Journal of Power Sources 382 (2018) 77–94

Contents lists available at ScienceDirect

Journal of Power Sources

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

A systematic approach for electrochemical-thermal modelling of a large format lithium-ion battery for electric vehicle application

Elham Hosseinzadeh*, Ronny Genieser, Daniel Worwood, Anup Barai, James Marco, Paul Jennings

WMG, University of Warwick, Coventry CV4 7AL, United Kingdom

HIGHLIGHTS

- A large format pouch cell over a wide range of ambient temperatures is characterised.
- The full parameter-set for the model are provided.
- Power and capacity significantly drop by decreasing the ambient temperature.
- The battery optimal operating range is between 25℃ - 35℃.

ARTICLE INFO

Keywords:
Electric vehicle
Electrochemical-thermal model
Large format cells
Lithium-ion battery
Drive cycle

ABSTRACT

A 1D electrochemical-thermal model is developed to characterise the behaviour of a 53 Ah large format pouch cell with $LiNi_xMn_yCo_{1\text{-}x\text{-}y}O_2$ (NMC) chemistry over a wide range of operating conditions, including: continuous charge (0.5C-2C), continuous discharge (0.5C-5C) and operation of the battery within an electric vehicle (EV) over an urban drive-cycle (WLTP Class 3) and for a high performance EV being driven under track racing conditions. The 1D model of one electrode pair is combined with a 3D thermal model of a cell to capture the temperature distribution at the cell scale. Performance of the model is validated for an ambient temperature range of 5℃–45℃. Results highlight that battery performance is highly dependent on ambient temperature. By decreasing the ambient temperature from 45 °C to 5 °C, the available energy drops by 17.1% and 7.8% under 0.5C and 5C discharge respectively. Moreover, the corresponding power loss is found to be: 5.23% under the race cycle as compared with 7.57% under the WLTP drive cycle. Formulation of the model is supported by a comprehensive set of experiments, for quantifying key parameters and for model validation. The full parameter-set for the model is provided ensuring the model is a valuable resource to underpin further research.

1. Introduction

Lithium ion (Li-ion) batteries play a key role in emerging electric vehicles (EVs) and hybrid electric vehicles (HEVs) due to their high energy and high power density [1]. It has been widely reported that many of the battery characteristics such as cycle life, reliability, cost, and in particular energy and power density are highly affected by the operating temperature [2,3]. The choice of the cell as well as the energy/power requirement of the pack, define the framework for designing the thermal management system (TMS) [4]. The primary function of the TMS is to regulate the battery temperature within the optimum range, typically defined to be between 15 and 35 °C [5,6], and to ensure battery safety and durability [5,6]. Higher temperatures improve the performance of li-ion batteries due to temperature dependency of the electrochemical parameters which result in lower internal resistance. However, higher ambient temperatures are known to accelerate the degradation rate due to increased side reactions within the cell [6,7]. Conversely, low temperatures deteriorate cell performance mainly due to the reduced reaction kinetics resulting a high internal resistance [5,6,8]. The impact of low temperature operation is known to become more severe during periods of high current charging or "fast charging" that may result in the onset of lithium plating [9]. Many studies in recent years have focused on analysing the thermal behaviour of the batteries [10]. For example the impact of geometry and position of the tabs on the temperature gradient of a 10 Ah and 75 Ah has been discussed in Refs. [11,12]. Kim et al. [13] investigated the thermal behaviour of a 14.6 Ah pouch cell under 1C, 3C and 5C at 25℃. Taheri et al. [14] used a 2D electro-thermal approach to develop a

* Corresponding author. Tel.: +44(0)24 7615 1374; fax: +44(0)24 7615 1374.
E-mail address: e.hosseinzadeh@warwick.ac.uk (E. Hosseinzadeh).

https://doi.org/10.1016/j.jpowsour.2018.02.027
Received 21 November 2017; Received in revised form 19 January 2018; Accepted 10 February 2018

Nomenclature

List of symbols

A_{surf}	surface area of the cell (m^2)
A_{tab}	cross sectional area of the tab (m^2)
a_s	reaction surface area
$brugg_n$	Bruggeman porosity exponent
C	Li^+ concentration ($mol\ m^{-3}$)
C_p	heat capacity (J ($kg.\ K$)$^{-1}$)
D	diffusion coefficient ($m^2\ s^{-1}$)
E_{act}	activation energy
F	Faraday's constant ($C\ mol^{-1}$)
h	heat transfer coefficient ($W/(m^2.\ K)$)
I	current load (A)
I_{pair}	current of a single-pair electrode (A)
i_e	ionic current density ($A\ m^{-2}$)
	electronic current density ($A\ m^{-2}$)
i_0	exchange current density ($A\ m^{-2}$)
j^{Li}	reaction current density ($A\ m^{-2}$)
k	thermal conductivity ($W.\ (m.\ K)^{-1}$)
k_i	reaction rate ($m^{2.5}\ mol^{-0.5}s^{-1}$)
L	thickness of the electrode (μm)
N_{pairs}	number of electrode-pairs
Q	heat generation (W)
q	volumetric heat generation ($W\ m^{-3}$)
q''	the heat flux at the exposed cell surface
R	resistance of the current collector (Ω)
R_c	contact resistance between the current collecting tab and the lead wire (Ω)
R_{uni}	universal gas constant ($J\ mol^{-1}K^{-1}$)
R_{SEI}	resistance of the SEI layer ($\Omega.cm^{-2}$)
r	radial coordinate in spherical particle (μm)
r_p	particle radius (μm)
T	temperature °C
t	time (s)
t_{dif}	diffusion time (s)
t_{dis}	discharge time (s)
t_+^0	transference number
$U_{ref,i}$	open circuit potential of the electrodes
U_{OCV}	open circuit voltage of the cell
V_t	terminal voltage
x	local state of charge of the negative electrode
y	local state of charge of the positive electrode

Greek letters

α	symmetry factor
δ_{cell}	capacity of a cell (Ah)
ε	volume fraction
η	overpotential (V)
k_D^{eff}	diffusional conductivity ($S\ m^{-1}$)
σ	electronic conductivity ($S\ m^{-1}$)
κ	ionic conductivity ($S\ m^{-1}$)
ρ	Density ($kg\ m^{-3}$), resistivity (Ω.m)
ϕ	potential (V)
ψ	a general parameter

Subscripts/superscripts

a	anode
amb	ambient
c	cathode
cc	current collector
e	electrolyte
eff	effective
elec	electronic
f	filler
irr	irreversible
neg	negative
pos	positive
r	reaction
rev	reversible
s	solid
sep	separator
surf	surface
x	direction through the cell thickness
y	direction along the cell width
z	direction along the cell height

Terms and abbreviation

Al	Aluminium
Cu	Copper
exp	experimental
OCV	open circuit voltage
sim	simulation
SOC	state of charge

reliable model for a 20 Ah NMC prismatic cell. Wu at al. [15] extended their research, combining a 2D electro-thermal with a 3D thermal model and applied it for a 25 Ah pouch cell. They discuss the tab heat generation as the main source for the temperature non-uniformity throughout the battery. Samba et al. [16] developed a 2D thermal model of a 45 Ah cell considering radiation effects, and detailed tab heat generation. Murashko at al. [17] coupled an equivalent electrical circuit with a 3D thermal model and validated their model against experimental data for a 60 Ah pouch cell at 25°C ambient temperature for a 1C, 3C and 5C current discharge. Bazinski at al. [18] developed an analytical model to predict the heat generation of a 14.5 Ah LFP cell under different discharge rates.

Even though the topic of thermal modelling of li-on batteries has been broadly investigated, relatively few researchers within the literature have investigated the impact of ambient temperature over a wide range and most of them are limited to 25°C ambient temperature. In addition, simple lumped parameter models, such as those presented in Refs. [19,20], cannot provide sufficient details regarding power/capacity loss under different drive cycles/ambient conditions. To capture it, higher fidelity models, such as electrochemical models are required. Examples of electrochemical-thermal models validated at 25°C can be seen in Ref. [15] for a 2.3 Ah LFP cylindrical 26650 type cell operating up to 10C, a 10 Ah cylindrical LFP (a commercial type 38120) cell operating up to 2C [21], a 3D model of 10 Ah LFP pouch cell [22], a 15.7 Ah LiMn2O4/graphite pouch cell operating up to 5C [23,24] and a 3D thermal-electrochemical model for a single layer 45 Ah LFP pouch cell operating up to 4C [25]. As mentioned despite the importance of the ambient temperature only a few studies considered it. Smith et al. [26] developed a mathematical model coupling the1D electrochemical model to the lumped thermal model. They employed temperature dependent electrochemical properties in their model through application of the Arrhenius expression. Their model was validated for a 6 Ah, LCO/graphite lithium ion battery at 1C charge and discharge. They have also adapted the single cell model to model a battery pack containing 72 serially connected cells and the heat generation for a range of driving cycles and operating temperatures (e.g. −15 to 65°C). Wu et al. [27] developed a similar model using the same electrochemical parameters as in Ref. [26] and employed the model for investigation of the load