Abstract—Lithium-ion batteries are currently amongst the leading technologies for electrical energy storage. In automotive industry they are recognized as the most promising alternative to gasoline powered engines. State estimation of the state of the battery can provide useful information regarding the state of charge (SOC) and state of health (SOH) of the battery which play a crucial role in optimal and safe utilization of the battery. Although the electrochemical dynamics of the battery are described by nonlinear system of PDAEs, most works in the area of condition monitoring of the battery resort to empirical or equivalent electrical circuit models. These models don’t provide any physical insight into the battery and lack insight into physical limitations of the battery. This work presents a particle filter algorithm for state estimation and condition monitoring of the Li-ion battery. This filter can effectively deal with the nonlinear and complex nature of the PDAEs describing the dynamics of the battery. It provides accurate estimation of the average as well as spatial distribution of concentration in the battery. The simulation results demonstrate the effectiveness of the proposed estimation algorithm.

I. INTRODUCTION

There has been an ever-growing trend towards finding a reliable alternative for replacing the gasoline powered engines during the last two decades. Among all the proposed and practiced technologies, batteries, and more particularly Li-ion batteries, could gain the most attraction by the car manufactures thanks to their unique characteristics. High energy density, no memory effect and low self-discharge rate have made Li-ion batteries a promising alternative that could change the future of portable energy storages. However, not only for Li-ion batteries but actually for all batteries, state-of-charge (SOC) and state-of-health estimation remain to be a challenge that needs to be effectively addressed. This work is an effort to address the SOC estimation using the nonlinear electro-chemical equations of the battery using a powerful estimation algorithm.

In this regard, model-based battery monitoring algorithms are of high importance in battery estimation. The fundamental battery dynamics can be described by electrochemical (EC) equations consisting of a set of nonlinear partial differential equations. However, due to the complicated nature of these equations, most of the works in the area of monitoring have resorted to equivalent circuit models or empirical models [1], [2]. These models, though easier to work with, have limited range of reliability, hence, not appropriate for the whole range of battery operation. Moreover, they don’t provide any physical insight into the battery and lack insight into physical limitations of the battery.

Changing underlying conditions and parameter changes during the battery operation has made the SOC estimation a troublesome task that calls for sophisticated algorithms capable of handling all of these difficulties. In recent years, there have been some attempts to use EC model for battery estimation by applying Kalman filtering (KF) or observer design techniques. Nevertheless, still most of these works resort to a simplified model (e.g. Single-Particle model) [3] for estimation where spatial distribution of concentration and current density in the battery is not being engaged in the equations. The operating range over which the model is valid is also limited. Observer-design is also hindered by some issues affecting the observability in both electrodes [4].

Ref. [5] applies an EKF to single particle (SP) model of the battery to estimate the state of charge of the battery. However, as mentioned in [5], SP model is valid for a limited range of currents. Moreover, voltage and current density are basically dependent on solid and electrolyte potentials where the corresponding equations are not considered in SP model. Hence, the applied EKF need to resort to numerical calculation of output derivatives which could be a source of error accumulation. The work in [4] presented a more accurate model, namely average model, where still the spatial dependence of Butler-Volmer current is ignored. Based on this model, an EKF is applied for state of charge estimation. This algorithm is limited to a confined range of operation in terms of current and temperature as well.

Refs. [6] and [7] try to design an observer for the estimation of the battery. Ref. [6] presents a simple Luenberger observer for the PDE equations of the battery, where the stability properties of the observer are not addressed. Thus, the observer gains cannot be chosen in a systematic manner considering that [4] and [7] also suggest the weak observability conditions for the battery equations. Ref. [7] develops a PDE backstepping observer for the battery model where the stability of the observer is systematically studied. However, due to the complexity of the full electrochemical model equations and weakly observable conditions of battery states, the model of the battery is significantly reduced by considering a single particle model for the negative electrode dynamics and assumption of an instantaneous diffusion for the cathode dynamics.

Alternatively, particle filter (PF) has emerged as a powerful estimation technique where it removes the
restrictive assumptions imposed on dynamic and form of conditional density by Kalman filtering methods. In fact, PF presents an implementation of the Bayes filter that can approximate the posterior distribution of the states with a set of weighted samples. This property introduces PF as an appealing estimator candidate to handle a wide range of general, non-Gaussian and nonlinear processes. Recent works have demonstrated the superiority of PF over Kalman based variants in dealing with nonlinear systems [8]. More importantly, the enticing feature of PF for us is that it is not necessary to simplify the partial differential equations describing the battery dynamics to a similar-state space model to be KF-applicable. Particle filters are potentially applicable to any kind of equations without the need to change the form. Hence, it can provide us with the desired feature of tracking the system in its entire range.

The paper is organized as follows. Section II briefly reviews the fundamentals of battery and underlying electrochemical model. Definition of the state of charge is presented in this section. Section III summarizes the particle filter concept and presents the corresponding algorithm. Simulation experiments will be conducted in Section IV to demonstrate the performance and effectiveness of the proposed algorithm. Finally, Section V summarizes the results with some concluding remarks and proposes future work.

II. FUNDAMENTALS OF ELECTROCHEMICAL MODEL OF BATTERY

A. Principles of battery

A battery consists of three basic parts, namely the positive and negative electrodes and electrolyte. Li-ion battery has a similar structure where the negative electrode (n) is composed of carbon and the positive electrode (p) is a metal oxide. Fig. 1 depicts a schematic of a Li-ion cell, where, as shown, the active material of each electrode is approximated with continuum of sphere particles. Fundamentally, the electrochemical governing equations of a Li-ion battery can be described by considering four basic equations, namely conservation of Lithium in solid and electrolyte phase, and conservation of charge in solid and electrolyte phase. These equations are mainly expressed in terms of field quantities, i.e. solid and electrolyte concentration \( c_s(x,t), c_e(x,t) \) and solid and electrolyte potentials \( \phi_s(x,t), \phi_e(x,t) \). The equations are also coupled with a Butler-Volmer electrochemical kinetic equation expressing the volumetric rate of electrochemical reaction \( j_{\text{Li}} \). Early work on Li-ion battery modeling is traced to the original work of Doyle, Fuller and Newman [9,10]. The reader is referred to [11-13] and references therein for a comprehensive overview of Li-ion battery principles. The nomenclature of the battery equations is given in the appendix.

B. 1D-Spatial EC model

For the sake of brevity in presentation and processing speed in simulation, we demonstrate the performance of the proposed algorithm on a simplified model where the spatial distribution of parameters could still be obtained. However, the proposed algorithm could be readily applied to the fundamental pseudo 2-D model as well.

The electrolyte concentration \( (c_e(x,t)) \) is assumed to be uniform and the radial distribution of the concentration is approximated with a fourth order polynomial [14]. The mass transfer in the solid material is expressed in terms of volume averaged concentration \( (\bar{c}_s(x,t)) \), particle surface concentration \( (c_{se}(x,t)) \), and averaged concentration flux \( (\bar{q}_s(x,t)) \), where the volume is \( V_R = 4/3\pi R_s^3 \).

\[
\bar{c}_s(x,t) = \frac{1}{V_R} \int_{r=0}^{R_s} c_s(r,x,t) \cdot 4\pi r^2 dr
\]
\[
c_{se}(x,t) = c_s(r = R_s, x, t)
\]
\[
\bar{q}_s(x,t) = \frac{1}{V_R} \int_{r=0}^{R_s} \left( \frac{d}{dr} c_s(r, x, t) \right) \cdot 4\pi r^2 dr
\]

Accordingly, the solid concentration is approximated by the following polynomial.

\[
c_s(x, t) = \gamma_1(t) + \gamma_2(t) \left( \frac{r^2}{R_s^2} \right) + \gamma_3(t) \left( \frac{r^4}{R_s^4} \right)
\]

where \( j = n, p \) corresponds to negative and positive electrodes and,

\[
\begin{align*}
\gamma_1(t) &= \frac{39}{4} c_{se,j} - 3R_s \bar{q}_{s,j} - \frac{35}{4} \bar{c}_{s,j} \\
\gamma_2(t) &= -35c_{se,j} + 10R_s \bar{q}_{s,j} + 35 \bar{c}_{s,j} \\
\gamma_3(t) &= \frac{105}{4} c_{se,j} - 7R_s \bar{q}_{s,j} - \frac{105}{4} \bar{c}_{s,j}
\end{align*}
\]

The system of PDAE dynamic equations for positive and negative electrodes \( (j = n, p) \) can be shown as [6]:

\[
\begin{align*}
\frac{\partial}{\partial t} \bar{c}_{s,j}(x,t) &= -\frac{3}{R_s} \bar{j}_{\text{Li},j}(x,t) \\
\frac{\partial}{\partial t} \bar{q}_{s,j}(x,t) &= -\frac{30 D_e}{R_s} \bar{q}_{s,j}(x,t) - \frac{45}{2R_s^2} \bar{j}_{\text{Li},j}(x,t)
\end{align*}
\]
\[ c_{se,j}(x, t) = \bar{c}_{x,j}(x, t) + \frac{8R_{s,j}}{35} q_{x,j}(x, t) - \frac{R_{s,j}}{35D_{s,j}} I_{Li,j}(x, t) \]  
\[ i_0,j(x, t) = k_j(c_e(x, t))^{a_\alpha} \left( c_{\text{max},j} - c_{se,j}(x, t) \right)^{a_\alpha} \left( \bar{c}_{x,j}(x, t) \right)^{a_\alpha} \eta_j(x, t) = \phi_{x,j}(x, t) - \varphi_{e,j}(x, t) - U_j \left( c_{se,j}(x, t) \right) \]  
\[ J_{Li,j}(x, t) = i_0,j(x, t) \times \left[ \exp \left( \frac{\alpha F}{RT} \eta_j \right) - \exp \left( - \frac{\alpha F}{RT} \eta_j \right) \right] \]
\[ \frac{\partial}{\partial x} i_{e,j}(x, t) = \frac{3e_{x,j}}{R_{s,j}} J_{Li,j}(x, t) \]
\[ \frac{\partial}{\partial x} \varphi_{e,j}(x, t) = \frac{i_{e,j}(x, t) - I(t)}{\kappa_{j}^e} \]
\[ \frac{\partial}{\partial x} \varphi_{se,j}(x, t) = \frac{e_{x,j}(x, t) - \bar{c}_{x,j}(x, t)}{\kappa_{j}^e} \]

The open circuit voltage \( U \) which is a function of the solid concentration at the electrolyte surface \( c_{se,j}(x, t) \) is calculated by equations given in Eqs. (13) and (14) of Ref [4]. The electrolyte dynamics can simply be added by \( \frac{\partial}{\partial x} \varphi_{se,j}(x, t) = - \frac{1}{\kappa_{j}^e} \). This set of equations can be solved by considering the following set of initial and boundary conditions.

The input of the system is the current \( I(t) \) and output of the system is the voltage which is the potential difference between the two ends of electrodes.

\( V(t) = \varphi_{se,j}(x = L^+ , t) - \varphi_{se,j}(x = 0^- , t) - R_j I(t) \)

The reader is referred to consult with [14] and [15] for the validation of the presented model. We will later show that by employing this set of equations, we can estimate the battery states using the output obtained from solving of the full model of the battery. It should be noted that if the estimation accuracy drops out of a certain range due to model mismatch, we can readily apply the proposed filtering algorithm to full dynamic model of the battery.

The parameter of interest in estimation is basically the solid concentration by which the different measures for state of charge can be calculated. Using the reference stoichiometry equations, the bulk SOC of a battery can be defined as follows.

\[ \text{SOC}_j(t) = \frac{1}{L_j R_j} \int_{x=0}^{L_j} I_{x,j}(x, r, t) \left( \frac{c_{x,j}(x, r, t)}{c_{\text{max},j}} \right) dx \]

In the simulation studies, the following measure of average solid concentration at the surface is also defined and compared.

\[ \text{SOC}^s_j(t) = \frac{3}{L_j R_j} \int_{x=0}^{L_j} I_{x,j}(x, r, t) \left( \frac{c_{x,j}(x, r, t)}{c_{\text{max},j}} \right) dx \]

III. PARTICLE FILTER

A. Basics

Particle filters (PF) belong to the family of sequential Monte Carlo methods which are utilized to estimate the states of a system using sample points based on Bayesian models. Given a system with nonlinear and/or non-Gaussian noise, particle filters offer an appealing alternative approach compared to Kalman filtering-based methods for which no restrictive assumptions about the nature of the dynamics and form of conditional density has been made.

The basics of the standard particle filter algorithm can be explained by considering a dynamic process described by the state-space model given in the following equation.

\[ x_t = f(x_{t-1}, u_t, t) + v_t \]
\[ y_t = g(x_t, t) + n_t \]

The process observations \( \{y_t\} \) are assumed to be of marginal distribution \( p(y_t|x_t) \) and conditionally independent of all other states given the current state \( \{x_t\} \). The system state \( x_t \) can be estimated by calculating the posterior probability density function (PDF), denoted by \( p(x_t|y_{1:t}) \), in which \( y_{1:t} = \{y_i; i=1, \ldots, t\} \) represents the measurement sequence from the initial time step to the present time step \( t \). This can be accomplished sequentially by the following prediction and updating stages:

\[ p(x_t|y_{1:t-1}) = \int p(x_t|x_{t-1}) p(x_{t-1}|y_{1:t-1}) dx_{t-1} \]
\[ p(x_t|y_{1:t}) = \frac{p(y_t|x_t) p(x_t|y_{1:t-1})}{\int p(y_t|x_t)p(x_t|y_{1:t-1}) dx_t} \]

assuming that the prior distribution \( p(x_0) \) is known [16].

The above equations represent the optimal solution from a Bayesian perspective to the nonlinear state estimation problem. In all these equations, the integration is a key operation and so the closed form solutions are rarely tractable, except in a very small number of situations. An important case is the linear model with an additive Gaussian noise for which the solution is the well-known Kalman filter. When the models in Eq. (5) are nonlinear or the noise is non-Gaussian, the state estimation leads to a difficult problem to be solved analytically. An efficient practical solution is to use PF algorithm as a sequential Monte Carlo technique to approximate the state estimation solution. For this purpose, PF algorithm bases its operation on representing relevant densities by random measures, composed of particles and weights, and hence computes integrals by Monte Carlo methods. Specifically, \( p(x_t|y_{1:t}) \) can be approximated as follows using a set of evolving random samples or particles, denoted by \( \{x^k_t; i=1, \ldots, N\} \), with their corresponding adjustable weights, represented by \( \{w^k_t; i=1, \ldots, N\} \):

\[ p(x_t|y_{1:t}) \approx \sum_{i=1}^{N} w^k_t \delta_{x^k_t} \]
where \( \sum_{i=1}^{N} w_i^t = 1 \) and \( \delta \) is the Kronecker delta function employed as an indicator function. The generation of particles is performed by sampling from the space of unobserved states. Their number \( (N) \) should be sufficient to cope with complexity of state space. A trade-off between accuracy and computational effort would determine the number of particles.

### B. PF Algorithm

The standard PF algorithm typically involves three basic steps, as summarized in Table I.

Though, the describing equations of battery are not presented in the conventional format of equation (1), the concept of particle filtering will not change. In the battery dynamics, the states are changing in a two-dimensional space composed of time and position. At each time step, the posterior distribution of particles will be updated based on the measured output of the system (voltage), and importance weights are determined based on the significance of each particle. This scheme is applied to the system of battery equations and results are discussed in the next section.

### TABLE I. BASIC PARTICLE FILTER ALGORITHM

<p>| | |</p>
<table>
<thead>
<tr>
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<tbody>
<tr>
<td>1.</td>
<td>Initialization</td>
</tr>
<tr>
<td></td>
<td>• For ( i = 1, \ldots, N ), sample ( x_0^i ) from the prior distribution ( p(x_0) ) at ( t = 0 ) to effectively approximate the posterior and then set ( t = 1 ).</td>
</tr>
<tr>
<td>2.</td>
<td>Prediction</td>
</tr>
<tr>
<td></td>
<td>• For ( i = 1, \ldots, N ), evaluate the importance weights according to ( \tilde{r}_t^i = p(y_t</td>
</tr>
<tr>
<td></td>
<td>• Normalize the weights.</td>
</tr>
<tr>
<td>3.</td>
<td>Resampling</td>
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<tr>
<td></td>
<td>• Resample ( N ) new particles ( {x_t^i, i = 1, \ldots, N} ) with replacement from the set ( {x_t^i, i = 1, \ldots, N} ) according to the importance weights. A new sample ( x_t^i ) is a copy of a particular particle ( \tilde{x}_t^i ) with a probability proportional to the weight of ( \tilde{x}_t^i ). So, high-weight particles may be copied several times, and low-weight particles may disappear.</td>
</tr>
<tr>
<td></td>
<td>• Set ( t = t + 1 ) and go to step 2.</td>
</tr>
</tbody>
</table>

### IV. SIMULATION STUDIES

#### A. Simulation Tests

The dynamic state evolution of the battery is obtained by discretizing the PDE equations (Eqsns. 1, 4) by applying finite difference method choosing a proper step-length for time \( (\delta_t) \) and position \( (\delta_x) \). This set of differential equations along with the algebraic equation corresponding to surface concentration and volumetric rate (Eqns. 2, 3) constitute a DAE set of equations that need to be solved at each instant. The PF algorithm introduced in Section III-B is then applied for state estimation of the battery, where output of the system \( y_t = V(t) \), and observation noise is \( \sigma^2_{\epsilon_t} = 1e^{-4} \). The estimated values are compared with actual values obtained from solving the full dynamic model of the battery. The performance results show the effectiveness of the proposed algorithm. In the following, the estimated values of \( SOC_t^h(t) \) and \( SOC_t^l(t) \) versus their actual values obtained from nonlinear model are illustrated. As mentioned, using the above model, the spatial distribution of all parameters is also achievable from proposed algorithm. Accordingly, some samples of the spatial distribution of \( \tilde{c}_{x,j}(x,t) \) has been brought in the results.

The particle filter is initiated with 50 particles corresponding to \( SOC_t^h(t = 0) \). Particles are initiated with some guess about the initial concentration at the negative electrode. Note that Li concentration at negative and positive electrodes are dependent based on the conservation of mass law (i.e. total lithium contained in active material of the cell is assumed to be constant) (see [6] for more details). The battery parameters used in simulations are adopted from [15]. The results are shown in Fig. 2. It can be seen that after a very short transient the proposed algorithm is capable of finding the correct SOC and tracks the correct value (Fig. 2 (b)). Fig. 2 (c) shows the spatial distribution of concentration \( t = 300 \) sec. The spatial distribution of different parameters (such as \( \tilde{c}_{x,j}, \varphi_{x,j}, \varphi_{e,j} \)) could have a particular significance in studying the battery health in future studies.
The robustness of the algorithm is confirmed by increasing the observation noise in the simulations. Fig. 3 shows the results where the estimation performance is still satisfactory and the algorithm can cope with the noise effect quite well.

CONCLUSION AND FUTURE WORK

A particle filter-based estimation scheme was developed for a lithium-ion cell using the fundamental electrochemical model. Comparing the proposed PF-based algorithm versus other methods shows a trade-off of complexity versus accuracy. The appealing feature of this algorithm is that it provides the opportunity to consider the very basic electrochemical model of the battery. In comparison with KF-based algorithms, there is no need to average the field variables in order to eliminate the position dimensional (x-dimension) of equations. Therefore, the spatial distribution of field variables in a battery can also be obtained using this algorithm. Results confirm the effectiveness of the proposed algorithm.

The promising results lead the authors to look at electrochemical model-based filter estimation of state of health of the battery using PF as a future work. Failure detection of batteries using particle filter is also another potential future area of research.

APPENDIX

The nomenclature of the presented battery model is given in this section.

TABLE II. NOMENCLATURE OF BATTERY

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
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<tbody>
<tr>
<td>$a_{i,j}$</td>
<td>active surface area of an electrode ($\text{cm}^{-2}$)</td>
</tr>
<tr>
<td>$c_{i,j}$</td>
<td>solid concentration ($\text{mol cm}^{-3}$)</td>
</tr>
<tr>
<td>$\bar{c}_{i,j}$</td>
<td>volume averaged concentration ($\text{mol cm}^{-3}$)</td>
</tr>
<tr>
<td>$c_{e}$</td>
<td>electrolyte concentration ($\text{mol cm}^{-3}$)</td>
</tr>
<tr>
<td>$c_{\text{max},i,j}$</td>
<td>maximum solid-phase concentration in sphere ($\text{mol cm}^{-3}$)</td>
</tr>
<tr>
<td>$D_{i,j}$</td>
<td>diffusion coefficient in solid phase ($\text{cm}^2\text{s}^{-1}$)</td>
</tr>
<tr>
<td>$F$</td>
<td>Faraday’s constant ($\text{Cmol}^{-1}$)</td>
</tr>
<tr>
<td>$i_{0,i,j}$</td>
<td>intercalation (exchange) current density ($\text{A cm}^{-2}$)</td>
</tr>
<tr>
<td>$i_{e,i,j}$</td>
<td>electrolyte current density ($\text{A cm}^{-2}$)</td>
</tr>
<tr>
<td>$j$</td>
<td>negative electrode(n), positive electrode (p), or separator (sep)</td>
</tr>
<tr>
<td>$I_{\text{vol},i,j}$</td>
<td>volumetric rate of electrochemical reaction ($\text{A cm}^{-3}$)</td>
</tr>
<tr>
<td>$k_{i,j}$</td>
<td>rate constant of reaction ($\text{A cm}^{-2}(\text{mol cm}^{-3})^{1+\alpha}$)</td>
</tr>
<tr>
<td>$L_{i,j}$</td>
<td>length of different parts of cell (anode, separator, cathode)</td>
</tr>
</tbody>
</table>
(cm)

\( \bar{q}_a \) volume averaged concentration flux (mol cm\(^{-4}\))

\( R \) gas constant (J K\(^{-1}\)mol\(^{-1}\))

\( R_f \) current collector contact resistance (mΩ)

\( R_0 \) radius of sphere (cm)

\( T \) Temperature (K)

\( U_j \) open circuit voltage at electrode j (V)

\( V \) cell voltage (V)

\( \alpha_a \) anodic transfer coefficient of electrochemical reaction

\( \alpha_c \) cathodic transfer coefficient of electrochemical reaction

\( \eta_{i,j} \) volume fraction of electrode j

\( \varphi_{s,j} \) solid potential (V)

\( \varphi_{e,j} \) electrolyte potential (V)

\( \eta_f \) overpotential (V)

\( \kappa_{eff} \) electrolyte phase effective conductivity (Ω\(^{-1}\)cm\(^{-1}\))

\( \sigma_\phi \) conductivity of electrode (Ω\(^{-1}\)cm\(^{-1}\))

REFERENCES


