1D-thermal analysis and electro-thermal modeling of prismatic-shape LTO and NMC batteries

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***Abstract*—In order to accurately predict and optimize the thermal behavior of batteries, a thermal model using heat equation and thermal parameters, such as the specific heat capacity, is developed. The specific heat capacity is an important parameter for this type of modelling and is determined with a simple method without using any calorimeter. This paper chooses two types of prismatic cells: lithium titanate (LTO) anode-based cell and nickel manganese cobalt oxide (NMC) with 23 Ah and 43 Ah, respectively. Validation was made by comparing the simulation results with experimental work for which an error of less than 3% was shown.**

Keywords—Lithium-ion battery; thermal behavior; specific heat capacity; LTO; NMC

I. Introduction

Thermal modeling of LiBs has been well documented in the literature [1]–[6]. It often starts with the simple heat balance equation of point that estimates the evolution of the temperature with the generated heat and the heat losses over a transient state of energy.

Differences in modeling complexity can be found in the literature such as 1D, 2D or 3D[7]–[9]. They use either few points to program a temperature calculation model or for more detailed modeling, many points like in finite element modeling. As a general rule in modeling, a tradeoff between complexity and accuracy must be reflected.

Moreover, for all these models, parametrization is a crucial step in which thermal parameters are assessed to ensure the functionality of the model. One parameter which is critical in the establishment of a thermal model is the specific heat capacity or C_p [10], [11]. The C_p reflects the energy required for a system to change its temperature (1°C). Thus, the specific heat is essential for temperature calculation. However, depending on the level of complexity of the model, several values of C_p can be used to represent the different parts or materials of the dedicated system [6], [7].

One usual manner to determine the C_p is to use calorimetry [12], [13]. However, such equipment is quite expensive especially when the tested cell presents high volume such as prismatic-shape cells. Another way is to deconstruct the cell and calculate the weighted sum of the specific heat capacity of the materials inside the cell. Except by having detailed information of the cell which is often disclosed by manufacturers, again thorough equipment is required which is not commonly available in a battery research lab.

In this paper, we propose a method to assess this parameter without the use of any calorimeter. The methodology lies in applying pulse discharge and charge capacity test at a certain SOC point. For that, battery tester, thermocouples, and climate chambers are the only equipment required for this method. We investigated this method on two battery technologies: high-power and high-energy, lithium titanium oxide (LTO) and nickel manganese cobalt oxide (NMC), respectively.

Moreover, in order to validate the values of the C_p, an electro-thermal model of the cells is developed based on the semi-empirical principal. The methodology is validated at different temperatures and with fairly-representative driving cycle. This provides robust validation of the models as well as solid and novel data of LiB technologies.

The paper is organized as follow: section II describes the model development, section III the experimental setup, section IV discusses the results and finally, conclusions are given in section V.

II. Model development

A. Modeling description

In this study, a 1D electro-thermal model is used. The model is based on the semi-empirical approach in a MATLAB/Simulink® interface. The aim of the model is to reproduce the cell's electrical and thermal performances with two parts: the electrical and thermal parts, as shown in Fig. 1.

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The complete detail of the model will be presented in the full paper

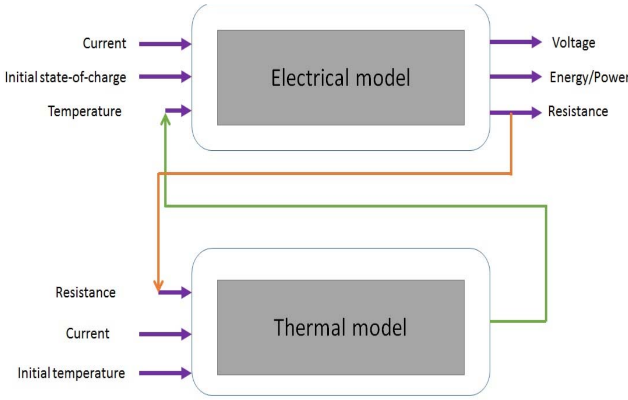


Fig. 1. Schematic of the modeling methodology [2].

B. Estimation methodology

In this paper, the method used to assess the specific heat capacity and the convective heat transfer coefficient involves high current rate in order to reach the thermal steady state of the system for which the Q_{gen} is equal to Q_{loss}. In this state, the cell starts to lose the same amount of heat it is gaining. Thus, equation 5 can be written:

$$Q_{conv} = h_{conv} S_{area} (T_s - T_{air}) = Q_{gen} \tag{6}$$

In equation 6, there is one unknown, h_{conv}, the other parameters are either inputs, obtained from the experimental test (T_s) or estimated by the electrical model (Q_{gen}).

Once the convective heat transfer coefficient is obtained, an estimation fitting algorithm in Matlab/Simulink is used to fit the simulation and experimental data and extract the specific heat capacity parameter in the transient state. In this algorithm, the pre-estimated value of h is used to remove one unknown and least-square regression is employed resulting from its fair accuracy. The estimation is then repeated for different temperatures. Fig. 2 reports the parameter estimation methodology chart.

III. Experimental Setup

In this section, the test bench, as well as the experiment protocol for characterizing the specific heat capacities of the cells, is described.

A. Battery overview description

In this paper, two cells are investigated. Both are prismatic and their chemistries are lithium nickel manganese cobalt oxide (NMC), and lithium titanate oxide (LTO). Specific details can be found in the table I

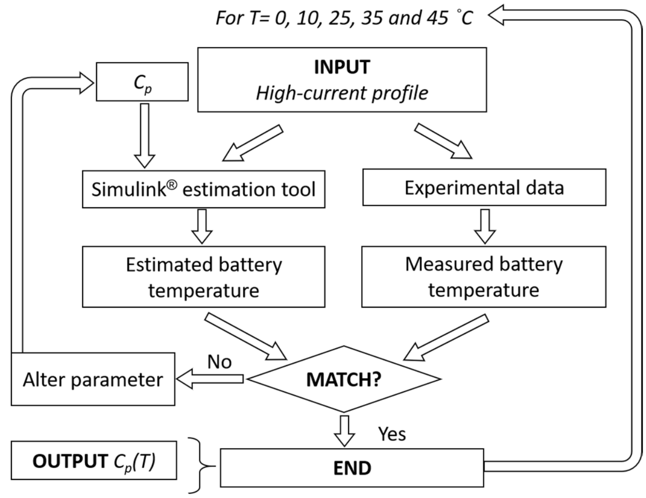


Fig. 2. Schematic of the parameter estimation methodology

TABLE I. Characteristics of the prismatic cells

Information	NMC					
	Dimensions (mm)	*Weight (kg)*	*Nominal capacity (Ah)*	*Operating voltage (V)*	*Max charge current (A)*	*Energy density (Wh/kg)*
Value	27.5*148*91	0.840	43	3-4.2	96 (2C)	200
Information	LTO					
	Dimensions (mm)	*Weight (kg)*	*Nominal capacity (Ah)*	*Operating voltage (V)*	*Max charge current (A)*	*Energy density (Wh/kg)*
Value	115*22*103	0.550	23	1.5-2.7	184 (8C)	96

a. According to the manufacturer's data

b. According to the manufacturer's data

B. Test setup description

In this study, for the experimental part, a test bench was built in the MOBI laboratory of the Vrije Universiteit Brussel. It consists of equipment commonly found in a battery dedicated laboratory:

- Battery tester is able to charge and discharge a cell and monitor the voltage, current, and temperature.
- One K-type thermocouple for the surface of the cell.
- Climate chamber to control the environmental temperature.
- Infra-red (IR) camera for validation.

In more details, a module ACT 0550 (80 channels) battery tester (PEC®) was used for the testing of the cells. For the validation, a Ti25 thermal camera captured IR images at regular time intervals. Because of the non-reflective casing of the LiBs, the surface of the cell was directly exposed to a climate chamber to recreate the environmental condition of any ambient temperature. The LTO cell was characterized at 0°C, 10°C, 25°C, 35°C and 45°C while the NMC cell was characterized at 0°C, 10°C, 25°C and 45°C. At the start of the test, all cells are charged to the same level and during the test, the voltage is monitored and controlled by the PEC tester.

C. Test profile

The profile used in this paper to assess the specific heat capacity involves charging and discharging pulses at the manufacturer's recommended maximum rates. The profile is called a micro-pulse and is conducted at a fixed SOC of 50% and it is shown for the LTO cell in Fig. 3. The first goal of this profile is to extract and inject the same number of Ah to the cell, in order to not have a dependency of the SOC, which can influence electrical and thermal parameters such as the cell resistances. The second aim to this profile is to reach rapidly a constant temperature at which the cell starts to lose the same amount of heat it is gaining (steady state), where thermal parameters such as convective heat transfer can be obtained. As for the C_p, the period for which the surface temperature is increasing (transient state) is considered for comparison with the model. Then, the test profile is repeated at different temperatures to obtain the parameters against the thermal gradient.

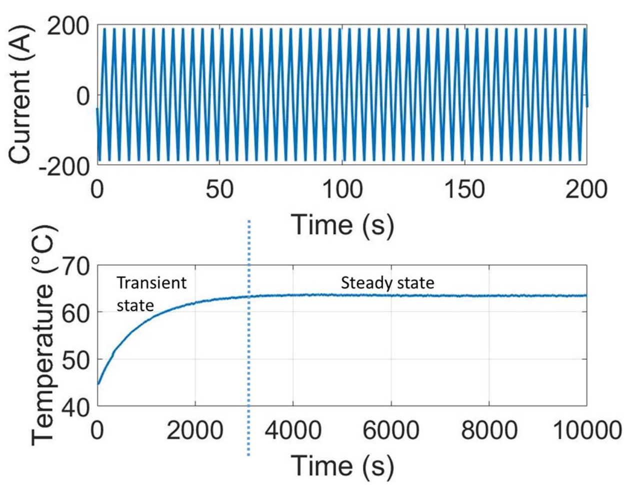


Fig. 3. Example of a micro-pulse test at 25°C.

D. Model parameters

The model parameters will be presented in the full paper.

E. Temperature measurement

For every test, a maximal allowable temperature is defined to prevent gassing and critical failure of the cell resulting from overheating and thermal runaway. Also, the evolution of the temperature is an important parameter for designing a thermal model. Thus, it is necessary to have a reliable way of measuring battery temperature.

Because only one point of the battery can be measured for temperature, this point has to be carefully chosen. Heat source diffusion has already been made with the cells chosen in this study.

To verify the proper place of the thermocouple, high-current discharge tests at maximum discharging C-rate, 8C and 2C for LTO and NMC, respectively, were performed and recorded by using infrared (IR) imaging. In this context, the experimental result of the cell's surface temperature distribution at 25°C was obtained and it is displayed in Fig. 4.

From the figure, it can be observed that the point of high interest is located near the negative tab. Therefore, the k-type thermocouple will be placed on this spot during the thermal characterization.

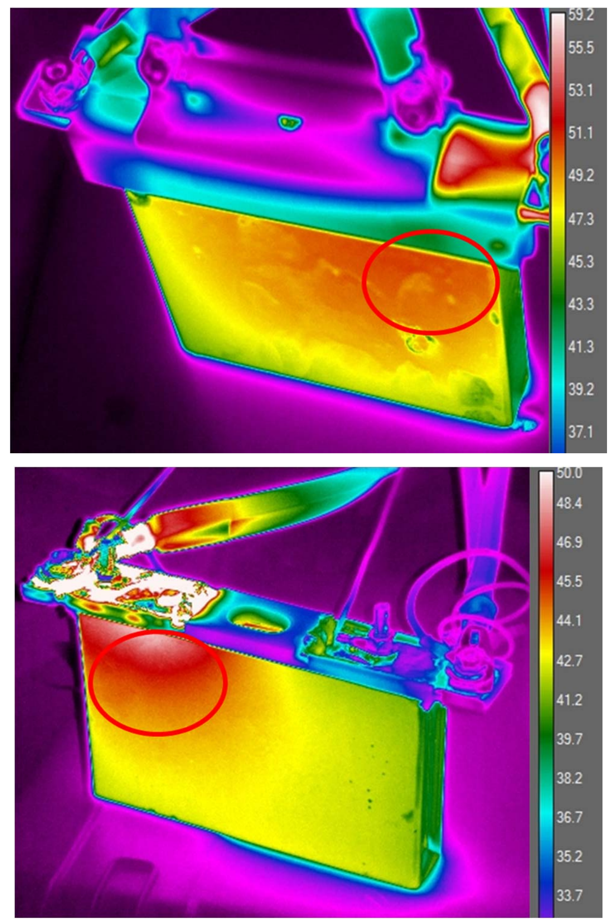


Fig. 4. Temperature points of interest for the LTO (top) and NMC (bottom) cells.

IV. Results and Discussion

The experiments using the micro-pulsing profile are conducted and, in this section, the results for the specific heat capacities and convective heat transfer are given. The thermal results are presented first with the specific heat.

As explained in the previous section, to assess the C_p, the micro-pulse test is carried out. However, the convective heat transfer coefficient is unknown and requested for the C_p

assessment. To determine the external convective coefficient, h, equation (6) is used in a parameter estimation algorithm in a time period describing the steady state, which is reached when the maximal temperature is attained and remains constant.

For Q_{gen}, the average value of the heat generation of the test after 20 min is used. The heat generation is calculated with the electrical model described before and is 8W for a 2C-micro-pulse test for the NMC-based cell and 20.5W for an 8C-micro-pulse test for the LTO-based cell. The ambient temperature is fixed to the tested temperature (0°C, 10°C, 25°C, 35°C and 45°C for the LTO cell and 0°C, 10°C, 25°C, and 45°C for the NMC cell), as for the final battery temperature, it is extracted from the experimental results as the final temperature point after 20 min of testing.

In order to assess the C_p, the same technique is used, however, only the period when the temperature of the surface of the cell is rising. The period of time goes from 0 seconds to the maximal surface temperature. Parameter estimation algorithm using least mean square fits equation (4) to the experimental curve by playing with the C_p with the pre-established value for h.

Fig. 5 illustrates the fitting method for the NMC 43 Ah cell. The least squares regression described above is also repeated at other temperatures to find the thermal gradient behavior. The specific heat capacities obtained with the method explained above are graphed in Fig. 6. From this figure, one can see that there is a weak positive correlation of the cell-specific heat capacity for the LTO cell with its temperature. Over the full temperature range subjected to the cell core, the average value of the specific heat capacity is 1150 kJ/(kg.K) for 50% of SOC for the LTO and 980 kJ/(kg.K) for the NMC-based technology.

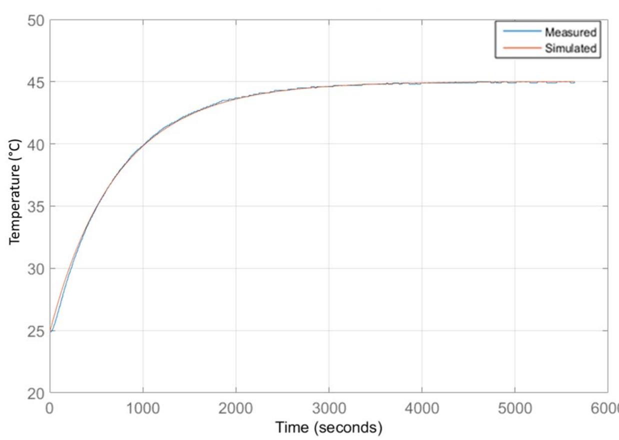
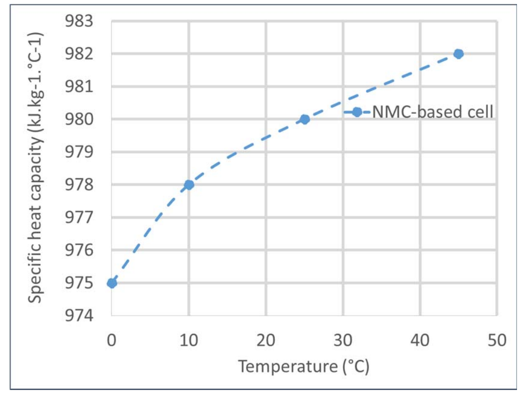


Fig. 5. Fitting of the simulated temperature to the measured surface temperature for the NMC 43 Ah cell at 25°C determined using least squares regression.



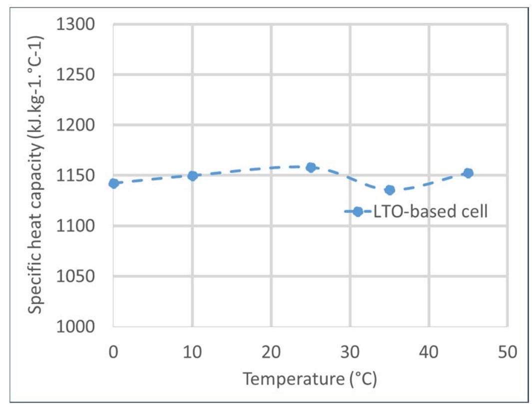


Fig. 6. NMC (top) and LTO (bottom) specific heat capacities at different temperatures and at 50% of SOC.

V. Conclusion

In this paper, a full-scale thermal analysis and model are proposed for LiBs for which the specific heat capacity is determined with a simple method without using any calorimeter. Two types of prismatic cells representing a high-power and a high-energy technology were investigating, namely: lithium titanate (LTO) cell and nickel manganese cobalt oxide (NMC) with 23 Ah and 43 Ah, respectively. The specific heat capacity was determined with micro-pulse testing.

Additionally, in order to validate the C_p values, the development of a 1D-electro- thermal and for predicting the thermal distribution and the voltage behavior under static and dynamic load profiles will be developed and presented in the full paper.

The model will be based on semi-empirical approach and preliminary results showed good results with the value pre-determined in the study for the electrical and the thermal part with less than 2.5% overall and 2°C error, respectively.

In the end, with the dynamic and static validation profiles performed on this cell, a solid foundation for a generalized model methodology is provided. Finally, future works will include the upgrade version of the model for which 3D simulation will be conducted in order to extend the study with the assessment of thermal conductivity parameters.

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