Journal of Energy Storage 18 (2018) 308–315

Contents lists available at ScienceDirect

Journal of Energy Storage

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

Dimensional analysis and modelling of energy density of lithium-ion battery

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ARTICLE INFO

Keywords:
Lithium ion
Battery
Energy density
Dimensional analysis
Modelling
Specific stiffness

ABSTRACT

A number of literature studies have shown that the energy density of lithium ion battery depends majorly on the particle radius, diffusivity, electric conductivity and thickness of the electrode. However, since the discovery of these major parameters, there has been no significant breakthrough in the present design technology to achieve successful design application in the Electric Vehicle industry. The energy density still ranges around 250Wh/kg on improvement and is insignificant compared to the energy produced by the internal combustion engine. Therefore, in this paper dimensional analysis is applied to lithium ion battery's energy density in order to obtain the sets of parameters that influence the performance with cathode material as reference. Five different cathode materials including; $LiMn_2O_4$, $LiFePO_4$, $LiCoO_2$, LiV_6O_{13}, and $LiTiS_2$ were used and the ranges for all material properties was selected based on reported data from literature. In order to bridge the gap in literature towards predicting the amount of energy obtainable from a specific electrode design, an empirical energy density model is proposed. Result showed that the specific modulus of the battery's electrode is a dominant factor for improving the energy density of the lithium ion battery compared to the particle radius, diffusivity and electrode thickness. Thus, in order to achieve a significant breakthrough, electrodes with high specific modulus are required. Designing an electrode with the characteristics of very low density, high compressibility factor, and high young modulus is necessary for an improved system performance. Thus, material combination of $LiCoO_2$/Aqueous-Lithium-air could give a practical breakthrough in achieving very high specific modulus and consequently high energy density. It is therefore suggested that focus on the mechanical/elastic property should not be geared only to its durability but also towards the energy density.

1. Introduction

In recent years, Lithium-ion batteries have attracted significant attention due to their high voltage and low weight, resulting in much higher achievable energy density than other battery technologies [1]. Their successful development and implementation in portable electronic devices has created further interest in their application in electric vehicles and aircraft [2]. Despite significant disparity in projections for oil prices and reserves, it is very likely that future oil prices will continue to increase, hence increasing the attraction of electric automobiles and aircraft. [3]. Batteries for electric vehicles are described by their relatively high power to weight ratio, energy to weight ratio. Smaller batteries reduce both cost and weight of the vehicle. It also enhances the performance of electric vehicle. Presently, battery innovations have much lower specific energy compared to fossil fuel, which also reduces the distance range of the vehicle. The energy density of presently available battery systems is limited to about 250 Wh/kg, which is about half of what is required in several classes of vehicles [4]. This is in large part due to a limited understanding of battery physics and limited use of systematic modelling and optimization techniques in the battery design process. Therefore, there exists a need to apply efficient schemes to gain a better understanding of the relevant physical phenomena occurring within battery cells.

Existing literatures has focused on improving the battery packs which yields little significance in the improvement of battery technology [5–7]. It has also been observed that on investigating the energy density of lithium ion batteries most studies concluded on specific significant parameters which can be varied to give an optimal battery performance. Such parameters include; Particle size, electrode surface area, porosity, electrode thickness and dimensions of current collectors [8–10]. An analytical model was developed by Newman et al. and co-workers [11] in order to optimize the thickness and porosity of the lithium ion battery for improved specific energy. Their result showed that the energy/current density is dependent on the C-rate, electrode thickness and porosity of the electrode. An experimental study on the maximum extractable energy from a battery cell was investigated by

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https://doi.org/10.1016/j.est.2018.05.002
Received 3 March 2018; Received in revised form 2 May 2018; Accepted 2 May 2018

Nomenclature

A,B	Regression coefficients
a_s	Reaction surface area
D^{eff}	Effective diffusion coefficient (Sm^{-1})
D_i	Diffusivity (m^2/s)
DOE	Design of experiment
E	Energy density(Wh/kg)
E_{cell}	Specific Energy(Wh/kg)
F	Faradays constant
I	Load current density (Am^{-2})
J	Reaction current density(Am^{-2})
K^{eff}	Effective conductivity(Sm^{-1})
L	Length
m_{cell}	Total weight of cell (kg)
R	Radial coordinate in spherical particle (μm)
R^2	Correlation factor
r_p	Particle radius (μm)
T	Time
t_{dis}	Discharge time(s)
T_e	Temperature(°C)
T_i	Electrode thickness
t_+^0	Transference number
U_{ocp}	Open circuit potential (V)
V	Terminal voltage
y	Dependent variable(Regression)

Greek letters

σ^{eff}	Effective conductivity (Sm^{-1})
Z	Dimensionless energy
Λ	Dimensionless diffusivity
Φ	Specific modulus(m^2/s^2)
Ψ	Experimental correlation coefficient function
δ	Dimensionless electrode thickness
ε	Volume fraction
θ	Correlation coefficient
φ_1	Electronic potential (V)

Singh et al. using a 320 μm thick electrode and 70 μm electrode for a lithium/graphite nickel manganese cobalt oxide. They showed that there is a reduction in capacity loss when using thicker electrode at low C-rates based on poor kinetics [12]. They suggested that using thick electrode will be suitable for applications which will require low C-rates. A gradient based method was applied by Golmon et al. [13] on a multiscale battery model in order to maximize the capacity using the porosity and particle size with the stress level of the cathode electrode as constraints. Timon et al. used the Newmans Psedo-2-Dimensional electrochemical model to investigate the influence of different particle size on the operation of porous electrode [14]. They found that smaller sizes of electrode solid particles improve the thermal characteristics of the battery, especially in higher charge and discharge currents. Their result also showed that as the solid particle sizes decrease, the battery capacity increases for various C-rates in charge and discharge cycles. The impact of particle size and electrode thickness on heat generation and battery performance was investigated by Wu et al. [15] using an electrochemical model-thermal model. Their result showed better performance with thin electrode coupled with temperature rise. Sensitivity analysis of a 2.3 Ah cylindrical battery was performed by Zhang et al. [16] using the Newman's P2D thermal model. They used about 30 parameters subjected under different operating condition in which 10 was found to be highly significant such as; the particle radius, volume fraction, diffusivity, contact resistance, activation energy and ionic conductivity. An electrochemical thermal model was developed by Edouard et al. [17] to investigate the sensitivity of major parameters involved in the aging of battery. They observed that the limiting factors are not consistent and could change depending on the battery design and operating conditions. A mathematical approach was conducted by Ghaznayi et al. [18] to study the lithium-sulfur battery using sensitivity analysis. They found out that fine size of electrode particles increases the performance of the cell. Du et al. [19] performed an experiment to quantify the relative parameter affecting the energy density of Lithium-ion battery using four significant parameters including particle radius, diffusivity and conductivity on the Li-ion based on data available in literature. They used kriging method, radial basis and polynomial response. They found that the particle radius and diffusivity are the most significant parameter when energy density is the major concern and that the electronic conductivity is of less importance.

Although, the dependence of battery cell performance on various morphological and operational variables has been investigated experimentally, they consist typically of sensitivity sweeps which involves varying one parameter at a time. For instance, the effect of cycling rate was investigated by Tran et al. which involve parametric sensitivity analysis [20]. Their result showed that the cycling rate changes differently for different particle size. Lu and Lin experimental investigation of the battery performance found that the coulomb efficiency and capacity of $LiMnO_2$ substantially increases as the particle size reduces [21]. Also, experimental investigation by Monge et al. [22] observed that the particle size of the $LiMnO_2$ have critical influence on the performance of the battery. By considering most these studies, it has been established that the particle radius, diffusivity, electrode thickness and conductivity are the most significant factors needed to optimize the present state of the lithium ion battery. However, there has been no significant change in the energy density of the lithium ion battery.

Dimensional analysis can be used to develop a form of generalized model equation which can further be fit into an experimental data for specific characterization and performance prediction. Dimensional analysis is the basis of the similarity concept. Generally, most energy systems make use of this concept of modelling and have been successfully applied in internal and external combustion engines such as gas turbines, rocket engine Stirling engines e.t.c. However, the validity of the empirical correlations or equations obtained depends on the respective assumptions made to simplify the theoretical model or ranges taken into account during the design of experiment and experimental measurements.

This paper uses the concept of dimensional analysis to model and locate the fundamental parameters necessary to achieve a significant breakthrough in energy density of lithium ion battery technology with the possibility of extending towards other battery technology.

1.2. Governing Equations of lithium ion battery

Generally, battery models can be classified into; (a) Equivalent circuit models (b) Multiphysics models (c) Electrochemical models and (d) Molecular models. The complexity of these battery models differs depending on the level of details included. Electrochemical models are often commonly used to carry out investigations. The most common electrochemical model used in literature is the Pseudo-2-dimensional model which was first developed by Newman [23]. The set of governing equations typically used in the electrochemical model are derived in Eqs. (1)–(14) along the axial distribution in the solid and liquid phase.

$$\nabla(\sigma^{eff}\nabla\phi_1) - J = 0 \tag{1}$$

$$\nabla K^{eff}\nabla\phi_2) + \nabla(K_D\nabla(lnc_2)) + J = 0 \tag{2}$$

According to [16], the diffusion in the liquid phase is given by Eq. (3) as follows;