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Development of a 2D-thermal model of three battery chemistries

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Abstract— The growing need for accurate estimation of battery temperature and electrical performances at different operating conditions are crucial in its applications especially in electrified vehicles. This paper presents an effective method for developing a thermal and electrical modelling methodology for calculating thermal behavior of a lithium-ion (Li-ion) cell and the voltage response under a current solicitation. The model was elaborated on three pouch cells with different battery chemistries for use in electrical vehicles/hybrid electrical vehicles, namely: lithium iron phosphate (LFP), lithium nickel manganese cobalt oxide (NMC) and lithium titanium oxide (LTO). The model, implemented in a Matlab/Simulink interface, uses an equivalent circuit and heat generation equations coupled a thermal model. The three cell chemistries have been investigated using test procedures and thermal images at room temperature. The results of this study show that a temperature distribution to be fairly uniform after a complete discharge for the three chemistries with the lowest temperature gradient found for the LTO-based cell. Finally, comparison between simulation results and measured data under a dynamic profiles shows a good correspondence with the measurements of the validation tests with errors lying between ±4% and 2°C for the electrical and thermal model, respectively.

Keywords—Entropy, thermal model, LFP, LTO, NMC, temperature predictions.

I. INTRODUCTION

Fossil fuel depletion and environmental concerns have spurred world-wide interest in the development of lithium-ion batteries (LiBs) for electrified vehicle application. LiBs have been the favorite technology for hybrid electric vehicles (HEVs), plug-in hybrid electric vehicles (PHEVs) and battery electric vehicles (BEVs) thanks to their better performance in terms of high power and energy density. Different lithium-ion (Li-ion) technologies distinguish themselves to supply the HEV and EV applications in terms of size, weight capacity, etc [1]. Among them we find for example: NMC, LFP, and LTO.

Nonetheless, despite offering advantages, market penetration of HEVs/EVs is limited by a series of technical barriers of Li-ion cells. Typically, in a MSMD battery model, there are two scales: microscopic (focuses on the molecular-level quantum behavior) and macroscopic (temperature distribution throughout the cell area) or in a pack system [22]. Unfortunately, microscopic MSMD models require a significant amount of computation time and will therefore not be studied in this paper. Regarding the macroscopic level, a number of models have already been developed to study the thermal behavior of Li-ion batteries [21], [23], [24], [25].

In most of the models, the thermal model is coupled with simplified-electrochemical equations which simulates the battery temperature profile with various operating conditions. For instance, Panchal et al. [26], investigated thermal modelling in a prismatic LFP battery. A neural network approach was used to accurately give the surface temperature profiles observed in the experimental results. In addition, Saw and Ye [27] investigated thoroughly the well-studied commercial 18650 LFP cell and developed also a pseudo two dimensional electrochemical coupled based on the physical dimensions (layer structure of the spiral wound, cylindrical casing, gasket). Although various thermal-model techniques have been suggested, Bazinski and Wang [28] proposed a new technique to predict the heat generation of a LFP pouch cell using lumped capacitance method (LCM). The technique performed very well in reconstructing each known hot spots on the surface. Regarding the NMC chemistry, recently, Samba et al [29]...
proposed a 2D-NMC thermal model where uneven temperature distribution is observed, leading to hot and cold spots on the surface. Some thermal models using one dimension are also proposed in the literature [23], [24], and [30]. They specify used thermodynamic equations for one direction only, without considering the tabs or the multiple-direction conductivity of the cell. However, despite the efficiency of the above mentioned thermal models, most of the 1D and 2D thermal models involve current technologies such as NMC or LFP, only a few studies focus on well-established and attractive chemistries, like LTO. The latter has indeed attracted lots of attention [31], [32] but it is no fully documented when it comes to thermal modelling. Moreover, the heat generation and its impact on the voltage behavior is not generally fully investigated in the present 2D-thermal models. Given these observations, this paper presents the development of a 2D-thermal and electrical model which will take into account geometrical properties of three lithium-ion pouch cells. The goal of this model is to give accurate predictions of the temperature distribution through the cell surface and the voltage behavior under various operating conditions. Indeed, the key contribution of this study is to establish a generalized battery thermal and electrical model that accounts for three commonly used LiB chemistries in EV/HEV applications, namely: LTO, NMC and LFP. An accurate method for estimating the battery parameters is also presented involving load test and infrared (IR) images recorded by a thermal camera. The test results of the parameters estimation are also marked as a key contribution as thermal or electrical investigations in the literature usually lack of studies on LTO-based cells. The paper is organized in this way: Section II gives the experimental protocol along with the developed tests. Section III presents the model methodology. Section IV discusses the simulations results performed under different operating conditions. Finally, the conclusions are established in Section V.

II. EXPERIMENTAL SETUP

A. Batteries feature

Three types of cell chemistries are tested in this study, namely NMC, LTO and LFP all rated at different nominal capacities: 20 Ah, 5 Ah, and 14 Ah, respectively. The thermal characterization and validation tests were carried out according to the conditions presented in Table I.

<table>
<thead>
<tr>
<th>Properties</th>
<th>NMC</th>
<th>LTO</th>
<th>LFP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length of the cell, mm</td>
<td>217</td>
<td>276</td>
<td>216</td>
</tr>
<tr>
<td>Thickness of the cell, mm</td>
<td>7.1</td>
<td>4</td>
<td>7.1</td>
</tr>
<tr>
<td>Width of the cell, mm</td>
<td>130</td>
<td>173</td>
<td>130</td>
</tr>
<tr>
<td>Width of the tabs, mm</td>
<td>30</td>
<td>85</td>
<td>45</td>
</tr>
<tr>
<td>Length of the tabs, mm</td>
<td>40</td>
<td>40</td>
<td>40</td>
</tr>
<tr>
<td>Weight of the cell, g</td>
<td>428</td>
<td>262</td>
<td>380</td>
</tr>
</tbody>
</table>

B. Description of the test bench

Three cells were tested with the test bench displayed in Fig. 1. An 80-channels battery cycler (ACT 0550) was employed for cycling (in this case charging and discharging), and capacity measurement. The current \( I_{\text{batt}} \), temperature and cell voltage, \( V_{\text{cell}} \), are monitored with an interface computer / PEC software. Regarding the temperature sensors, the PEC battery cycler permitted the use of a thermistor (NTC 5K) to measure the cell temperature with an allowable tolerance of 1%. It was placed near the positive tab where with these batteries, studies [12], [33], have shown that is a spot where the maximum heat is observable. A climate chamber, free from the test bench and autonomous, was used to recreate a stable environmental temperature, called in this study, \( T_{\text{nch}} \), (the temperature of the chamber).

C. IR imaging

To obtain the surface-heat distribution of the three pouch cells, surface temperature of the cells were recorded. A Ti25 thermal camera captured IR images at regular time intervals. To achieve accurate results from the IR camera, pitch-black paint covered entirely the surface of the cells to be placed in a dark environment (less reflected heat interference).

D. Protocol

The electro-thermal model needs several parameters to be operated. The purpose of this subsection is to present the specific details and procedures to be carried out for extracting the required model parameters. The specific details and procedures are standard-based and can be found in numerous studies about thermal modelling [29], [34]. The proposed protocol for the data collection procedure for the 2D modelling consists of:

1) Capacity test;
2) Open circuit voltage (OCV) [30], [35];
3) Hybrid pulse power capability (HPPC) [36];
4) Worldwide harmonized light vehicle testing cycle (WLTC)

The data extraction is fairly straightforward for the first test. The capacity discharged expressed in Ah at different discharge C-rates and temperatures can be directly obtained from the test results. Three temperatures are tested: 25, 35 and 45°C. The OCV test determines the relation between the relaxation voltage and the state of charge (SoC) of the battery. The profile consists of a complete discharge pulses following by a complete charge pulse of the cell in steps of 2% steps between a 100% and 90% SoC window, 5% steps between 90% to 10% SoC window and 2% steps between 10% and 0% SoC window. The OCV test is performed under four temperatures (15°C, 25°C, 35°C, and 45°C) to have a temperature- and SoC-dependency of the OCV term for the based calculation of the entropic coefficient which will be described in the next section.

Thanks to the HPPC tests, the three chemistries’ internal impedances were obtained and stored in look-up tables to steer the electrical part of the model. The pulse currents for the HPPC test were C/3, 1C, 1.5C, 2C, and 2.5C with a 10-second discharge pulse and 10-second regen pulse for each given C-rate. For the LTO technology, the test was pushed further to 3C and 4C due to the low capacity. The pulses were performed from 100% to 0% with a 5%-step at 25°C.

Finally, in order to correctly validate the electro-thermal model created, some independent validation tests are additionally performed. This test can be used to compare the output of the model with the voltage response of the cell. Two different tests have been selected in order to acquire the validation of the electrical model. The validation test procedure that has been used is the so-called the WLTC test procedure. During the 1990s, the emergence of electric road vehicles powered by alkaline batteries pushed the development of suitable test procedures and standards. Conventional constant current discharge tests, as were defined for lead-acid batteries, did not reflect the actual use pattern of the batteries in electric vehicles. Thus, a current load profile based on an actual driving profile (WLTC) has been realized.

III. ELECTRO-THERMAL MODELLING

A. Description of the used methodology

In this paper, an electro-thermal methodology has been developed and applied to obtain a surface heat distribution of a pouch cell. A full outline of the methodology is illustrated on Fig. 2. This approach requires the knowledge of various input parameters such as electrical and thermal parameters, all obtained experimentally. To apply this methodology in practice, as mentioned in the previous section, experimental tests have been performed. Then, numerical simulations under the same various, operating and loading conditions, have been realized. For this, the simulations, and beforehand, the development of the electro-thermal model were achieved within the Matlab interface. Basically, the two main models (electrical and thermal) were coupled together and then, calibrated and validated, based on experimental sets of data.

![Electrical model](image)

![Thermal model](image)

Fig. 2. Presentation of the used methodology.

B. Description of the electrical model

In this section, the electrical part of the methodology is presented. As shown by Fig. 3, the model is a 2nd-order Thevenin model based the electrical equivalent circuit (EEC) approach [37]. The bi-directional structure of the model, using a combination of voltage sources, resistors, and capacitors, was set to determine the battery voltage under current solicitations.

In its most basic form, the Thevenin-based model uses a resistance in series and two RC-parallel networks to predict the battery’s response at an initial SoC. The two RC circuits refine the description of polarization characteristics and simulate the concentration polarization and the electrochemical polarization separately [37], [38]. As mentioned before, the OCV has a dependency on the SoC and temperature, as for the internal resistance, it depends on the current, the temperature and the SoC. The latter is defined as [39], [40]:

\[
SoC = SoC_{init} - \int \frac{1}{C_{init}} dI
\]  
(1)

with \(C_{init}\) the initial capacity (Ah) dependent on the temperature, and \(SoC_{init}\) the original state-of-charge of the cell. The output voltage is calculated based on the following equation [21]:

\[
V_{batt} = OCV - R_{d}I_{batt} - R_{i1}I_{1} - R_{i2}I_{2}
\]  
(2)

with OCV the open-voltage source (V), \(I_{batt}\), the battery current \(A\) and \(I_{1}\) and \(I_{2}\), the currents in the RC circuits, \(R_{d}/C_{1}\) and \(R_{i2}/C_{2}\), respectively.
C. Description of the thermal model

Fig. 4 displays the three different domains and sizes of the tested cells with the casing, electrodes, and tabs. It is assumed that the lithium-ion pouch cells have a small thickness, so, in this model, the heat distributions are only calculated in two planar directions (x and y axis on Fig. 4). The battery is made of three distinct computational domains, i.e., the electrodes, the casing (cold housing), and the tabs. The energy balance equation used to calculate the dynamic temperature response of the cell over a volume is defined as [41]:

\[
mC_p \frac{dT}{dt} = q_g + k \left[ \frac{\delta T}{\delta x^2} + \frac{\delta T}{\delta y^2} \right] - q_{conv}
\]

(3)

where \( m \) is the mass of the cell (kg), \( C_p \) is the specific heat of cell (J/kg.K), \( T \) is the cell temperature (K), \( q_g \) is the internal generation heat (W), and \( k \) is the average thermal conductivity (W/m.K) along the x-direction and y-direction, respectively. \( q_{conv} \) is the convective heat with surrounding air (W). The heat generation rate depends on the thermodynamic properties of the reactions inside the cell, the potential-current characteristics of the cell, and the rates of charge and discharge. In this study, the heat sources can be distinguished in two terms: the ohmic heat \( Q_{ohmic} \) generated by the internal resistances, and the reversible heat \( Q_{rev} \), resulting from the entropy heat. These thermal sources can be determined by [21], [41]:

\[
q_g = q_{ohmic} + q_{rev}
\]

(4)

\[
q_{ohmic} = R_o l_1^2 + R_1 l_1^2 + R_2 l_2^2
\]

(5)

\[
q_{rev} = IT \frac{\delta OCV}{\delta T} \frac{\delta T}{\delta \text{SoC}}
\]

(6)

where \( \delta OCV/\delta T \) is the entropy coefficient derivative to the SoC (mV/K). This term varies both with temperature and state-of-charge (SoC) and can be either negative or positive, differing if a charging current (negative) or discharging current (positive) is applied [42], [43]. In our case, this parameter was measured experimentally during OCV tests at 4 temperatures with results shown in the next section. In addition, for NMC and LFP, it could have been possible to look in the literature for this coefficient. Regarding the LTO technology, it is not fully documented but experimental tests were performed and the entropy coefficient of a LTO pouch cell is shown in the next section. Finally, the heat loss (\( Q_{rev} \)) is given by the convection heat with surrounding air [41]:

\[
q_{conv} = hS(T_{amb} - T)
\]

(7)

where \( S \) is the cross-section area (m²), and \( h \) is the convective heat transfer coefficient (W/m².K). Natural convection is considered solely for cooling, thus \( h \) is small. A value of 5 W/m² has been chosen to represent this natural convection effect. Table II lists the dynamic parameters used for the thermal model.

### Table II. Dynamic Parameters

<table>
<thead>
<tr>
<th>Chemistry</th>
<th>( \rho ) (kg/m³)</th>
<th>( C_p )-(J/kg.K)</th>
<th>( h )-(W/m².K)</th>
<th>( k )-(W/m.K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>NMC</td>
<td>2247 [29]</td>
<td>785 [29]</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Furthermore, each temperature profile obtained by the thermal camera (Section II.C) was used in a 1D-thermal model. The output surface temperature of the model was compared to the measured one in a parameters estimation algorithm found in Simulink Design Optimization™. By fitting between the experimental and simulated data, the algorithm determined the overall conductivity heat transfer parameters (\( k \)). The result of this estimation is reported in Table II.

IV. EXPERIMENTAL RESULTS

All test results of the characterization tests are presented in this section. The latter is divided in three subsections: electrical parameters, entropy coefficient and surface-heat distribution, respectively. From these tests, the model parameters are extracted and integrated in the electro-thermal model.

A. Electrical parameters

The HPPC test is intended to measure the battery impedance using a test profile that incorporates both discharge and regen pulses. The primary objective of this test is to extract the resistances and capacitances parameters required for the electrical model. As an example, Fig. 5 shows as a function of SoC and current rate, the ohmic resistance, \( R_o \), of the three technologies cells obtained from discharging pulses. From these graphs, one can conclude that a low SoC engenders a high ohmic impedance for the NMC, LFP and LTO cells.

Additionally, the resulting voltage profiles of the OCV tests as function of SoC are presented in Fig. 6. Based on the obtained OCV values, a look-up table can be generated for the prediction of the OCV in function of the battery SoC at different temperatures.
Fig. 4. Graphics and sizes (mm) of the three Li-ion chemistries, from left to right: NMC, LFP and LTO.

Fig. 5. From top to bottom: ohmic resistance measured by HPPC test at steps of 5% SoC of NMC, LFP and LTO, respectively.

Fig. 6. OCV curves of the three technologies at 25°C.

B. Entropy

To determine the variation of the reversible heat with the SoC, the OCV measurements were performed over the whole SoC at different temperatures. Fig. 7 presents the entropy coefficient for the three technologies. As shown in Fig. 7, in the case of the NMC chemistry, between SoC=30% and SoC=70%, the NMC entropy coefficient rises as the temperature increases.

Indeed, the available heat is absorbed by the battery during discharge (endothermic reaction), while it is released at the end of the discharge (exothermic reaction). Note that the opposite scenario occurs during the charge.

As for the LFP-based technology, they have a high change in entropy with at high- and low-SoC extremities which is in line with what as it has been reported in the literature [44]. Finally, regarding the LTO-based chemistry, a plateau is observed in Fig. 7 which is a common feature to the LTO chemistry as discovered by other researchers [45].
V. MODEL VALIDATION

For the validation part, the results of the electro-thermal model simulations were compared to the experimental data under different operating solicitations.

A. Electrical model validation

The electrical model was simulated using Matlab for validating its response, the validation was done using a dynamic current profile: the WLTC current profile. Fig. 8 shows the measured and estimated voltage for the three chemistries under the loading condition. A good agreement can be observed for all technologies. In the same way, Fig. 9 displays the model deviation between the measurement and simulation plotted for the three chemistries against time. It can be observed that the error remains below 2% (4% for the LTO-based cells) over almost the full duration of the validation test, except for the increase in error at the end of the test for the NMC and LTO cells. Indeed, when the SoC level of those cells drops below 10%, the simulated voltage differs with more than 3% from the measured voltage. At this deep DoD, the battery cell behaves in a non-linear way, which could explain the increase of error with the simulation. As a result, the 2nd Order Thevenin model discussed earlier can be also used successfully to reproduce a dynamic profile. Furthermore, the methodology proposed for the electrical modelling can be used for simulating at least three different LiB technologies, which was one of the key objective in this study.

B. Thermal model validation

During the capacity test the cell (section II.D), the surface-heat distribution of the three pouch cells was recorded with a thermal camera. Since the heat generation rate depends mostly on the rates of the current rate, the 1C capacity test for NMC and LFP and a 6C for the LTO chemistry are shown in this section. Fig. 10 displays the thermal distributions results of the cells at the conclusion of the capacity tests with the simulated heat distribution by the 2D thermal model. Regarding the experimental results, an overview of the three schematics shows that the similar temperature distribution patterns of the surface in the case of the three lithium technologies. The spatial distribution is more uniformly located at the center of the cell. A hot region is also observed for the NMC cell near the positive tab (Fig. 10A). The reason results from the high thermal resistivity of the aluminum composing the positive tab which produces more heat than the copper-based negative tab [33]. The LTO chemistry showed the same temperature distribution, but the only difference is a lowest
temperature gradient compared to the two others cells, which emphasizes LTO as a good candidate against thermal runaways.

Fig. 10 also shows the outcomes of the 2D-thermal model of the three cells at 25°C and under the same operating conditions. The simulated thermal distributions at the end of the capacity show a good agreement with the experimental data, repeating that the cells surface temperatures are nearly uniform with the maximum temperature located in the middle with a maximum difference of 2°C for each chemistry.

VI. CONCLUSION

In this study, a method is presented for developing a 2D-thermal and electrical model for predicting the thermal distribution and the voltage behavior under static and dynamic load profiles of three Li-ion pouch cells. This method, based on Matlab/Simulink interface was elaborated on three Li-ion chemistries, NMC, LTO and LFP. The experimental results used for validation showed a temperature distribution to be fairly uniform after a complete discharge with 1°C of maximal temperature difference. Regarding the LTO technology, the lowest temperature gradient was found even after a high c-rate discharge. This demonstrates the favorable thermal performance of this chemistry in an automotive application. In addition, from the comparison of both simulations and the experimental results, a good agreement was found with a maximum error of 2% (4% for LTO) and 2°C for the electrical and thermal, respectively, for the three chemistries. Therefore, with the dynamic and static validation profiles performed on three chemistries, a solid foundation for a generalized model methodology is provided, since in the literature there is a lack of universal electro-thermal models that are able to account for three LiB technologies. However, future works will include the validation of the model at different ambient temperatures (from -15°C to 45°C), which will change the thermal distribution. Also, future works will include the study on a battery pack but a more sophisticated method would be required, such as finite element method.

ACKNOWLEDGMENT

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REFERENCES

Fig. 10. IR images at the end of the capacity test of the three chemistries. (t=3600s for NMC and LFP, t = 600 for LTO; A = NMC, B = LFP and C = LTO.


