data-driven models. A Battery DT is a digital replica of a physical battery, which attempts to replicate battery operation in real-time and forecast its state.

Fig. 1 shows the concept of battery DTs. For a battery DT, battery historical data and operational data are required, such as cell voltage, electrical current, and operating temperature, which need to be measured using sensors and stored in a database. Physics-based models consist of electrochemical models, equivalent circuit models, and thermal models of battery systems. Various data-driven models consist of regression, machine learning, and artificial intelligence. Database links to DT-based physics-based and data-driven models. Using DT not only physical batteries will be synchronized with the DT function, but it also connects to the various external energy-based applications as shown in Fig. 1. Updated parameters of the physical battery need to be stored in the database and use as input to the DT[4,7–9]. In this research work, the preliminary modelling of battery storage is discussed using physics-based and data-driven least square models[1]. Highlights of this research as are follows:

- An equivalent circuit model (Thevenin model) was used to represent the battery system's electrical behaviour. Thevenin model is an equivalent circuit model of a battery that uses one equivalent series resistance (R_0) and one parallel RC circuit with resistance (R_1) and capacitance (C_1) to replicate the dynamic properties of batteries[1].
- Experimental current and voltage data of the LTO battery were used to estimate parameters for the Thevenin model[1].
- Model-based state estimation using a Kalman filter was used for the SOC estimation of battery storage[1].
- Using the experimental dataset of the LTO battery and estimated SOC, weighted least square (WLS) regression was used to estimate the total cell capacity of the battery[1].
- Equivalent series resistance was estimated using LTO battery voltage and current data[1].
- Output terminal voltage was analyzed and validated.

2. METHODOLOGY

2.1. Equivalent circuit model of battery storage.

An equivalent circuit model (Thevenin model) of lithium titanium oxide (LTO) battery was used in this research work as shown in Fig. 2 This model is used to simulate the transient behaviour of an LTO battery cell

[1,10]. The terminal voltage of the Li-ion cell was defined by equation 1 [11].

$$v(t) = OCV\big(z(t)\big) - v_{c_1}(t) - i(t).R_0 \tag{1}$$

Voltage drops across the R-C parallel circuit are,

$$v_{c_1}(t) = v_{R_1}(t) = R_1 i_{R_1}(t) \tag{2}$$

Where v is terminal voltage, OCV is open circuit voltage, z is SOC of the cell, v_{c_1} is voltage drop across capacitor C_1, i is cell current R_0 is equivalent series resistance(Internal resistance), v_{R_1} is the voltage drop across the resistor R_1 and $i_{R_1}$is current passing through the resistance R_1[1,10].

$$v(t) = OCV\big(z(t)\big) - R_1 i_{R_1}(t) - i(t).R_0 \tag{3}$$

Resistor current i_{R1} is calculated by

$$i_{R_1}(t) = exp\left(\frac{-\Delta t}{R_1 C_1}\right) i_{R_1}(t) + \left[1 - exp\left(\frac{-\Delta t}{R_1 C_1}\right)\right] i(t) \tag{4}$$

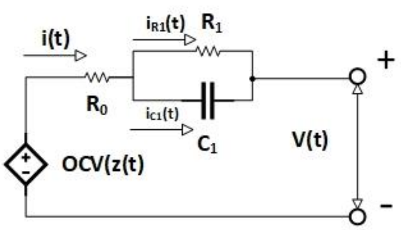

Fig. 2. Thevenin model proposed for LTO battery

2.2. Experimental data from an LTO battery cell

A DT for battery storage was developed using a large dataset of experimental LTO battery operation data from a robot application. Data was available per second for the period whenever the robot was booted. The battery is subjected to a multiple-charge discharge cycle for 32 hours of operation in 2.5 months. On each robot, LTO cells were used [12]. Fig. 2 depicts the cell current for an LTO battery cell. The terminal voltage of the cell to the corresponding dataset is shown in Fig. 3. Firstly, the battery is subject to charge at 4 amperes from 2.15 V to 2.64 V. Furthermore, the battery is subjected to multiple charge-discharge cycles as shown in Fig. 3 and Fig. 4. The first 2 discharge-charge cycles are considered to estimate equivalent circuit model parameters as shown in Fig. 5. Estimation of equivalent series resistance (R0), resistance (R1) and capacitance (C1) from RC parallel circuit is carried out based on experimental cell voltage data based on voltage drop and time constants as defined in Fig. 5. Equivalent series resistance was estimated by calculating instantaneous voltage drop divided by cell current whereas R1 and C1 were estimated using tome constant(R1C1) and voltage recovery as shown in fig. 5.

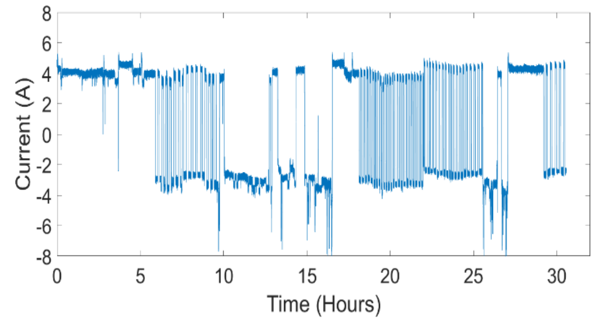

Fig. 3. Experimental data for cell current

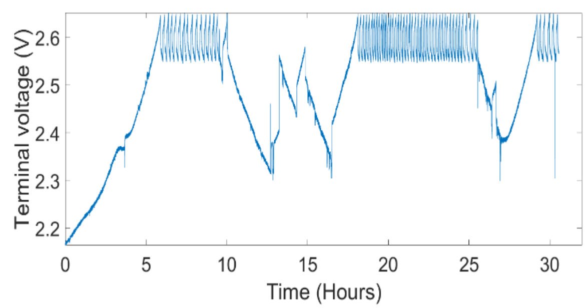

Fig. 1. Experimental data for terminal voltage

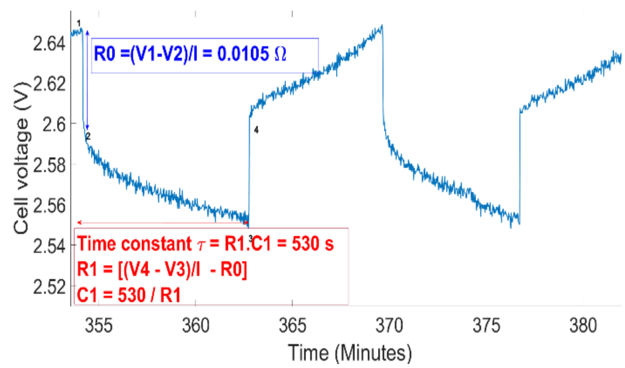

Fig. 5. Parameter estimation

2.3. OCV vs SOC Relation

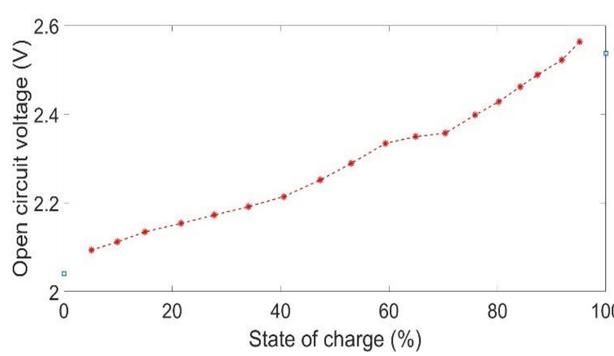

Fig. 6. Open circuit voltage and SOC relation

For SOC estimation of LTO battery cells, OCV-SOC relation plays a crucial role. In the voltage-based method

OCV is estimated and using the lookup table for OCV vs. SOC, the state of charge needs to be estimated whereas this relation is required to get an output equation parameter of the Kalman filter as well. Fig. 6 shows the relation between OCV and SOC of LTO battery storage [11].

2.4. SOC estimation

There are several methods used by researchers for SOC estimation such as the voltage-based method and coulomb counting method[1,9,13,14]. For a more accurate estimation of SOC, the Kalman filter is used. The Kalman filter is an optimal recursive algorithm that combines system dynamics and measurement data to estimate the true state of a system while accounting for noise and uncertainties. Kalman filtering (KF) is a state estimation algorithm based on a prediction-correction approach that estimates the SOC of the cell by using the state equation and output equation, with the cell's current as input and terminal voltage as output. The Kalman filter is widely used for SOC measurements, and provides an optimal estimate of the true SOC, considering noise and uncertainties. Its real-time capabilities and adaptability to changing conditions make it a popular choice for accurate SOC estimation, benefiting battery management and energy storage utilization. The SOC of the battery cell was estimated using the following equation[1,10,13,14].

$$z_{k_2} = z_{k_1} - \frac{1}{Q}\sum_{k=k_1}^{k_2-1} \eta[k]i[k] \qquad (5)$$

The value of the SOC needs to be initialized first. Kalman filter is divided into 2 major steps prediction and correction steps. Each step includes 3 sub-steps as follows. [1,15]

Step 1a: SOC prediction time update

$$z_p(k) = A.z_e(k-1) + B.i(k-1) \qquad (6)$$

Step 1b: Error covariance time update

$$\Sigma z(k) = A.z_e(k-1).A^T + \Sigma_p \qquad (7)$$

Step 1c: Predict terminal voltage.

$$v_{T,p}(k) = C.z_p(k) + D.i(k) \qquad (8)$$

Step 2a: estimator (Kalman) gain matrix

$$L(k) = \Sigma z(k).C[C.\Sigma z(k).C^T + \Sigma_s]^{-1} \qquad (9)$$

Step 2b: SOC estimates measurement update.

$$z_e(k) = z_p(k) + L(k).(v_T(k) - v_{T,p}(k)) \qquad (10)$$

Step 2c: error-covariance measurement update

$$\Sigma z_e(k) = (I - L(k).C)\Sigma z(k) \qquad (11)$$

2.5. SOH Estimation

Apart from accurate SOC monitoring of SOC, one of the key factors to consider for battery DTs is the degradation of the battery cells. The battery SOH shows battery degradation and residual capacity of the battery due to chemical reactions, cycling, and many more electrochemical parameters [1,16]. Capacity fade was estimated by the following equation.

$$SOH_Q = \frac{Current\ cell\ capacity\ (Q)}{Initial\ capacity(Q_0)} \qquad (12)$$

The SOC of the battery cell

$$z_{k_2} = z_{k_1} - \frac{1}{Q}\sum_{k=k_1}^{k_2-1} \eta[k]i[k] \qquad (13)$$

$$(z_{k_2} - z_{k_1})Q = -\sum_{k=k_1}^{k_2-1} \eta[k]i[k] \qquad (14)$$

By rearranging the equation, a linear equation of y = Qx is formed where with a regression method total cell capacity was estimated. To estimate total capacity, Q for y =Qx using the need to measure N -vectors of measured data x_i and y_i which links to battery from a cell over time interval i, where x_i is the change in state-of-charge over that interval [1]

$$x_i = z_{k_2} - z_{k_1} \qquad (15)$$

y_i is the net accumulated ampere hours passing through the cell during that period.

$$y_i = \sum_{k=k_1}^{k_2-1} \eta[k]i[k] \qquad (16)$$

Store measured value of (x_i,y_i) and using the WLS method, the total capacity of the cell was estimated. Various steps for least square methods are as follows:[1]

Estimate weighted-least-squares (WLS) cost function.

$$\chi^2_{WLS} = \sum_{i=1}^{N} \frac{(y_i - Y_i)^2}{\sigma_{yi}{}^2} = \sum_{i=1}^{N} \frac{(y_i - \hat{Q}x_i)^2}{\sigma_{yi}{}^2} \qquad (17)$$

minimize weighted-least-squares (WLS) cost function.

$$\frac{\delta\chi^2_{WLS}}{\delta\hat{Q}} = -2\sum_{i=1}^{N} \frac{x_i(y_i - \hat{Q}x_i)}{\sigma_{yi}{}^2} = 0 \qquad (18)$$

$$\sum_{i=1}^{N} \frac{x_i y_i}{\sigma_{yi}{}^2} = Q\sum_{i=1}^{N} \frac{x_i{}^2}{\sigma_{yi}{}^2} \qquad (19)$$

Each time a new data pair (x_i,y_i) is available, compute

$$c_1 = \sum_{i=1}^{N} \frac{x_i{}^2}{\sigma_{yi}{}^2} \quad ; \; c_2 = \sum_{i=1}^{N} \frac{x_i y_i}{\sigma_{yi}{}^2} \qquad (20)$$

Estimate Total cell capacity.

$$\hat{Q} = \frac{c_2}{c_1} \qquad (21)$$

Similarly, Power fade is a decrease in a battery's ability to deliver output power due to a rise in internal resistance (R0). Discharge power is computed by setting the cell terminal voltage to v_{min}. As internal resistance R_k increases over time, output power decreases.[1]

$$SOH_R = \frac{R_{present} - R_{Beginning\ of\ life}}{R_{End\ of\ life} - R_{Beginning\ of\ life}} \qquad (22)$$

The value of R_0 at the beginning of life is usually available from the manufacturer description whereas R_0 at the end of life is assumed to be 1.5 to 2 times R_0 at the beginning of life[1]. To estimate R0 terminal voltage was measured and current from the battery. The terminal voltage of the cell was estimated by

$$v[k] = OCV[z(k)] - i[k].R_0 \qquad (23)$$

$$v[k-1] = OCV[z(k-1)] - i[k-1].R_0 \qquad (24)$$

Subtracting equation 24 from rquation 23

(Neglecting changes in OCV value because cell SOC z_k changes relatively slowly compared to how quickly i_k changes)

$$v[k] - v[k-1] \approx (i[k-1] - i[k])R_0 \qquad (25)$$

$$R_0 \approx \frac{v[k] - v[k-1]}{(i[k-1] - i[k])} \qquad (26)$$

R_0 estimation of the LTO cell was done using the above equation for the LTO current and voltage dataset. Furthermore, the estimated equivalent series resistance (Internal resistance) signal is filtered using the one-pole digital filter.

$$R_{0,k,filt} = \alpha\ R_{0,k-1,filt} + (1-\alpha)R_{0,k} \qquad (27)$$

3. RESULTS AND DISCUSSIONS

3.1 Terminal Voltage

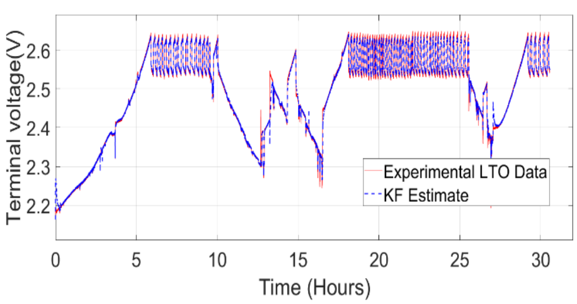

Fig. 7. Model results terminal voltage comparison with experimental data.

Physics-based models, Kalman filter and WLS models are discussed in previous sections for battery modelling, SOC, and SOH estimation. Based on the experimental dataset, battery parameters were estimated and used in the models. Voltage response to the input current profile from Fig. 3 and Fig. 4 is estimated and compared with experimental data in Fig. 7. Figure shows model results of terminal voltage are found to be compared well with experimental LTO battery data.

3.2 State of charge

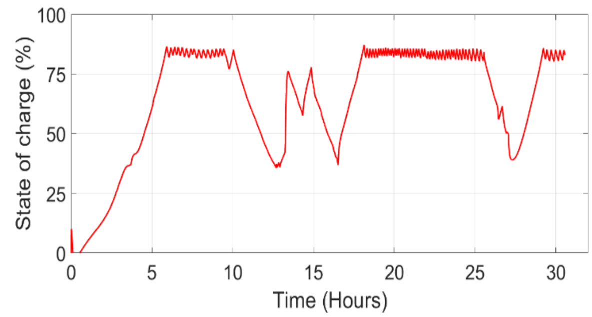

Fig. 8. State of charge

In section 2.3 Kalman filter is discussed for SOC estimation of the battery. For the given input current to state space model of Kalman filter SOC of LTO is estimated as shown in Fig. 8. Battery is operated between SOC range of 0 % to 90%. Estimated SOC is considered for capacity estimation using the WLS method described in section 2.5.

3.3 Cell Capacity

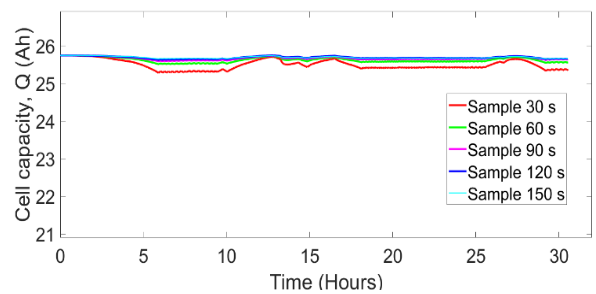

Fig. 9. Battery cell capacity

WLS regression technique is discussed for total cell capacity estimation of LTO cells. Since data collection from the robot was random whenever the robot was booted, due to lack of battery cycling data, a timestep independence study was done by considering various sample times for capacity estimation.

3.4 Equivalent series resistance/ Internal resistance

As described in section 2.5, the power fade of the battery depends on the rise in internal resistance(R_0). Fig. 10 shows the estimated R_0 and filtered value of R_0 using one pole digital filter. During the initial operation of the battery, R_0 value is around 0.0105Ω. over the operation of 32 hours, a slight rise was observed in internal resistance to 0.125Ω. Due to noisy data, some rise and fall in R_0 estimation was observed since the model covers all major changes in cell current during the charge and discharge of the battery.

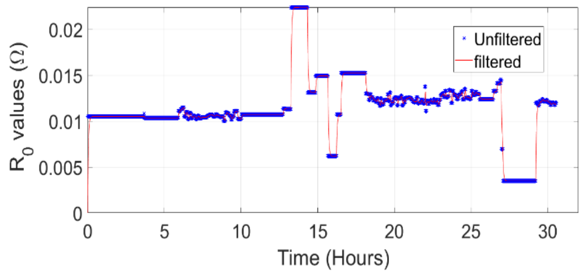

Fig. 10. Internal resistance R_0

In future work, a major focus will be on battery pack integration for battery storage and battery management systems. In this study, model parameters were estimated from real-world data which is a complex task due to factors like temperature and battery variations. While the Kalman filter method was used for estimating battery SOC and the WLS method for SOH estimation, the next challenge is to integrate this model for a large-scale battery pack for power system applications.

4. Conclusion

In this paper, an outline of the battery DT of a LTO battery is discussed. A physics-based Thevenin equivalent circuit model is developed. The experimental dataset of LTO battery storage is analyzed and leads to battery cell parameter estimation. Estimated parameters were used as input to physics-based models. Kalman filter is used for SOC estimation of LTO battery storage. The estimated terminal voltage was validated with experimental data. The SOH estimation method is discussed as the capacity and power fade of the battery cell. The WLS method was used for the total cell capacity estimation of the battery and internal resistance (R_0) was estimated for power fade. This paper defines an overview of battery modelling of battery DT. In future research, battery models will be coupled together on pack level with a battery management system as DT of a use case study of a power system application.

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