State of charge estimation of a lithium ion cell based on a temperature dependent and electrolyte enhanced single particle model

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Abstract

SOC (state of charge) estimation provides critical information to system engineers and end users of consumer electronics to electric vehicles. The accuracy of model-based SOC estimation depends on the accuracy of the underlying model, including temperature effects that greatly influence cell dynamics. This paper uses a 7th order, linear, ESPM (electrolyte enhanced single particle model) as the basis for a Luenberger SOC observer for a lithium ion cell. Isothermal and non-isothermal simulations compare the SOC from a commercially-available finite volume code and the SOC estimate for a wide range of temperature (0 < T ≤ 50 °C) and pulse C-rates (|I| ≤ 15C). Arrhenius relationships between the ESPM model parameters and the sensed temperature improve SOC estimation. At low temperature (T < 10 °C) and low C-rates, temperature measurement reduces the RMS (root-mean square) SOC estimation error by up to ten times. At high temperature (T ≥ 40 °C) and high C-rates (|I| ≤ 15C), temperature measurement decreases SOC estimation error by more than three times.

1. Introduction

Reducing greenhouse gas emissions and improving the fuel efficiency of automobiles, trucks, and buses can be achieved by partial and full electrification of the vehicle sector [1]. The U.S. CAFE (corporate average fuel economy) standard will double the conventional internal combustion engine’s fuel efficiency to 54.5 miles per gallon [2] by 2025, saving consumers $1.7 trillion in fuel costs and reducing oil consumption by 12 billion barrels. Most of the vehicles in the U.S. are expected to be HEVs (hybrid electric vehicles) and PHEVs (plug in hybrid electric vehicles) by 2034 and 2045, respectively [3,4], to meet the CAFE standard.

Lithium ion batteries offer 40–50% weight reduction, 30–40% volume reduction, and superior Coulometric and energy efficiency compared to Ni - MH batteries [5], making them well suited to electric vehicles. Lithium ion battery packs require an advanced and real-time BMS (battery management system) to ensure safe and efficient power management. One of the major tasks of a BMS is to estimate the SOC (state of charge), the percentage of maximum available charge at the current time. SOC can not be measured directly, so the measured voltage and current are used to estimate the SOC. Coulomb counting through current integration is a SOC estimation method but it requires accurate knowledge of the initial state of the cell. As with all open loop estimators, the estimated SOC may drift away due to sensor error and model mismatch. Model-based SOC estimation using feedback, is more reliable but requires an accurate cell model that captures the cell dynamics under varied operating conditions over the life of the pack. Equivalent circuit models are often used to estimate SOC [6–9] but they lack underlying physiochemical processes of the cell and require extensive empirical parametrization. Plett [10–12] first introduces the use of Kalman filtering for equivalent circuit models of Li-ion cells. Lee et al. [13] report a reduced order extended Kalman filter based on equivalent circuit model. Hu [14] designs a Luenberger observer based on an equivalent circuit model.

Full order, physics based, electrochemical models are often not the best candidates for state estimator design because they consist of non-linear, coupled, PDEs (partial differential equations), that must be simplified and discretized to be used for real-time estimation on-board a vehicle. Reduced order models have been developed by many researchers that simplify the full order electrochemical models. These reduced order models capture the dominant cell dynamics at a specific SOC and temperature and sufficiently low C-rates. Smith et al. [15,16] develop a 7th order isothermal model in state variable form using residue grouping that...
predicts internal cell potentials, concentration gradients, and estimate SOC from current and voltage measurements. The model does not provide explicit relationships between the cell internal parameters and the coefficients of impedance transfer function. Lee et al. [17] extend this work by obtaining an analytic transfer function for solid phase potential, electrolyte phase potential, and concentration distribution. Klein et al. [18] reduce the full electrochemical model by assuming constant electrolyte concentration and approximating solid phase diffusion using volume averaging. Incorporating a temperature corrective term in the energy equation enables accurate SOC estimation at moderate C-rates (current/battery capacity) [19].

SPM (single particle model) based observers have also been reported in literature [20–22]. The SPM is a simplified, physics-based, fundamental model where the current density is assumed to be uniform in each electrode and all of the active material particles are in parallel. The associated diffusion equations are solved assuming average electrochemical reaction rate. The electrolyte dynamics modeled by a diffusion resistance, assuming instantaneous Li-ion transfer across the cell leads to significant error at high C-rates [23]. Rahimian et al. [24] derived an isothermal SPM by polynomial approximation of electrolyte dynamics in terms of 13 differential algebraic equations which are solved by COMSOL Inc. Marcicki et al. [25] recently proposed an SPM that includes a time-varying resistance and first order truncated liquid diffusion dynamics. Tanim et al. [26,27] analytically augment the SPM model with electrolyte diffusion dynamics (ESPM) and Arrhenius relations for the model parameters to account for temperature variations (ESPM-T).

The performance and dynamic response of a Li-ion cell is strongly dependent on temperature and C-rate. The accuracy with which one can estimate SOC is directly related to the accuracy of the underlying model [5]. SOC estimators drive the voltage and SOC estimate to zero if the model is accurate. Model mismatch introduces phantom currents that contribute the inaccurate SOC estimate. ESPM-T is a control-oriented and physics-based model that adds electrolyte dynamics and temperature effects to the conventional SPM and much more accurately predicts the voltage response given the current input and sensed cell temperature [26–28].

This paper presents a Luenberger state estimator for Li-ion cells based on the ESPM and ESPM-T models from Refs. [26,27]. The temperature is typically measured in a Li-ion pack so the temperature sensor signal is used to update the ESPM-T model’s parameters and improve its accuracy. The proposed model-based estimators are co-simulated with a commercial, 1D, fully nonlinear, and thermally coupled Li-ion cell model namely AutoLion-ST™ [29,39,40]. The ESPM and ESPM-T-based SOC estimates are compared with AutoLion-ST™ to identify the operating temperature and C-rate ranges with accurate SOC estimation.

2. Mathematical modeling

The three domains of the 1D Li-ion cell model, schematically shown in Fig. 1, are the porous anode with spherical graphite particles, porous separator, and porous cathode with spherical active material particles (e.g. lithium NCM (nickel manganese cobalt oxide), LCO (lithium cobalt oxide), LMO (lithium manganese oxide), or LFP (lithium iron phosphate)). The electrolyte (typically 1.2 M LiPF6 in PC (propylene carbonate)/EC (ethylene carbonate)/DMC (dimethyl carbonate)) saturates all the three cell domains. The separator allows Li-ions to diffuse through but isolates the direct electron path between the positive and negative electrodes using a micro porous polymer or gel polymer separator. Very thin aluminum (Al) and copper (Cu) foil current collectors are attached at the ends of the positive and negative electrodes, respectively.

During discharge, Li-ions de-intercalate from the negative electrode.

\[
\text{Li}_x\text{C} \xrightarrow{\text{discharge}} \text{C} + x\text{Li}^{+} + xe^{-}, \quad (1)
\]

and intercalate into the positive electrode.

\[
\text{Li}_{1-x}\text{MO}_2 + x\text{Li}^{+} + xe^{-} \xrightarrow{\text{discharge}} \text{LiMO}_2, \quad (2)
\]

where M stands for Ni_{1/3}Co_{1/3}Mn_{1/3} (NCM). The opposite reactions occur during charge.

2.1. Governing equations

Four governing equations: Conservation of Li-ion (Li^{+}) and conservation of charge (e^{-}) in both the solid and electrolyte phases are used to describe the electrochemical model of a Li-ion cell. Fick’s law of diffusion governs the conservation of Li^{+} in a single, spherical, solid phase particle [5]:

\[
\frac{C_{\text{Li}^{+}}}{D_{\text{Li}^{+}}} \frac{\partial^2 C_{\text{Li}^{+}}}{\partial x^2} = 0,
\]

where \(D_{\text{Li}^{+}}\) is the diffusion coefficient of Li-ion in the solid phase.

\[
\frac{C_{\text{E}}}{D_{\text{E}}} \frac{\partial^2 C_{\text{E}}}{\partial x^2} = 0,
\]

where \(D_{\text{E}}\) is the diffusion coefficient of Li-ion in the electrolyte phase.

\[
\frac{\partial C_{\text{Li}^{+}}}{\partial t} = \frac{\partial}{\partial x} \left( D_{\text{Li}^{+}} \frac{\partial C_{\text{Li}^{+}}}{\partial x} \right) + j_{\text{Li}^{+}},
\]

where \(j_{\text{Li}^{+}}\) is the current density of Li-ions.

\[
\frac{\partial C_{\text{E}}}{\partial t} = \frac{\partial}{\partial x} \left( D_{\text{E}} \frac{\partial C_{\text{E}}}{\partial x} \right) + j_{\text{E}},
\]

where \(j_{\text{E}}\) is the current density of electrolyte.

\[
\frac{\partial C_{\text{Li}^{+}}}{\partial t} = \frac{\partial}{\partial x} \left( D_{\text{Li}^{+}} \frac{\partial C_{\text{Li}^{+}}}{\partial x} \right) + j_{\text{Li}^{+}} + j_{\text{E}},
\]

where \(j_{\text{Li}^{+}} + j_{\text{E}}\) is the total current density.

\[
\frac{\partial C_{\text{E}}}{\partial t} = \frac{\partial}{\partial x} \left( D_{\text{E}} \frac{\partial C_{\text{E}}}{\partial x} \right) + j_{\text{E}} + j_{\text{Li}^{+}},
\]

where \(j_{\text{E}} + j_{\text{Li}^{+}}\) is the total current density.
\[
\frac{\partial c_s}{\partial t} = \frac{D_s}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial c_s}{\partial r} \right),
\]

where \(r\) and \(t\) are the radial and time coordinates, respectively, and \(c_s\) is the concentration of \(Li^+\) in the solid phase active material particles. The solid phase potential depends on the particle surface concentration, \(c_s(x,t) = c_s(x,R_{el,t})\).

Planar diffusion governs the conservation of \(Li^+\) in the electrolyte phase [5]

\[
\frac{\partial c_e}{\partial t} = D_e \frac{\partial^2 c_e}{\partial x^2} + \frac{1 - \frac{\epsilon_0}{\epsilon F} \bar{j}^{li}}{x}.
\]

where \(c_e(x,t)\) is electrolyte concentration and \(D_e\) and \(\epsilon_e\) are different in each domain (anode, separator, and cathode). The tortuous path of \(Li^+\) transport through the porous electrode and separator is accounted for by using the Bruggeman relation \(D_e^{\text{eff}} = D_e c_s^{\epsilon_5}\). The boundary conditions ensure continuity of concentration and flux through the adjoining domains within the cell and zero flux at the current collectors.

Conservation of charge in the solid phase of each electrode is [5]

\[
\sigma^{\text{eff}} \frac{\partial^2 \phi_s}{\partial x^2} = \bar{j}^{lii},
\]

where \(\phi_s\) is the solid phase potential, the reference conductivity of the active material is \(\sigma\), and the effective conductivity of the solid phase \(\sigma^{\text{eff}} = \sigma_{s}\).

The linearized electrolyte phase charge conservation is governed by Ref. [5]

\[
\sigma^{\text{eff}} \frac{\partial^2 \psi_e}{\partial x^2} + \kappa_{s0}^{\text{eff}} \frac{\partial^2 c_e}{\partial x^2} + \bar{j}^{li} = 0,
\]

where \(\psi_e\) is the electrolyte phase potential and Bruggeman relation \(\kappa_{s0}^{\text{eff}} = c_s^{\epsilon_5}\) calculates the effective ionic conductivity. The effective diffusional conductivity is

\[
\kappa_d^{\text{eff}} = \frac{2RT\sigma}{F} \left( \frac{\rho^e}{\rho^s} - 1 \right) \left( 1 + \frac{d\ln \epsilon}{d\ln \rho} \right),
\]

according to concentrated solution theory. The Butler-Volmer (B-V) kinetic equation [5]

\[
\bar{j}^{li} = a_i i_0 \exp \left( \frac{\epsilon_i F \eta}{RT} \right) - \exp \left( - \frac{\epsilon_i F \eta}{RT} \right),
\]

couples the four conservation Eqs. (3) through (6) through \(c_s\), \(c_e\), \(\psi_e\), and \(\phi_s\) variables, respectively, where the exchange current density is

\[
i_0(x, t) = k(T) c_s^{\text{max}}(c_s) a_i c_s^{\epsilon_{s,i}}.
\]

Overpotential is the extra potential required to overcome the surface reaction:

\[
\eta = \phi_s - \phi_e - U(c_s),
\]

where \(U(c_s)\) is the open circuit potential of the individual electrode.

Finally, the cell voltage can be evaluated from.

\[
V(t) = \phi_e(L, t) - \phi_s(0, t) - \frac{R_e}{A} I(t).
\]

### 2.2. Development of the 7th order ESPM

In the ESPM, current density is assumed uniformly distributed across each electrode making all the active material particles in parallel and simplifying each electrode’s dynamics to be represented by a single spherical particle with radius \(R_s\) but with Li-ion storage capacity equal to the electrode storage capacity. The conservation equations are linearized, and all properties are evaluated at the equilibrium point (50% SOC).

The solid state diffusion impedance transfer function of a spherical particle provides the particle’s surface concentration corresponding to an input current. Taking the Laplace transform of Eq. (3) and applying the associated boundary conditions produces.

\[
\bar{C}_s x(R_s, s) = \frac{1}{\bar{D}_e} \left( \frac{R_e}{D_b} \left[ \frac{\tanh(\beta)}{\tanh(\beta) - \beta} \right] \right),
\]

where \(\beta = R_s \sqrt{\beta}\) [31] and the tilde indicates a small perturbation from the equilibrium condition \(\bar{C}_s x(t) = \bar{C}_e x + \bar{C}_s x(t), \bar{\eta}, \bar{\epsilon}_s\), and \(\bar{\epsilon}_e\) are zero at equilibrium so, tildes are unnecessary and capital letters indicate a Laplace transformed variable. The equilibrium particle concentration \(\bar{C}_s x\) depends on the SOC setpoint.

Assuming infinite solid phase conductivity in the electrodes, Eq. (5) is integrated in each electrode domain using the boundary conditions to obtain the uniform current distributions.

\[
\frac{\bar{J}_s^{lii}(s)}{\bar{I}(s)} = \frac{1}{\bar{A}_L},
\]

\[
\frac{\bar{J}_p^{lii}(s)}{\bar{I}(s)} = \frac{1}{\bar{A}_P},
\]

Where \(\bar{J}_s^{lii}(s) = \frac{1}{L_s} \int_0^L \bar{J}_s^{lii}(x, s) dx\) and \(\bar{J}_p^{lii}(s) = \frac{1}{L_p} \int_{L_p}^L \bar{J}_p^{lii}(x, s) dx\).

Substituting Eqs. (13) and (14), Eq. (12) can be written as.

\[
\frac{\bar{C}_s x(s)}{\bar{I}(s)} = \frac{1}{\bar{A}_e F \bar{A}_n \left( \frac{R_e}{D_b} \left[ \frac{\tanh(\beta)}{\tanh(\beta) - \beta} \right] \right)}.
\]

\[
\frac{\bar{C}_p x(s)}{\bar{I}(s)} = \frac{1}{\bar{A}_e F \bar{A}_p \left( \frac{R_e}{D_b} \left[ \frac{\tanh(\beta)}{\tanh(\beta) - \beta} \right] \right)}.
\]

for the negative and positive electrodes, respectively. Eqs. (15) and (16) are in transcendental transfer function form and infinitely differentiable. A 3rd order Padé approximation [32,33] is used to convert Eqs. (15) and (16) into polynomial transfer functions.

\[
\frac{\bar{C}_s x(s)}{\bar{I}(s)} = \frac{21}{s^3 + 189 s^2 + 3465 s + \frac{495}{4}}.
\]

\[
\frac{\bar{C}_p x(s)}{\bar{I}(s)} = \frac{21}{s^3 + 189 s^2 + 3465 s + \frac{495}{4}}.
\]
The 3rd order Padé approximation is experimentally validated by Prasad et al. [23] with a 10 Hz bandwidth, sufficiently high for current EV applications.

The B–V Eq. (8) is linearized as

$$\frac{\eta(s)}{I_n(s)} = \frac{R_{ct}}{\Delta s}. \tag{19}$$

where the charge transfer resistance, $R_{ct} = \frac{RT}{\Delta \mu_{eq}}$. Combining Eqs. (13), (14) and (19), overpotentials in the individual electrodes are

$$\eta_n(s) = \frac{R_p^m}{\Delta \mu_{eq}} \frac{1}{A_{eq}} L_n. \tag{20}$$

$$\eta_p(s) = \frac{R_p^p}{\Delta \mu_{eq}} \frac{1}{A_{eq}} L_p. \tag{21}$$

Combining Eqs. (10) and (11) and linearizing around an equilibrium production the voltage deviation.

$$\tilde{V}(t) = \eta_n(L, t) - \eta_n(0, t) + \phi_e(L, t) - \phi_e(0, t) + \frac{\partial U_p}{\partial \mu_{eq}} c_{eq}(L, t)$$

$$- \frac{\partial U_p}{\Delta \mu_{eq}} c_{eq}(0, t) - \frac{R_{ct}}{A} I(t). \tag{22}$$

The impedance transfer function is obtained by taking Laplace transform of Eq. (22) to produce

$$\tilde{V}(s) = \frac{\eta_n(L, s) - \eta_n(0, s)}{I(s)} + \frac{\Delta \phi_e(L, s) + \frac{\partial U_p}{\Delta \mu_{eq}} c_{eq}(L, s)}{I(s)}$$

$$- \frac{\partial U_p}{\Delta \mu_{eq}} c_{eq}(0, s) - \frac{R_{ct}}{A}. \tag{23}$$

The OCP (open circuit potential) slopes $\frac{\partial U_p}{\Delta \mu_{eq}}$ and $\frac{\partial U_p}{\Delta \mu_{eq}}$ are evaluated at any SOC from the empirically measured open circuit potential functions provided in Table 1.

To obtain the electrolyte potential difference in Eq. (23), the $Li^+$ conservation Eq. (4) is solved first by using IMA (integral method analysis) [5,20,34–36] across the three domains of the cell. Finally, the charge conservation Eq. (6) in electrolyte phase is solved by using the known concentration profiles. Substituting Eqs. (13) and (14) into Eq. (4) for the anode, separator, and cathode and taking the Laplace transform.

$$e_{en}^{s}C_{eq}^{i}(s) - D_n \frac{\partial^2 C_{eq}^{i}(s)}{\partial x^2} - b_1 I(s) = 0 \quad \text{for} \quad x=0, L_n, \tag{24}$$

$$e_{es}^{s}C_{eq}^{i}(s) - D_n \frac{\partial^2 C_{eq}^{i}(s)}{\partial x^2} = 0 \quad \text{for} \quad x=L_n, L_n + L_s, \tag{25}$$

$$e_{ep}C_{eq}^{p}(s) - D_p \frac{\partial^2 C_{eq}^{p}(s)}{\partial x^2} + b_2 I(s) = 0 \quad \text{for} \quad x=L_n + L_s, L. \tag{26}$$

where $b_1 = \frac{1}{\Delta \mu_{eq}}$, $b_2 = \frac{\Delta \mu_{eq}}{\Delta \mu_{eq}}$ and the superscript ‘eff’ on diffusivity has been removed for simplicity.

Spatially quadratic electrolyte concentration profiles are substituted into Eqs. (24)–(26), integrated, and simplified using the boundary conditions to obtain third order transfer functions for electrolyte concentration in the individual domains. Eqs. (13) and (14) are substituted into Eq. (6), integrated spatially, and simplified using the associated boundary conditions. The voltage drop between the cell terminals due to electrolyte dynamics is

$$\frac{\Delta \phi_e(L, s)}{I(s)} = \frac{R_0 s^2 + R_1 s + R_0}{L_s s^2 + L_s + L_0}. \tag{27}$$

where $\Delta \phi_e(L, s) = \phi_e(L, s) - \phi_e(0, s)$ and the coefficients $R_0, ..., R_2$ are listed in Ref. [26].

Eqs. (17), (18), (20), (21), and (27) are substituted into Eq. (23) to obtain the 7th order ESPM impedance transfer function.

$$\tilde{V}(s) = \frac{K_1 + K_2}{s}$$

$$+ \frac{b_{000} s^6 + b_{010} s^5 + b_{020} s^4 + b_{020} s^3 + b_{040} s^2 + b_{040} s + b_{06}}{s^6 + a_{010} s^5 + a_{020} s^4 + a_{030} s^3 + a_{040} s^2 + a_{050} s + a_{060}}, \tag{28}$$

where the coefficients $a_{010}, ..., a_{020}, b_{000}, K_1, K_2, s$ are explicitly given in terms of model parameters in Ref. [26]. The transfer
function Eq. (28) is converted to a state space realization [42] which
gives seven linear ODEs (ordinary differential equations) as follows,

$$\begin{align*}
\mathbf{x}(t) &= A\mathbf{x}(t) + Bu(t) \\
\mathbf{y}(t) &= C\mathbf{x}(t) + Du(t)
\end{align*}$$

(29) (30)

where \( \mathbf{x} = \frac{dx}{dt} \mathbf{x}, \mathbf{R}^2 \) is the state vector, \( \mathbf{u}(t) = I(t) \) is the input vector,
\( \mathbf{y}(t) = [V(t), \text{SOC}(t)]^T \), is the output vector, \( A\mathbf{R}^{2}\times2 \) is the state matrix,
\( B\mathbf{R}^{2}\times1 \) is the input matrix, \( C\mathbf{R}^{2}\times2 \) is the output matrix, and \( D\mathbf{R}^{2}\times1 \).

The SOC = \( \text{SOC} - \frac{1}{C} \int_{0}^{t} P(\tau) d\tau \), where \( C \) is the nominal cell capacity.
The system is observable from the voltage output [42].

2.3. Temperature dependent ESPM (ESPM-T)

The coefficients in the impedance transfer function (28) are explicit in terms of model parameters and thus, the temperature
dependent parameters of the cell can be easily updated throughout
the cell operation in the ESPM-T. The important physicochemical
parameters in ESPM-T are updated with cell temperature output
from AutoLion-STM to simulate the case of measuring cell tempera-
ture in a real battery pack.

The most important temperature dependent parameters for the
NCM chemistry modeled in this paper are solid phase diffusion
coefficients, exchange current density, electrolyte diffusion
coefficient, electrolyte ionic conductivity, and electrolyte diffusional
ionic conductivity. The Arrhenius equation.

$$
\psi = \psi_{\text{ref}} \exp \left[ \frac{E_{\text{act}}}{R} \left( \frac{1}{T_{\text{ref}}} - \frac{1}{T} \right) \right],
$$

(31)

where \( T = \text{Temperature and } R \) is ideal gas constant, is used to
calculate the temperature dependence of the solid particle diffusion
coefficient and exchange current density. The temperature
dependent property \( \psi \) (e.g. \( D_i^0 \), \( D_i^0 \), and \( i_0 \)) depends on the reference
value \( \psi_{\text{ref}} \) and the activation energy \( E_{\text{act}} \) associated with that
property and given in Table 1. Characterization of electrolyte properties at different
temperatures and concentrations is rare in the open literature. Value en et al.
[43] propose empirical correlations obtained from extensive experi-
ments of liquid electrolyte containing LiPF\(_6\) in propylene car-
bonate/ethylene carbonate/dimethyl carbonate (PC/EC/DMC) in the
temperature range of \(-10 \text{ to } 60 \text{ °C}\). This paper uses the following
temperature dependent empirical correlations obtained from
Ref. [43].

$$
D_i(T) = 10^{-\left\{4.43 + \frac{54}{(229 + T_{\text{ref}})} + 0.22c_{\text{e}}\right\}},
$$

(32)

$$
\kappa(T) = c_{\text{e},0} \left( -10.5 + 0.074T - 6.96 \times 10^{-5}T^2 \right) \\
+ c_{\text{e},0} \left( 0.668 - 0.0178T - 2.8 \times 10^{-5}T^2 \right) \\
+ c_{\text{e},0} \left( 0.494 - 8.86 \times 10^{-4}T^2 \right)^2,
$$

(33)

$$
\kappa_{\text{d},i} = \frac{2RTx_{i}^{\text{eff}}}{F} \left( t_i - 1 \right) \left( 1 + \frac{d \ln f_i}{d \ln c_{\text{e}}} \right) = \frac{2RTx_{i}^{\text{eff}}}{F} \left( t_i - 1 \right) \nu(T),
$$

(34)

where \( x_{i}^{\text{eff}} = \kappa(T)x_i^{1.5} \) for individual domains, \( c_{\text{e},0} \) is the average
electrolyte concentration, \( t_i \) is the Li\(^+\) transference number, and \( f_i \) is the mean molar activity coefficient. The empirical correlation

$$
\nu(T) = 0.601 - 0.24c_{\text{e},0}^{1/4} + 0.982(1 - 0.0052(T - 293))c_{\text{e},0}^{1/4}.
$$

(35)

In the ESPM-T simulations, the matrices in Eqs. (29) and (30) are
temperature dependent. The cell properties are given in Table 1.

2.4. Model-based Luenberger state estimator design

Fig. 2 shows a block diagram of a Luenberger observer for cell state
estimation. The cell dynamics are represented in state-
variable form (Eqs. (29)–(30)). \( V(t) \) is the measured cell voltage
from an actual battery pack. For the present study, AutoLion-ST™
provides the voltage, current, and temperature data in place of an
actual cell.

The state estimator equations are.

$$
\dot{\mathbf{x}}(t) = A(T)\mathbf{x}(t) + B(T)\mathbf{u}(t) + I(y - \mathbf{y}),
$$

(36)

$$
\dot{\mathbf{y}}(t) = C(T)\mathbf{x}(t) + D(T)\mathbf{u}(t),
$$

(37)

where \( \mathbf{x} \) is the state estimate, the observer gain matrix is \( K_i \mathbf{R}^{2}\times1 \),
and error \( e(t) = \mathbf{x}(t) - \mathbf{x}(t) \). The feedback term, \( I(y - \mathbf{y}) \) in the estimator equations compensate for model mismatch and noise.

When the actual and estimated outputs differ due to different
initial conditions, sensor noise, and model mismatch, then there is
a correction term and the estimator tends to reduce the error.

If the estimator and the cell have the same dynamics, initial
conditions, and input, then the estimated state (and voltage) will
perfectly track the actual state. The convergence is guaranteed if
the model and the experimental system are identical, there is no
sensor noise, and the gain matrix \( I \) is chosen to place the poles of
\( (A - IC) \) in the left half of the complex plane.

3. Results and discussion

HEVs require high C-rate charge-discharge pulses to assist a
vehicle within a strict SOC window [44]. Considering that, a 1020 s
hybrid pulse current input with a maximum C-rate of \( \pm 20 \text{C} \) is
simulated for a high power 1.78 Ah Li-ion cell. The ESPM and
ESPM-T-based observer’s performance are compared with Auto-
Lion-ST™. The accurate estimation ranges of ESPM and ESPM-T-
based observers are identified in terms of temperature and C-rates.
The AutoLion-ST™ outputs are current, voltage, and temperature.
ESPM and ESPM-T-based observers use this voltage and current
(and temperature for ESPM-T) measurements to estimate the SOC.
The hybrid current pulse profile in Fig. 3(g) is charge
conserving and operating around 50% SOC. Current and voltage
random noises of 100 mA and 10 mV, respectively, are added.

The observer gain matrix, \( I = [I_{i1} I_{i2} I_{i3} I_{i4} I_{i5} I_{i6}] \), is tuned manually to
obtain a reasonably fast transient decay and low steady state SOC
error and the same for all the simulations in this study.

3.1. Isothermal simulation with ESPM-based estimator

Fig. 3 compares the voltage and SOC estimates of the ESPM-
based Luenberger observer with AutoLion-ST™ response at a
representative temperature of 25 °C. The magnified views of the
voltage response in Figs. 3(a) and (b) at low and high C-rates,
respectively, show very good agreement between the observer
response and the AutoLion-ST™ voltage response. The insertion of electrolyte dynamics in the ESPM model significantly improves the performance relative to the traditional SPM that considers the electrolyte as a static resistor, resulting in voltage overshoots at higher C-rates.[23] The zoomed in Figs. 3(c) and (d) of the SOC plot (Fig. 3(f)) show the initial transient and steady state performance, respectively. The SOC error diminishes quickly <2.0% within 200 s from an initial estimator SOC error of 25%. During the most aggressive part (700 s–950 s) of the hybrid cycle, the maximum SOC error is <3.1%.

3.2. Non-isothermal simulation with ESPM-T-based estimator

Fig. 4 compares the ESPM-based observer, ESPM-T-based observer, and AutoLion-ST™ voltages and SOC responses for an adiabatic simulation of the hybrid cycle starting from 0 °C to 50 °C. An external cooling loop in AutoLion-ST™ regulates the cell temperature at 50 °C for 700 s. The temperature output of the AutoLion-ST™ is fed into the ESPM-T-based observer to update the state matrices. The ESPM estimator has constant state matrices corresponding to 25 °C.

The ESPM-based estimator’s voltage response significantly undershoots and overshoots at low and high temperatures as shown in Figs. 4(a) and (b), respectively. Thus, the ESPM-based SOC estimate is poor at temperatures away from the setpoint of 25 °C. ESPM-T updates the temperature dependent battery parameters and is much more accurate through out the temperature range for low C-rates at the beginning of the cycle. At high C-rates and low temperature (100–350 s), however, the ESPM-T estimated voltage overshoots the actual voltage. This is due to the unmodeled distributed current within the electrodes and sluggish reaction kinetics at low temperature and high C-rates. The ESPM-T-based estimator’s initial transients decay within 200 s. Once the battery warms up due to self heating, the ESPM-T-based observer estimates the AutoLion-ST™’s voltage response very well up to 50 °C and tracks the actual SOC (Figs. 4(c) and (d)) within a maximum error of 2.7% during that most aggressive part of the hybrid cycle. The ESPM observer, however, fails to provide accurate SOC estimate at higher temperature as shown in Figs. 4(b) and (d).

3.3. Accurate estimation ranges

The previous simulations show that estimation accuracy depends on C-rate and temperature. To further study these effects, we simulate a constant hybrid pulse cycle at different temperatures with zero initial estimator error and calculate the RMS error. The RMS error gives a good measure of the steady state error of the estimator. The temperature ranges from 0 °C to 50 °C for 1C–15C constant 20 s pulses are considered. Fig. 5 shows an example 1200 s long, 20 s-10C pulse charge–discharge cycle used to develop Figs. 6 and 7. The cell is power limited at low temperatures and high C-rates so those cases are not included.
Fig. 6 shows the RMS error contour plot for the ESPM-based SOC estimator. The ESPM-based estimator operates at a constant 25°C whereas the AutoLion-ST™'s temperature is changing due to adiabatic operation. The highly accurate region with less than 1% error is at low C-rate and near room temperature (25°C). If battery operates further away from 25°C and higher C-rate's, significant SOC estimation error is introduced.

Fig. 7 shows the ESPM-T SOC estimation error contour plot versus battery temperature and C-rate. Besides voltage, ESPM-T-based estimator also uses battery temperature (see Fig. 2) to correct
the model mismatch which reduces the estimation error. Unlike ESPM-based estimator (Fig. 6), the highly accurate region in Fig. 7 grows considerably for ESPM-T-based estimator. High temperature performance is specially very good, staying less than 3% for the entire high temperature range and C-rates. Cold temperature remain a problem at high C-rates. Overall, the ESPM-T estimator outperforms the ESPM estimator at low temperatures and C-rates by up to ten times. At high temperatures, the ESPM-T estimator is more than three times accurate.

4. Conclusion

The ESPM-based observer is capable of estimating only room temperature battery SOC for aggressive HEV current inputs. Inclusion of the temperature effect in the ESPM-T model is shown to be crucially important for accurate SOC estimation in scenarios where cell temperature varies during usage. Temperature updating of the estimator state matrices provides improved SOC estimation over a wide range of temperature and C-rates. At low temperature ($<10^\circ$C) and low C-rate ($<0.5C$), temperature measurement reduces the RMS SOC estimation error by up to ten times. For $T>40^\circ$C and $|I|<15C$, temperature measurement decreases SOC estimation error by more than three times.

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