Journal of Energy Storage 19 (2018) 120–134

Contents lists available at ScienceDirect

Journal of Energy Storage

journal homepage: www.elsevier.com/locate/est

An adaptive physics-based reduced-order model of an aged lithium-ion cell, selected using an interacting multiple-model Kalman filter

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ARTICLE INFO

Keywords:
Lithium ion battery
Electrochemical model
Battery management systems
Aged parameter estimation
Interacting multiple model Kalman filter

ABSTRACT

Reduced-order physics-based models of lithium-ion cells provide the opportunity for a battery-management system to define battery-pack operational limits in terms of cell internal electrochemical processes in order to mitigate degradation and to avoid failure modes. For these physics-based models to be relevant over the lifetime of the battery pack, they must somehow adjust to describe the internal processes accurately at every stage of battery life. Two possible approaches to do so suggest themselves. First, an algorithm might somehow *adapt* the parameter values of the model during operation to match presently observed current–voltage behaviors; but, this must be done very carefully to avoid making the model unstable or physically nonmeaningful. Alternately, a set of models could be pre-computed at different feasible aging points and the model from this set that most closely predicts presently observed current–voltage dynamics could be *selected* from the set. This second approach guarantees stable and physically meaningful models since all models in the pre-computed set meet these criteria. We propose such an approach here.

To do so, we first present a method for calculating *a priori* the changes to cell parameter values that will be produced by aging due to side reactions and/or material loss. These aged parameter values are utilized to produce reduced-order physics-based models at different stages of cell life. The reduced-order models are then used within a nonlinear interacting multiple-model Kalman filter to select the pre-computed model whose voltage predictions most resembles present measured voltage, so providing an estimate of the aged parameter values of a cell via the parameter values of this model. The selected model may then be used for state-of-charge estimation, state-of-power estimation, state-of-energy estimation, and other model-based battery-management tasks.

1. Introduction

Applications requiring high power and energy densities (e.g., utility-scale grid storage or hybrid and electric vehicles) have created significant demand for reliable and cost-effective energy-storage technologies. Lithium-ion batteries are perhaps the best energy-storage technology currently available to meet these demands due to their high energy density, high specific energy, and low self-discharge rates. Lithium-ion cells are not without drawbacks, the most significant being their cost and possible safety hazards when misused. To reduce the lifetime costs and to ensure the correct utilization of lithium-ion cells, battery management systems (BMS) are implemented between the battery and host application, to inform the host controller regarding energy and instantaneous power limits of the battery, as well as assessments of the cell's state-of-health [1–3].

Mathematical models of lithium-ion cell behavior are at the core of a BMS, by providing forecasts of variables that allow calculating the power and energy that can be delivered by its cells before predefined operating limits are reached. Modern BMS utilize equivalent-circuit models (ECMs) to predict cell behavior, with associated voltage operating limits that have been found to prevent rapid aging and catastrophic failure in the majority of circumstances [4,5,2]. By combining various linear and nonlinear circuit elements to represent empirically observed behavior, ECMs model cell voltage at the terminals. However, the models are valid only within the operating region for which they were created — they offer no predictive value outside of the data used to create them. Additionally, ECMs generally convey little or no information about the chemical processes at work within the cell. These empirically derived models and operating limits succeed in ensuring the safe operation of batteries, but are unable to optimize a tradeoff between performance and life directly since cell degradation depends most fundamentally on mechanisms dependent on the internal

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https://doi.org/10.1016/j.est.2018.07.004
Received 6 March 2018; Received in revised form 21 June 2018; Accepted 3 July 2018

Nomenclature

A	surface area of the electrode, m^2
A	state transition matrix of the state-space model
a_s	specific surface area of the porous electrode, $m^2\,m^{-3}$
B	input matrix of the state-space model
C	output matrix of the state-space model
c	concentration of lithium in phase indicated by subscript, $mol\,m^{-3}$
$c_{s,max}$	maximum lithium concentration in an electrode particle, $mol\,m^{-3}$
$c_{s,e}$	surface concentration of lithium in a spherical electrode particle, $mol\,m^{-3}$
D	input-output coupling matrix of the state-space model
$D_{e,eff}$	effective electrolyte diffusivity, $m^2\,s^{-1}$
D_s	solid diffusivity, $m^2\,s^{-1}$
F	Faraday's constant, 96 485 $C\,mol^{-1}$
i_{app}	applied cell current, A
j	reaction flux, $mol\,m^{-2}\,s^{-1}$
k_0	rate constant for the electrochemical reaction, $mol^{\alpha-1}\,m^{4-3\alpha}\,s^{-1}$
L	(without subscript) length of the cell, m
L	(with subscript) length of region of cell, m
m_k	operating mode of system at time k
p_{ij}	IMM transition probability matrix
Q	cell capacity, A hr
r	radial coordinate, m
R	universal gas constant, 8.31451 $J\,mol^{-1}\,K^{-1}$
R_f	film resistance, $\Omega\,m^2$
T	temperature, K
t_+^0	transference number
t	time, s
U_{ocp}	open circuit potential, V
x	lD linear coordinate across the cell, m
x	state of state-space model
y	linear output of state-space model

Greek

α	charge-transfer coefficient
α	capacity remaining in an aged lithium-ion cell
ε	volume fraction of phase indicated by subscript
ϕ	potential of the phase indicated by subscript, V
η	local overpotential, V
κ_{eff}	effective electrolyte conductivity, $S\,m^{-1}$
Λ_j	likelihood of measured output given model j is correct
μ	probability mass function for best fitting IMM model
σ_{eff}	effective solid conductivity, $S\,m^{-1}$
θ	stoichiometric coefficient of electrode

Subscript/superscript

n	pertaining to the negative electrode
p	pertaining to the positive electrode
s	pertaining to the solid phase

electrochemical state of the cell, which is not predicted by an ECM. The lack of transparency to the internal behavior of the cells means that excess capacity must be designed into the battery pack and conservative operating constraints must be used to avoid premature aging when using ECM with BMS.

To overcome the shortcomings of ECMs, models have been developed based on the physics of the chemical processes occurring within cells [6–9]. These physics-based models (PBMs) offer insight into electrochemical variables within the cell (such as electrical potentials, lithium movement, and lithium concentrations) in addition to the voltage measured at the terminals, and offer predictive value for a wide range of possible inputs. This information, however, comes with a significant computational cost. The coupled partial-differential equations (PDEs) that define PBMs are too demanding computationally to be evaluated in real-time by the hardware available within a BMS. Somehow, these models must be approximated with high accuracy but low computational complexity. This is generally done via model-order reduction. A number of model-order-reduction strategies appear in the literature. Most simplify the full-order model by approximating the PDE describing mass diffusion in the solid particles. Polynomial approximation [10–12], Padé approximation [13] and proper orthogonal decomposition [14,15] are some candidate methods.

While the method we propose in this paper could be applied to any reduced-order model in state-space form, we prefer a transfer-function approach coupled with a subspace-based model-identification method to reducing model order (e.g., the discrete-time realization algorithm [1,16]). This method gives a complete cell model of very low order (e.g., 6 independent linear ordinary difference equations (ODEs) provide "states" that are combined in a nonlinear way to predict values for all internal electrochemical variables of the cell at any desired set of locations as well as overall cell terminal voltage). The resulting computational complexity is often on the same order as for ECMs. These physics-based reduced-order models (ROMs) can enable BMS to provide energy and power availability estimates based on internal electrochemical variables, rather than voltage limits alone. For example, performance improvements might be realized by allowing terminal voltages to exceed typical limits when internal chemical quantity estimates indicate little chance of rapid aging, and by limiting or halting cell operation even within typical voltage limits when the internal estimates indicate a high likelihood of rapid or catastrophic degradation. For example, one reference [17] shows that electrochemically limited pulse charging a 6 Ah cell to the same negative-electrode phase-potential $\phi_s - \phi_e$ at the negative-electrode/separator boundary as encountered at equilibrium at 100% SOC increases usable charge power by 22% and usable energy by 212% versus voltage-limited charging.

Whether using ECMs or ROMs as the cell model within a BMS, unavoidable aging processes will occur [18]. Battery-management systems must have means to quantify this aging in a state-of-health (SOH) metric, which must indicate, at a minimum, how bulk attributes of the cell such as capacity and ohmic resistance change such that the ability of the cell to store energy and deliver power is reduced.[1] These degradation processes cause an aged cell to behave differently from a new cell whether using ECMs or PBMs. To ensure accurate estimates, an update to model parameter values is required over time. Methods for updating these parameter values fall into two general categories:

1. Parameter estimation: Similar to state estimation, parameter estimation seeks to use on-line measurements to estimate model parameter values (rather than the model's state). As the only on-line measurement data typically available to a BMS are the applied electrical current, terminal voltage, and cell temperature, both state and parameter estimation must be run simultaneously using the same measurements. There are several ways to approach this estimation problem (see below), but all solution techniques in some

[1] The method presented herein finds the closest pre-computed set of aged parameter values to the present operating condition of the cell, which means that it can closely track *all* aged parameter values, including aging in the stoichiometries of the open-circuit-potential functions of both electrodes, and thus in the overall cell open-circuit voltage relationship, for example.