U. Iraola, I. Aizpuru, J. M. Canales, A. Etxeberria and I. Gil, "Methodology for thermal modelling of lithium-ion batteries," IECON 2013 - 39th Annual Conference of the IEEE Industrial Electronics Society, 2013, pp. 6752-6757.

DOI: https://doi.org/10.1109/IECON.2013.6700250

Methodology for thermal modelling of lithium-ion batteries

U.Iraola, I.Aizpuru, J.M.Canales, A.Etxeberria
Computing and Electronics department
Faculty of Engineering, University of Mondragon
Mondragon-Arrasate, Spain

I.Gil
Electronics department
Orona eic s.coop
Hernani, Spain

Abstract— **Temperature is a determinant parameter in terms of performance, lifespan and safety working with li-ion batteries. Working above 45ºC, in hot climates, has direct influence in the cycle life of the battery and can cause a dangerous failure if higher temperatures are reached; besides, performance of li-ion batteries in cold climates is very poor due to the high internal resistance they present under these ambient conditions. Being able to predict the temperature of a li-ion cell or the temperature distribution in a module for any working condition without testing the device is considered important when designing energy storage systems based on li-ion batteries. Thus, this paper presents a methodology to achieve the equivalent thermal parameters governing the behavior of a single li-ion cell and the power losses within it; different experimental tests are combined with an analytical expression of the power losses inside a cell to reach this target. The parameters obtained are used to develop a model in *matlab/simulink* and another model solved with *CFD* software. Simulation results show good agreement with experimental results with a maximum error of 2ºC committed during the validation of the methodology.**

Keywords— Thermal equivalent model; Li-ion cell; behavioural model.

I. INTRODUCTION

Advances in the field of energy have contributed significantly to the development of society up to the present situation, and its consumption is increasing day by day. The lack of natural resources joined to the high consumption requires looking for the highest possible efficiency and adding alternatives to support the energy demand; renewable energies are a real alternative to support energy production, but there are other alternatives to improve the present situation. Energy storage is presented as an important option because it presents important advantages: the ability to work without a grid connection and make autonomous systems; and the capacity to accumulate energy from different energy sources and use it to support the grid when the energy demand is higher. There are different ways to accumulate energy; mechanically with flywheels, electrically with supercapacitors or thermally with steam accumulators... However, nowadays, energy storage systems based on electrochemical devices, also called batteries, are commonly used in several applications.

Different battery technologies have been grown up since the first battery appeared; lead-acid, nickel metal hydride, nickel cadmium and lithium-ion (li-ion) batteries are the most representative ones. However, li-ion technology is mostly used today in portable applications, and there is increasing interest in using this technology for power applications. High power applications require high voltage and current levels and thus, large battery packs. The high energy and power density of li-ion batteries is then an important advantage against other technologies when large battery packs are needed.

High power demands increase Joule effect power losses and temperature can reach undesirable values. This hot ambient directly affects the cycle life of the battery [1] and can be dangerous if temperature is not under control above 60 ºC because *thermal runaway* phenomenon can be triggered [2]. Conversely, cold climates (0-10ºC) also worsen the performance of the li-ion battery because of the increase in their internal resistance under cold environments; besides, cycling the battery in very cold climates (<10ºC) can damage the battery irreversibly and reduce its capacity under 80% in a few cycles [1]. Thus, it is important to keep the battery temperature within a safe range (commonly 20-40 ºC) for any working condition [3].

In this context, it is considered essential to study the thermal modeling and simulation as a tool to predict the behavior of the temperature within the battery under different working and ambient conditions without the necessity of doing the experimental test.

Internal heat generation (*q)* is the first parameter to calculate for any thermal model. In bibliography different equations are found depending on the assumptions made by the author. In *electrochemical models* chemical and electrical aspects are taken into account when calculating *q* [4–7]. However, *models based on experimental tests* commonly use the equation proposed by *Bernardi et al.* in [8]; experimental data and electrical variables are needed to calculate the internal heat generation parameter with this equation [9–12].

Temperature distribution is the other parameter achieved in a thermal model; two different modeling techniques have been identified in this field, *behavioral models* and *analytical models*. The *analytical models* solve the differential equation governing the energy balance in the battery [12], as in *finite element models*, since *behavioral models* use electrical equivalent circuits to predict the evolution of the cell

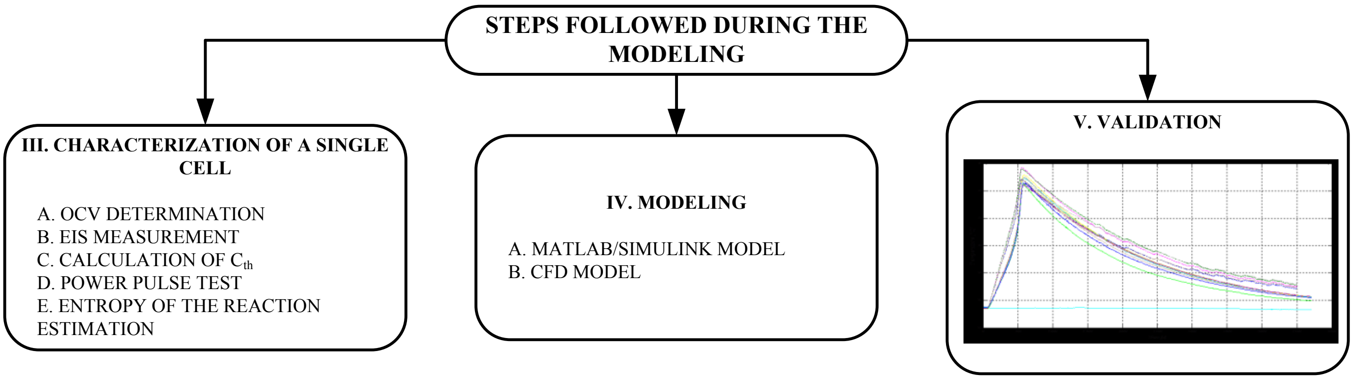


Fig. 1. Steps followed during the modeling of a single cell.

temperature [13]. *Finite element models* are commonly time consuming but also more accurate since a temperature distribution is calculated throughout the battery. *Behavioral models* instead, are faster and easier to develop but usually calculate an average temperature for the whole battery and thus, are less accurate.

The lack of information concerning the different materials within the cell in terms of thermal properties and dimensions makes the option of the *behavioral model* very attractive to reach the desired thermal model. Thus, this paper presents a methodology to obtain the parameters of a *behavioral model* for a concrete li-ion battery, the parameters of the equivalent electrical circuit that predicts the behavior of the cell under different working conditions.

Besides, the average thermal properties of the cell obtained from the *behavioral model* are used to define a simple 3D model solved with *CFD*; the target is to conduct module level simulations with different ambient conditions.

The cell used in this work to obtain the results presented is a prismatic 6.5 Ah $LiFePO_4$ power cell.

II. CHARACTERIZATION OF A SINGLE CELL

The following chapter presents the experimental tests done to do the thermal characterization of a single lithium-ion cell.

A. *OCV determination*

In this work a *linear interpolation method* [14] has been developed to determine the *OCV*. The *linear interpolation method* consists of doing a complete charge and discharge to the battery with a very low current rate *(C/20)*; the overpotential effect is neglected and the *OCV* is considered equal to the terminal voltage. Resulting *OCV* curves for the cell under test are shown in Fig. 2.

B. *EIS measurement*

An *electrochemical impedance spectroscopy* analysis has been done to measure the impedance of the cell in different points of the *SOC* at different frequencies. The frequency range used for this analysis has been 6.5 kHz to 1Hz. The goal is to find the value of the frequency at which the impedance of the cell is purely resistive for a concrete *SOC*, and the value of this impedance. Fig. 3 shows the resulting curve for a *SOC* value of 50% and at room temperature.

C. *Power pulse generation test*

After determining the values of the impedance R_0 and the frequency f_0 for a concrete *SOC*, in this case *50%*, the *power pulse generation test* has been conducted. This experimental test consists of applying a sinusoidal current of frequency f_0 and big amplitude (30 A rms in this work) to the cell to generate a constant power losses profile within it (1). In this case the amplitude of the constant pulse has been 0.879 W.

$$q_0 = R_0 (I_{rms})^2 \tag{1}$$

This procedure has been obtained from Schmidt et al. work [15]. Fig. 4 shows the results obtained from this test; the evolution of the measured temperature is similar to a 1st order model response.

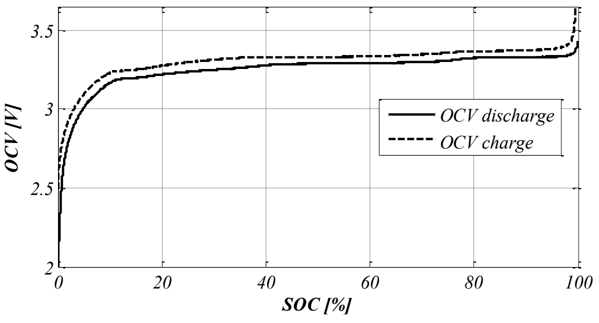


Fig. 2. *OCV* results for the cell under test.

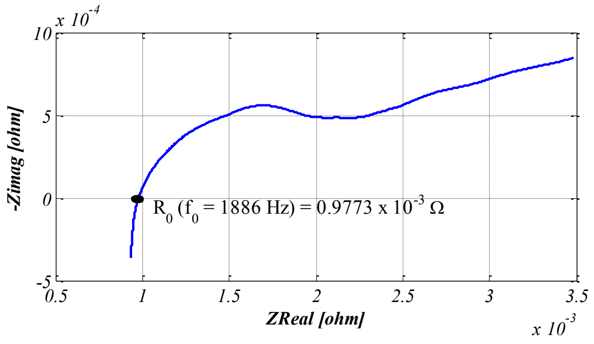


Fig. 3. EIS measurement at 50% of the *SOC*.

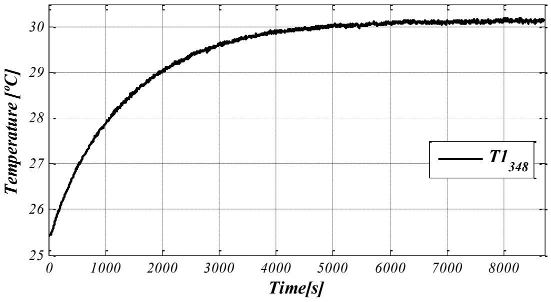


Fig. 4. Experimental results of the temperature on the surface of the cell during the power pulse generation test.

D. *Calculation of the heat capacity of the cell (C_{th})*

An important parameter to be able to predict the thermal behavior of the li-ion cell is the heat capacity C_{th}. In this work an average value of the heat capacity for the overall cell has been calculated conducting an experimental test. Other authors estimate it from the heat capacities of each material within the li-ion cell; however, this data about the materials and their thermal properties is not usually accessible and experimental estimations are conducted with calorimeters in some studies.

Due to the absence of such equipment, another experimental test has been conducted to estimate C_{th}. Four thermocouples are placed on the surface of a single cell under test, and the cell is covered by a protection layer; then the cell and the protection layer are inserted in a tube and this tube is filled with a thermal insulation material. This material solidifies and the cell is trapped in it with the connection and measurement wires out from the structure; Fig. 5 shows the final assembly of the experimental test. With this assembly heat cannot be evacuated to the environment and all the heat generated inside the cell is accumulated within it.

In order to generate heat inside the cell the same procedure as in *power pulse generation test* is followed. In this case a constant heat pulse of $q_0 = 0.543$ watts has been generated.

Fig. 6 shows one of the surface temperatures resulting from the experimental test. From these results the value of Δt/ΔT is obtained, and the average heat capacity C_{th} of the cell is calculated with (2). In this case, the value achieved for C_{th} is 272 [J/ºC].

Fig. 5. Final assembly of the experimental test.

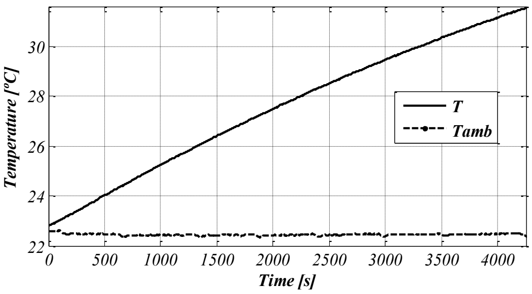


Fig. 6. Resulting evolution of the surface temperature of the cell.

$$C_{th} = \frac{q_0 dt}{dT} \tag{2}$$

E. *Experimental determination of the entropic heat coefficient ($\partial OCV_{avg}/\partial T$)*

The last step is to conduct another experimental test to evaluate the *entropic heat coefficient* of the li-ion cell. This experimental test consists of evaluating the variation of the *OCV* for different *SOC* values when the temperature of the cell changes. In order to do that, the cell is placed inside a climate chamber and the temperature is varied; meanwhile, the *OCV* of the cell and the surface temperature are measured and their variation is quantified. The same process is applied for 8 different *SOC* values.

Fig. 7 shows the resulting variation of *OCV* and surface

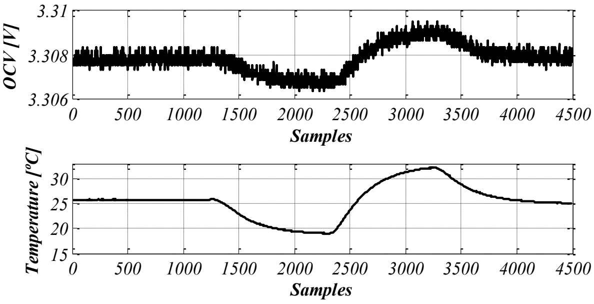


Fig. 7. Variation of the *OCV* when the room temperature changes.

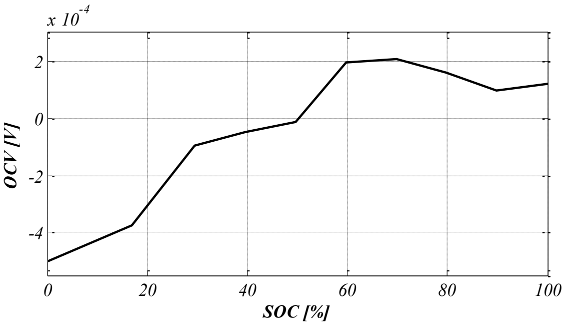
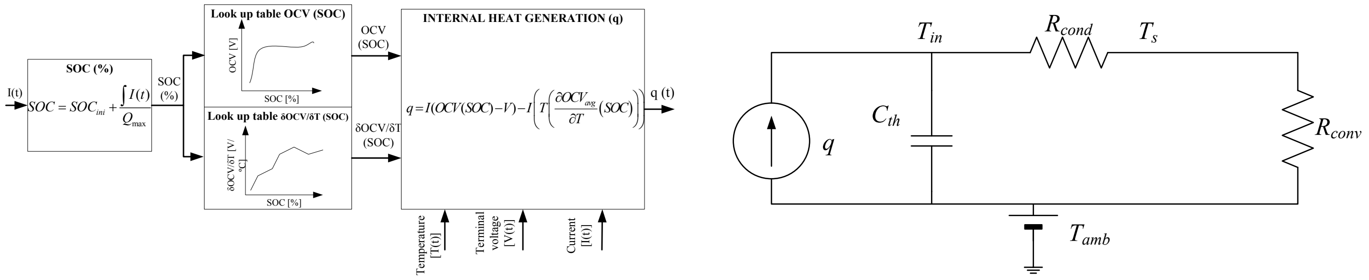


Fig. 8. *Entopic heat coefficient* depending on the value of *SOC.*



a)

b)

Fig. 9. a) Internal heat generation model in matlab/simulink; b) Thermal equivalent model of the cell utilized in matlab/simulink.

temperature for a *SOC* of 58%. The quantification of the *entropic heat coefficient* has been done when temperature rises from 18º C to 32º C following (3).

$$\frac{\partial OCV_{avg}}{\partial T} = \frac{OCV_{avg}(T_{\max}) - OCV_{avg}(T_{\min})}{T_{\max} - T_{\min}} \qquad (3)$$

After doing the same process for 8 different *SOC* values, Fig. 8 shows the resulting *entropic heat coefficient.* The values obtained show good agreement with other authors values; in power applications, the demanded current levels are quite high, and thus, power losses due to *Joule effect* will be high comparing them with the *entropic losses.* When a power application current profile is studied, the *entropic power losses* in li-ion cells could be neglected.

III. MODELING

During next chapter the simulation models used in this work are going to be explained. Firstly, a model developed with *matlab/simulink*, and after that, a simulation model solved with a *Computational fluid dynamics* (*CFD)* simulation tool. The parameters achieved during the *characterization chapter* are used to develop both simulation models.

A. Matlab/Simulink model

This model is divided into two main parts, the internal heat generation of the li-ion cell, and the estimation of the surface temperature. It is an iterative process, each time step the surface temperature of the cell is calculated and feed backed to the internal heat generation calculator because this variable is temperature dependent. Then, the internal heat generation is applied into the thermal equivalent model shown in Fig. 9 b) to calculate the surface temperature again.

1) Internal heat generation

The internal heat generation calculation in this work is based on the equation of Bernardi et al.[8], equation (4) in this document. The *q* value calculated is an average value of the whole cell, it is not spatially dependent.

$$q = I(OCV_{avg}(SOC) - V) - I(T(\frac{\partial OCV_{avg}}{\partial T}(SOC))) \qquad (4)$$

Fig. 9 a) shows the *internal heat generation* model used in this work. The *OCV* and the $\partial OCV_{avg}/\partial T$ are *SOC* dependent; the instantaneous values of these parameters are calculated using look up tables. Equation (4) also requires the instantaneous value of the terminal voltage *(V)* , the charge or discharge current *(I)*, and cell temperature *(T)*. The terminal voltage and the current are measured during the experimental test and are inputs of the equivalent model. Temperature instead is calculated by the equivalent model and fed back to calculate the *internal heat generation* of the cell.

2) Calculation of the parameters of the equivalent model

Once the *internal heat generation* is calculated, the estimation of the surface temperature is done. Fig. 9 b) shows the thermal equivalent model of the cell used in this work [13]; this model is composed by an internal heat generation inside the cell *q (W)*, a thermal capacity C_{th} *(J/ºC)*, a resistor modelling the conduction R_{cond} *(ºC/W)*, and a resistor modelling the convection R_{conv}*(ºC/W)*. T_s*(ºC)* is the temperature on the surface of the cell, T_{amb}*(ºC)* is the ambient temperature and T_{in}*(ºC)* is the temperature inside the cell. The value of the conduction resistor determines the temperature difference between inside and the surface of the cell. The convective resistor instead, the temperature difference between the surface and the ambient. Heat capacity determines the dynamics of the temperature inside and on the surface of the cell.

The equation governing the evolution of the surface temperature *(T_s)* of the cell for a constant ambient temperature T_{amb} has been calculated (5).

C_{th} has been previously calculated in II.D; convection resistor R_{conv} and conduction resistor R_{cond} have been obtained from Fig. 4 results.

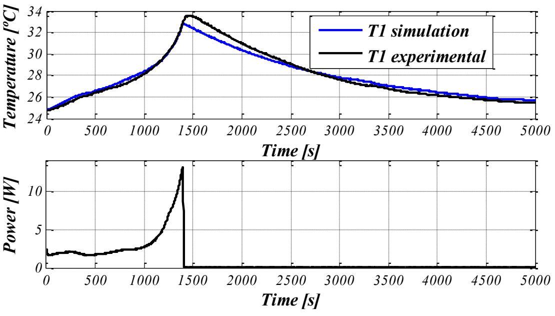


Fig. 10. Comparison between simulation and experimental results for a 3C complete discharge.

TABLE I

THERMAL EQUIVALENT CIRCUIT PAREMETERS

Parameter	Value
C_{th}	272 [J/ºC]
R_{cond}	1.8 [ºC/W]
R_{conv}	3.371 [ºC/W]

$$T_s(t) = T_{amb} + R_{conv} q \left(1 - e^{\left(\frac{-t}{C_{th}(R_{cond} + R_{conv})} \right)} \right) \tag{5}$$

When the surface temperature reaches the steady state, the convection resistor can be calculated with equation (6). Then, the conduction resistor R_{cond} is calculated from (5) because it is the last unknown term.

$$R_{conv} = \frac{(T_s - T_{amb})}{q_0} \tag{6}$$

The values of the parameters of the equivalent thermal circuit obtained for the cell under test are presented in TABLE I.

3) *Model validation*

Fig. 10 shows the results obtained by the model for a 3C complete discharge process. In the upper figure the predicted surface temperature and the experimental measurement; in the down figure the *internal heat generation* estimated by the model. This estimation has not been validated due to the absence of a calorimeter to compare the results. However, the results obtained predicting the surface temperatures of the cell under test are accurate enough to think that the error committed is not excessive. The error committed in the temperature approximation during the simulation is acceptable since a *behavioral model* with average parameter estimation has been used.

B. CFD model

The absence of information regarding to the materials within cells and their dimensions make difficult to build up a layered 3D model of a single li-ion cell like in [16]. Although the accuracy obtained with a layered model is high for a single cell model, the time consumed by the simulation in a layered 3D model for a battery module or pack could be excessive.

Thus, a simple 3D model has been developed in this work to evaluate the surface temperature of li-ion cells for single cells and modules. The assumptions made for a single cell level simulation are the following ones:

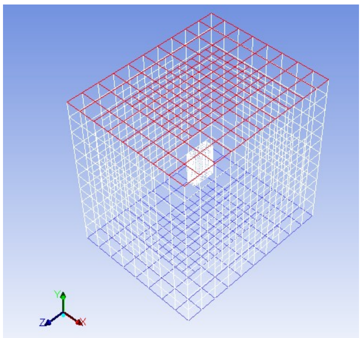


Fig. 11. Single cell simulation model.

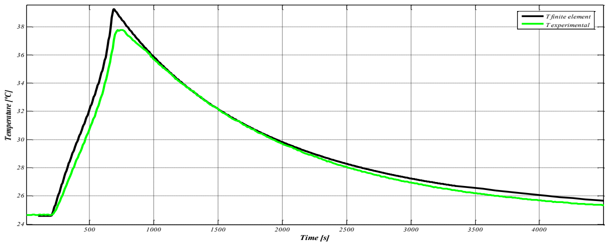


Fig. 12. 7.69C complete discharge results for the *CFD* model.

- Cell is considered a single body with user defined thermal properties; *specific heat (J/kgºC)*, *isotropic thermal conductivity (W/ºC m)* and *constant density (kg/m^3).*
- The *internal heat generation rate (W/m^3)* of the cell is considered uniform for the whole body.

The *specific heat* and the *isotropic thermal conductivity* are the same values as the ones obtained for the *matlab/simulink* thermal equivalent model III.A; the value of *density* is obtained from the specifications of the cell; the *internal heat generation rate* is also obtained from this model and applied as an input to the *CFD* model.

Fig. 11 shows the setup of the single cell level 3D simulation. In all the simulations, heat is transferred from the surface of the cell to the ambient by *natural convection*.

Fig. 12 shows the result obtained from the simulation for a 7.69C complete discharge of the cell under test. As mentioned before, the *internal heat generation* applied in this model is first obtained with *matlab/simulink*. The result shown is the average value of the surface temperature of the cell and it is compared with the measurement acquired on the surface of the cell experimentally. An error is committed in the prediction but it is considered a good result due to the simplicity of the model.

IV. CONCLUSIONS

This paper presents a methodology based on experimental tests to calculate the parameters of an equivalent thermal model for lithium ion cells. These parameters are used to build up a model in *matlab/simulink* and a 3D model solved with *CFD* software. According to the modeling of the internal heat generation of a li-ion cell, it is concluded that *Bernardi´s* equation and the assumptions made are adequate to achieve a good approximation of this parameter. The validation of the equation has been done in an indirect way, measuring temperatures on the surface of the cell and comparing them

TABLE II

THERMAL PROPERTIES OF THE CELL FOR THE 3D MODEL

Parameter	Value
Specific heat [c_{th}]	700 [J/kgºC]
Density [ρ]	2089 [kg/m^3]
Thermal conductivity [k]	1.08 [W/mºC]

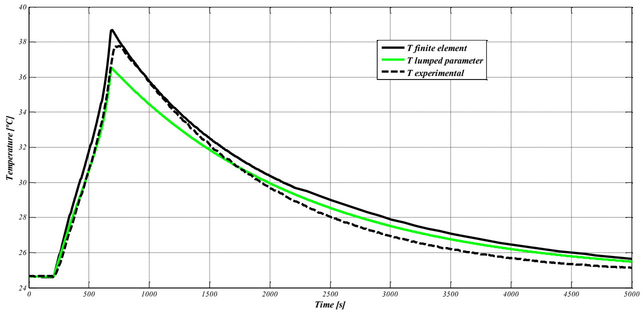


Fig. 13. Comparison between the experimental results and both models under a 7.69C discharge rate.

with the ones achieved from the *matlab/simulink* model, in which the heat generation is calculated. However, it is considered important to have special equipment to measure the amount of heat generated by the cell permitting a direct validation of the equation of *Bernardi*.

Talking about the *matlab/simulink*, it is concluded that a 1st order *RC* thermal equivalent circuit is able to predict the behavior of the surface average temperature in the cell under test. However, an error is committed during the simulations and improvements in terms of accuracy during experimental tests and increasing the order of the equivalent thermal circuit could benefit the overall results. On the other hand, the methodology described to estimate the parameters of the equivalent *RC* circuit is considered to be adequate according to the results obtained during the fitting of the parameters.

The main advantage of a 3D model is that temperature distributions can be calculated and in the model presented in this paper average surface temperatures are presented. The reason for this is because this model is going to be used in the future to calculate temperature distributions within li-ion battery modules, not in a single cell level. However, the validation of the model has been done with a single cell before including battery modules. Furthermore, in commercial battery packs it is typical to have at most a single measurement per cell; thus, it is considered useful to have a 3D battery model to get an average temperature per cell when battery modules or packs are under simulation.

REFERENCES

[1] J. Wang, P. Liu, J. Hicks-Garner, E. Sherman, S. Soukiazian, M. Verbrugge, H. Tataria, J. Musser, and P. Finamore, “Cycle-life model for graphite-LiFePO4 cells,” *Journal of Power Sources*, vol. 196, no. 8, pp. 3942–3948, Apr. 2011.

[2] T. M. Bandhauer, S. Garimella, and T. F. Fuller, “A Critical Review of Thermal Issues in Lithium-Ion Batteries,” *Journal of The Electrochemical Society*, vol. 158, no. 3, p. R1, 2011.

[3] A. Pesaran, S. Burch, and M. Keyser, “An approach for designing thermal management systems for electric and hybrid vehicle battery packs,” *Fourth Vehicle Thermal Management Systems Conference and Exhibition*, no. January, 1999.

[4] G. G. Botte, V. R. Subramanian, and R. E. White, “Mathematical modeling of secondary lithium batteries,” *Electrochimica Acta*, vol. 45, no. 15–16, pp. 2595–2609, May 2000.

[5] P. M. Gomadam, R. E. White, and J. W. Weidner, “Modeling Heat Conduction in Spiral Geometries,” *Journal of The Electrochemical Society*, vol. 150, no. 10, p. A1339, 2003.

[6] K. Kumaresan, G. Sikha, and R. E. White, “Thermal Model for a Li-Ion Cell,” *Journal of The Electrochemical Society*, vol. 155, no. 2, p. A164, 2008.

[7] M. W. Verbrugge, “Three-dimensional temperature and current distribution in a battery module,” *AIChE Journal*, vol. 41, no. 6, pp. 1550–1562, 1995.

[8] D. Bernardi, E. Pawlikowski, and J. Newman, “A general energy balance for battery systems,” *Journal of The Electrochemical Society*, vol. 132, no. 1, 1985.

[9] S. Al Hallaj, H. Maleki, J. S. Hong, and J. R. Selman, “Thermal modeling and design considerations of lithium-ion batteries,” *Journal of Power Sources*, vol. 83, no. 1–2, pp. 1–8, Oct. 1999.

[10] S. Chen, Y. Wang, and C. Wan, “Thermal analysis of spirally wound lithium batteries,” *Journal of the Electrochemical Society*, vol. 153, no. 4, 2006.

[11] K. Onda, T. Ohshima, M. Nakayama, K. Fukuda, and T. Araki, “Thermal behavior of small lithium-ion battery during rapid charge and discharge cycles,” *Journal of Power Sources*, vol. 158, no. 1, pp. 535–542, Jul. 2006.

[12] S. Chen, C. Wan, and Y. Wang, “Thermal analysis of lithium-ion batteries,” *Journal of power sources*, vol. 143, no. 9, 2005.

[13] C. Forgez, D. Vinh Do, G. Friedrich, M. Morcrette, and C. Delacourt, “Thermal modeling of a cylindrical LiFePO4/graphite lithium-ion battery,” *Journal of Power Sources*, vol. 195, no. 9, pp. 2961–2968, May 2010.

[14] V. Pop, H. J. Bergveld, D. Danilov, P. P. L. Regtien, and P. H. L. Notten, *Battery Management Systems: Accurate State-of-Charge Indication for Battery-Powered Applications (Philips Research Book Series) (Philips Research Book Series)*, 1st ed. Springer Publishing Company, Incorporated, 2008.

[15] J. P. Schmidt, D. Manka, D. Klotz, and E. Ivers-Tiffée, “Investigation of the thermal properties of a Li-ion pouch-cell by electrothermal impedance spectroscopy,” *Journal of Power Sources*, vol. 196, no. 19, pp. 8140–8146, Oct. 2011.

[16] S. C. Chen, C. C. Wan, and Y. Y. Wang, “Thermal analysis of lithium-ion batteries,” *Journal of Power Sources*, vol. 140, no. 1, pp. 111–124, Jan. 2005.