

Advances in Science, Technology and Engineering Systems Journal Vol. 2, No. 4, 180-188 (2017) www.astesj.com ASTES Journal ISSN: 2415-6698

Kalman filter Observer for SoC prediction of Lithium cells

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ARTICLEINFO
Article history:
Received: 09 August, 2017
Accepted: 29 August, 2017
Online: 23 September, 2017
Keywords:
Li Ion batteries
SoC estimation
non linear fractional model
Impedance Spectroscopy
Fractional Order Calculus
Kalman Filter

ABSTRACT

The SoC estimation of Li Ion batteries presents a difficult task for almost applications in order to ensure their higher energy density and their safety. Hence, there have been several methods to optimize the state of charge of the Lithium cells such as observer strategies which have been considered in this work. Kalman filter observer has been selected for state optimization. It has been considered to stabilize the error estimation of battery state thanks to its gain through the following non linear fractional model. The fractional model has been deduced from analysis of Impedance Spectroscopy data and it has been well defined by Fractional Order Calculus. The performance of Kalman filter has been evaluated through the simulation results. They have improved the efficiency and limits of Kalman theory to determine the actual internal state of cells.

1 Introduction

The optimization of state of charge for Lithium batteries presents the main effect on their internal states in several applications [1]. It leads to maintain the activities of applications in permanent way.

The state of charge (SoC) is meaningful parameter that is defined in case of discharge of the battery [2]. It presents the shift time of battery capacity through the following expression [3]:

$$SoC(t) = 100 * \int_{t_0}^t \frac{I_b(\tau)}{Q} d\tau$$
 (1)

with I_b : the current of the battery, Q: the nominal capacity of the battery and τ : Time of energy storage.

The SoC optimization is a difficult issue for different domains due to its dependency on some factors such as battery capacitance, temperature and internal resistance and also the problem of defining it easily [4]. Therefore, many researches have focused on the possibility to estimate the SoC of the Lithium cells through different techniques [5,6,7] such as Direct measurements [8], Book keeping estimation [9], SoC estimation based on models [10].

The most considered technique for SoC optimization is Observer techniques [11,12].

This method is based on puting the following battery model to the observer and update the optimization of the states by calculating their erros which are the set of difference data between the measured and desired state [13]. The model based methods presents among the diagnosis technology and especially fault diagnosis. They are designed for extraction parameter from impedance spectra and optimization the state of the electrochemical systems. It has been described in figure 1.



Figure 1: Properties of the model based method for fault mechanism and diagnosis

The equivalent battery models permit to make conformity between electrochemical impedance and electric impedance measured by Electrochemical Impedance Spectroscopy (EIS). They own medium mathematical complexity and they ensure good precision in field of optimization.

In general, there is a fractional order aspect of equivalent models for electrochemical systems [14, 15,

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16]. Moreover, the fractional models have been well defined by Fractional Order Calculus (FOC) [17]. Thanks to fractional order calculus, the several dynamic and chemical phenomena of Lithium battery have been perfectly characterized. Many researches have improved the efficiency of fractional order in electrochemical fields [18] for example: according to Ichise et al., fractional calculus has been used for analysis of electrode processes through an analog simulation of non-integer order transfer functions [19].

SoC estimation based on model for electrochemical systems requires an accurate fractional descriptor observers [20]. In addition, there are some researchers who have focused on this direction like Yan Ma and Xiuwen Zhou have considered the fractional kalman filter observer to optimize the state of charge of Li Ion batteries [21] and also Fei Zhang et al. has proposed the extended Kalman filter to ensure the stability of error estimation of SoC [22].

The objective of this research work consists on presenting new strategy for SoC estimation based on observer for Lithium cells.

Kalman Filter has been proposed to determine correctly the state of Lithium batteries. It has been more explained and described in section 4.2. Indeed, Kalman filter has been theoritically checked and there has been improved that it is efficient method in field of prediction of State of Charge (SoC).

2 Dynamic model for Lithium battery

The Lithium battery considered in this paper is Lithium cell LiFePO4, model (SP-LFP40AHA). This part has focused on defining the dynamic phenomenon of selected Lithium battery by analysis of Impedance spectroscopy data in each frequency range.

In fact, Impedance Spectroscopy (IS) has been the most considered strategy in field of estimation of state of charge of electrochemical systems thanks to its benefits. It is direct measurement that precises a suitable circuit related to characteristics of impedance curve at the level of frequency domain [23]. The measurement of impedance has been carried out in frequency range from 0.01 Hz to 1 KHz. Futhermore, impedance spectroscopy may identify the parameters of the several components for the equivalent circuit such as diffusion coefficient and kinectic variables [24, 25, 26]. The Lithium battery is closely non linear system and there is difficulty to identify its chemical coefficients and variables. So, thanks to impedance spectroscopy, there is possibility to determine the several chemical internal reactions which then can be defined by equivalent model.

Figure 2 shows the measured impedance diagram in 50% of SoC for wide range of frequencies. The several dynamic phenomena of Lithium battery have been appeared in each frequency range.:

- Parasitic effects and electro migration in the electrolyte and connectors at high frequency part (300Hz < f < 355 Hz).
- Charge transfer inside the battery and exactly in the interface between the electrode and electrolyte at mid frequency part (354.8Hz < f < 3.54 Hz). It is identified by $Z_{C_{PE}}$ which is defined in next section.
- Diffusion phenomena of ionic species in low frequency (f < 3.54 Hz). It is identified by Z_w which is defined in next section.



Figure 2: Measured Impedance spectra for LiFePO4, model (SP-LFP40AHA) in 50% of SoC

Hence, the topology of equivalent model for chosen Lithium cell has been presented in figure 3. Dynamic battery has been modelled by set of electrical components.



Figure 3: Topology of equivalent model for Lithium cell LiFePO4, model (SP-LFP40AHA)

With *I*: the Current of LiFePO4 battery, *Z*: Impedance of LiFePO4 battery , U_b : the terminal of LiFePO4 battery.

The several effects over frequency range have been illustrated as:

- High frequency effects have been defined by inductance *L* in parallel with his interne resistance *r*.
- Electrode effects have been presented by ohmic resistance *R_e*.
- Mid frequency effects have been defined by parallel circuit constant phase element CPE- transfer resistance R_{ct} .

• Low frequency effects have been identified by Warburg impedance Z_{ω}

Li Ion cells is non linear electrochemical system and there is difficulty to deduce its appropriate properties. So, in order to obtain the optimal values of battery model variables which have been shown in figure 3, there has been used the genetic algorithm (G.A) as fitting procedure.

The optimal values of model have been determined through mechanism of evolutionnary algorithm which is described in figure 4.



Figure 4: Mechanism of Genetic Algorithm

The dynamic model for LiFePo4 has been described in figure 5 and its structure is based on hysterisis phenomenon which is presented by open circuit voltage OCV and from impedance spectroscopy analysis.



Figure 5: Dynamic Model topology for Lithium cell

The inductance element L hasn't been involved in the battery model because the Lithium ion cells are less applied in high frequencies range.

2.1 Parameters of battery model

There are different parameters related to equivalent model such as:

• The double layer capacitance *CPE* models the imperfect capacitors that appear in experimental spectra. It is defined by its fractionnary impedance through the following expression [24]:

$$Z_{C_{PE}} = \frac{1}{Q(j\omega)^{\beta}} \tag{2}$$

with : Q > 0 , $0 \le \beta \le 1$

• Z_{ω} is fractionnary impedance for warburg element. Its main characteristic consists in its straight line with constant slope at the level of Nyquist diagram in low frequency values. The impedance Z_{ω} can be written as in semi infinite diffusion [25]:

$$Z_{\omega}(j\omega) = \frac{\alpha \sqrt{2}}{(j\omega)^{\sigma}}$$
(3)

with : α : the diffusion parameter and $\sigma = 0.5$.

• OCV: Open Circuit Voltage and it is considered as crucial variable that expresses many criterias of performance for the battery. The open circuit voltage is used for SoC estimation [26].

A non linear relationship between OCV and SoC has been illustrated in the litterature. In fact, some recent works have proposed some approximations for this relationship in order to facilitate its calculation.

Among these approximations, the relation between *OCV* and *SoC* is considered as [27]:

$$OCV(z) = K_0 + K_1 \frac{1}{e^{\lambda_1(z-\Theta_1)}} + K_2 \frac{1}{e^{\lambda_2(z-\Theta_2)}} + K_3 \frac{1}{e^{\lambda_3(z-1)}} + K_4 \frac{1}{e^{\lambda_4 z}} + K_5 z$$
(4)

with z is the state of charge of the battery, $K_{i=1...5}$ are the linear parameters and $\lambda_{i=1..4}$, $\Theta_{i=1..2}$ are the non linear parameters.

Table 1 presents each values of the following coefficient K_i in order to fit the measured curve OCV. This set of values has been determined by Genetic Algorithm and it has been considered as optimal results by the process.

Table 1: Values of coefficient K_i

<i>K</i> ₀	<i>K</i> ₁	<i>K</i> ₂	<i>K</i> ₃	K_4	K_5
2.67	2.7	2.85	2.93	3.1	3.4

This approximation relationship has been plotted in figure 6.



Figure 6: Diagram of OCV over SoC range

The objectif of battery model is defining the several electrochemical reactions which own the fractional criterias. They are expressed by Fractional Order Calculus (FOC).

3 Non Linear fractional model

The dynamic model which has been shown in figure 5 is considered as non linear fractional model. The fractional order calculus is a tool for defining the fractional models. The fractional aspect in general presents among the characteristics of electrochemical systems. They have been developed and evaluated through fractional order calculus in some researches [28]. Besides, by recent works, the FOC has been defined as mathematic operator using differentiation with integration to non integer order aD_t^q where q: the order, a and t: the bounds of the operation. It is applied in science fields like bioengeneering [29], electronics [30, 31] and control theory [32]. In addition, almost engineer applications have focused on FOC startegies which are based generally on describing the aspects of dynamic systems by condensed expressions and considering non local characteristics such as thermal diffusion phenomenon [33] and botanical electrical impedances [34].

Fractional order calculus is denoted as [35]:

$$aD_t^{\ q} = \begin{cases} \frac{d^q}{dt^q} & if \ q > 0\\ 1 & if \ q = 1\\ \int_0^t d\tau^{-q} & if \ q < 0 \end{cases}$$
(5)

with aD_t^q is initialized q^{th} order differintegration.

At the level of this work, FOC is fractional differentiation and according to Grunwald-Leitnikov, it can be written as [36, 37]:

$$D^{q}x(t) = \lim_{\Delta T \to 0} \frac{1}{T^{q}} \sum_{i=0}^{\frac{1}{\Delta T}} (-1)^{i} {q \choose i} x(t - i\Delta T)$$
(6)

with $\triangle T$: the sampling time, *q*: the order Grunwald-Leitnikov fractional derivative of *x*(*t*).

$$\binom{q}{i} = \frac{\Gamma(q+1)}{\Gamma(i+1)\Gamma(q-i+1)}$$
(7)

where $\Gamma(q)$ is the generalization of factorial function [38]. It is expressed as:

$$\Gamma(q) = \int_0^\infty y^{q-1} e^{-y} dy \tag{8}$$

In this part, the constant phase element *CPE* and the warburg element Z_{ω} have been considered as fractional elements [39].

In fact, the fractional element is defined as [39]:

$$Z_{fractional} = \frac{1}{Y(jw)^{\delta}}$$
(9)

where: *Y* is the coefficient; $-1 \le \delta \le 1$: the arbitrary

order of the fractional element which can be an integer or a fraction. It is characterized by straight vertical line in Nyquist plot for low frequency domain.

For *CPE*, its fractional model is given as [20]:

$$Z_{C_{pe}} = \frac{1}{C_1(j\omega)^{\beta}} \tag{10}$$

For Z_{ω} , its fractional model is given as [20]:

$$Z_{warburg} = \frac{1}{W(j\omega)^{\sigma}} \tag{11}$$

where: *W* is the coefficient and β , σ are the arbitrary orders of the fractional elements: $0 \le \sigma \le 1$ and $0 \le \beta \le 1$.

In this work, the double layer capacitance CPE has treated as perfect capacitor C_1 and then its following equation is given as:

$$Z_{C_{pe}} = \frac{1}{C_1(j\omega)} \tag{12}$$

Among the effectiveness of FOC for electrochemical systems, it defines precisely the chemical phenomenon of Lithium batteries. It has been improved in figure 7 for measured impedance spectrum in 50% of SoC of Lithium batteries.



Figure 7: Measured Impedance vs Impedance model presented by FOC

The dynamic behavior of the battery which has been presented by FOC has been given as:

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- For diffusion phenomenon: It has been defined by *Z_{warburg}*.
- For charge transfer phenomenon: It has been defined by capacitor *C*₁ in parallels with resistor *R*.

According to figure 7, the diffusion phenomena has been obvisiouly well defined by FOC. The straight line of $Z_{warburg}$ is similar to line with constant slope of Z_{ω} .

Thanks to FOC, the equivalent circuit of the battery can be deduced and hence the chemical reactions can be identified through many parameters related to different circuit components.

3.1 Fractional battery model

The equations of the fractional model from figure 4 has been expressed as in the following form:

$$D^{\beta}V_{1} = \frac{I_{b}}{C_{1}} - \frac{V_{1}}{R_{ct}C_{1}}$$
(13)

where V_1 : the voltage at the level of $R_{ct}C_1$ parallel circuit.

$$D^{\sigma}V_2 = \frac{I_b}{W} \tag{14}$$

where V_2 : the voltage at the level of warburg element.

$$D^1 z = \frac{I_b}{C_n} \tag{15}$$

where C_n : the capacity of the Li Ion battery .

The voltage of Lithium battery V_{bat} is the sum of open voltage and voltages at the level of the electrode resistance R_e , the *RC* parallel circuit and warburg element.

It can be written as:

$$V_{bat} = OCV(z) + R_e I_b + V_1 + V_2$$
(16)

3.2 State space for Lithium battery model

Through the different equations (13)-(16), the state space for Lithium cell can be given as:

$$D^{q}x(t) = Ax(t) + Bu(t)$$

$$y = Cx(t) + Du(t)$$
(17)

where: x(t): the vector of the following states;

$$x = \begin{pmatrix} z & V_1 & V_2 \end{pmatrix}^T$$

$$A = \begin{pmatrix} 0 & 0 & 0 \\ \frac{-1}{R_{ct}C_1} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, B = \begin{pmatrix} \frac{1}{C_n} \\ \frac{1}{C_1} \\ \frac{1}{W} \end{pmatrix}, C = \begin{pmatrix} K_5 & 1 & 1 \end{pmatrix},$$

 $D = R_e, q = (1 \ \beta \ \sigma), y = V_{bat}$: Output of state space.

u(t): Input of state space with $u=I_b$ (The current of the battery).

4 SoC optimization using fractional observer

The observers have been considered as an alternating tool for some problems which exist in practice like: the high cost of installation of the devices and long time of measurements of the missing variables. The main role of observers is determining the unknown variables related to the state vector and reducing the use of expensive sensors [40]. This area has been attractive by many researches [41,42] and many kind of observer strategies have been evolved especially for several classes of chemical systems to estimate their internal states [43, 44]. In addition, the use of observers becomes a challenge in front of many requirements of accuracy and suitable estimation performances. For the recent workers, there was set of types of observers which have been cited in electrochemical fields [45].

The design of observers owns an appropriate methodolgy. It has been firstly based on linear forms with presence of noises [46]. Then, there has been a developpement at the level of their forms due to the complexity of the systems. Hence, non linear observers have been widely considered [47]. They have based on mathematical models and they are evaluated by observer's equations. Indeed, the gain and the optimization of error dynamics are the main properties for model based observers.

Figure 8 presents the procedure of observer design.



Figure 8: Procedure of observer design

Moreover, the observer is among elements of control theory and it estimates in real time the state of given system from measurements of its inputs and outputs. Its principle has been described in figure 9.



Figure 9: Reconstruction of state space involving the state observer

4.1 Observability of non linear fractional model

The observability is criteria for control approach. It is based on defining the behavior of internal states of the system by knowledge of its measured outputs [48]. The observability condition is main part for observer designing and especially it depends on the formulation of the given system where there is choice of type of observability. Futhermore, there is two kinds of observability conditions: observability matrix and observability Gramian. In this work, the observability Gramian [49] has been considered to detect the aspect of given system.

The state space (17) for non linear fractional system has been firstly evaluated for its observability and then it has been put into the state observer. It is effectively observable at time *t* if there is $\theta < t$ where the state at time *t* can be finded by knowing its outputs over the interval $[\theta t]$ [50].

The observability Gramian matrix $W(\theta, t)$ is defined as [51]:

$$W(\theta, t) = \int_{\theta}^{t} E_{\gamma} (A^{T} (t - \tau)^{\gamma}) C^{T} C E_{\gamma} (A (t - \tau)^{\gamma}) d\tau$$
(18)

where E_{γ} is Mittag-Leffler function which is expressed as follows [52]:

$$E_{\gamma}(x) = \sum_{k=0}^{\infty} \frac{A^k}{\Gamma(1+\gamma k)}$$
(19)

with $\gamma > 0$

According to the battery model, the observability matrix $W(\theta, t)$ is expressed as:

$$W(\theta, t) = \begin{pmatrix} 6.100 & 5.8965 & 5.9512 \\ 5.75 & 5.9512 & 6.110 \\ 5.9512 & 6.12 & 7.110 \end{pmatrix}$$

This matrix is invertible and thus its inverse $W^{-1}(\theta,t)$ exists.

Futhermore, the non linear fractional model is observable and there is possibility to estimate its internal state from knowledge of its external outputs. Hence, this model would be synthetized through an observer by following method which has been shown in figure 10 :



Figure 10: Battery model based on SoC estimation through the feedback method Kalman filter observer

As described in figure 10, SoC estimation is ensured by feedback method Kalman Filter which has been explained in next sections.

4.2 Fractional Kalman filter (FKF) observer design

Model battery variables are not available directly to measure them. Hence, they need an accurate optimal tool to determine them which is fractional kalman filter (FKF).

Kalman filter is an estimator algorithm based on the informations about the given model and input, output signals in presence of noise [53]. Its operation can be done in real time using the actual input measurements and the previously calculated states. Kalman filter doesn't need past informations during its run where it tries to find the minimum mean square error optimization states of the actual Lithium states.

The objectif of fractional Kalman filter is getting an appropriate optimization results by reducing the cost function in the following steps [54]:

$$\arg\min_{x} [(\hat{x_{k}} - x)\hat{P_{k}}^{-1}(\hat{x_{k}} - x)^{T} + (y_{k} + Cx)R_{k}^{-1}(y_{k} + Cx)^{T}]$$
(20)

with $\hat{x_k}$ is the state vector prediction and $\hat{P_k}$ is the error covariance of state estimation.

The FKF is recursive algorithm and the form of state space (17) has been expressed as discrete form from stochastic theory:

For
$$k \ge 1$$
: $x(k+1) = [\triangle^q TA + diag(q)I]x(k)$
 $-\sum_{i=2}^{N+1} (-1)^i {q \choose i} x(k+1-i) + \triangle^q TBu(k)$ (21)
 $+ w(k)$
 $y(k) = Cx(k) + Du(k) + v(k)$

with
$$\binom{q}{i} = \gamma_i = C_q^i = \frac{q!}{i!(q-i)!}$$

w(k): Stochastic disturbance; v(k): Output noise.

Fractional Kalman filter owns two main steps where the state estimate is evaluated through several equations presented in figure 11:

- Prediction step: permits to compute and update the state estimate and error covariance through mathematical relation between the priori estimation $(\hat{x}_k^-, \hat{P}_k^-)$ and the posterior estimation $(\hat{x}_k^+, \hat{P}_k^+)$.

- Correction step: updates the measurements of state estimate and error covariance.

The formulation of FKF designed for state optimization [20, 55, 56] has been summarized in figure 11:



Figure 11: Fractional Kalman Filter for state optimization

5 Simulation results and analysis

The performance of fractional Kalman filter has been evaluated for SoC estimation of the battery by Logiciel Matlab Simulink and the run time of simulation is about 1000 secondes.

The several simulation results have been performed through set of conditions:

- The fractional model of Lithium battery is observable
- The initial SoC value has been considered as 0.88.
- Presence of stochastic disturbance and output noise w(k) and v(k).

5.1 Analysis of error for SoC estimation

Figure 12 shows the SoC optimization by proposed observer Kalman filter and its error estimation.



Figure 12: *SOC* estimation and its error by Fractional Kalman filter observer

According to figure 11, Kalman filter well optimize the SoC of the battery . It provides good state of charge estimation error thanks to its accuracy for parameter estimation. Hence, the stability between the model and the observer has been perfectly ensured by Kalman filter.

Besides, the dispersion of error of SoC estimation for fractional kalman filter is not totally concentrated at zero error. It is more dispersed and tends to -0.005 due to the problem of choice of initial parameters. This explains that the optimal values of SoC are not exactly equal to real SoC values.

5.2 Analysis of rise time for SoC estimation

The rise time of proposed estimation method may explain about its speed responses and improves its dynamic performance.

The desired state of charge by Kalman filter observer converges slowly to real state. Thus, it isn't considered for real time applications.

Kalman filter owns limits for convergence of the variables. It takes a long period to reach to real values of the following state of charge (SoC) due to its slowly operations. According to figure 11, the estimated state has been firstly fluctuated in narrow range and then it has been converged to real SoC. Hence, Kalman Filter observer is very slow method and it owns long rise time for SoC estimation.

So, Kalman filter doesn't operate perfectly in term of estimation rise time and it yields to get bad quality of state optimization for electrochemical systems. It has high time consumption due to the long time of calculation of the covariances (P_k , Q_k , R_k).

5.3 Discussion

The dynamic performance of Kalman filter has been synthetized through simulation results. Kalman filter observer can estimate the state of charge of Lithium battery despite of its limits.

In fact, it has high time consumption which depends on two reasons:

- The first reason: It is related to calculation of feedback coefficients. For Kalman filter, its gain is determined through the equations related to prediction and correction steps.
- The second reason: There is long time of calculation of complex covariances which makeS a big time consumption for Kalman filter.

Besides, Kalman filter has high estimation rise time due to its slow responses for SoC prediction of Lithium batteries.

In order to get better the state estimation for batteries, the extension form of these proposed techniques can be considered.

6 Conclusion and Outlook

A new strategy for SoC estimation has been described in this work which has based on state observer. Its main principle is using the equivalent fractional model of Lithium battery and determining from it the state of charge through observer methods. The battery model has been defined from impedance spectroscopy analysis. Each chemical property of the battery has been modelled through set of electrical components. The selected technique for state optimization is Fractional Kalman filter. Its operation for SoC estimation has been explained. The performance of this method and several aspects of SoC estimation (Rise time and time consumption) have been evaluated theoretically and there has been improved that Kalman filter observer has benefits and limits to predict the internal state of the batteries due to its long rise time and time consumption.

Future goals of this work is overcoming the limits of Kalman filter by considering its extension form or a robust and fast observer tool for SoC estimation which is Proportional Integral Observer (PIO). It well defines through its operations the actual states of electrochemical systems.

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