A CFD thermal analysis and validation of a Li-ion pouch cell under different temperatures conditions

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Abstract. Li-ion cells are one of the core components for the actual and future electric mobility. Differently from other types of applications and due to the high charge/discharge rates, the thermal-related issues in batteries for mobility are drastically relevant and can affect the reliability, the safety and the performance of the system. Indeed, limited temperature differences within a battery pack have a significant impact on its efficiency, thus it is important to predict and control the cell and battery pack temperature distribution. In the proposed study, a CFD analysis has been carried out to quantify the temperature and heat distribution on a single Li-ion pouch cell. The main objective of this work is to determine the temperature imbalance on the cell and the required cooling load in order to be able to correctly design the cooling system and the best module architecture. The internal heat generation occurs as a result of electrochemical reactions taking place during charge and discharge of batteries. An electric model of the cell allows to assess the thermal power generation; the model parameters are changed according to the operative conditions to improve the accuracy, specifically to take into account varying temperature conditions and C-rates. The high accuracy of the model with respect to experimental data shows the potentiality of the proposed approach to support the optimization of Li-ion modules cooling systems and architecture design.

1 Introduction

Lithium-Ion Batteries (LIBs) have emerged as a key energy storage technology and are widely used in the automotive industry to provide power in electric and hybrid vehicles. They have attracted considerable amount of attention due to their high energy density, efficiency and voltage, but also because of their long-life and slow self-discharge rate. However, the effective use of LIBs requires strict thermal control: operating temperatures have to be constantly monitored and maintained in a controlled range [1]. In fact, temperature changes affect the chemical reactions that take place in batteries, as well as the properties of the materials that compose them. One example of this is the electrodes and electrolytes ionic conductivity which changes with temperature variations [2]. A decrease in temperature leads to an increase of the electrolyte viscosity, which implies a consequent reduction in the ionic conductivity. In other words, the internal resistance will rise due to the increase in the impedance of the directional migration of chemical ions [2]. Moreover, as has been shown in different experimental studies [2,3], the increase of the charge-transfer resistance in LIBs contributes to the performance degradation at low temperatures. As reported in several studies [2,4], exposure to low-temperatures may cause drops in power and energy densities. Furthermore, the available capacity, which governs the LIBs State of Charge (SOC), was also found to decrease by more than 20% when the operating temperature was reduced from 25°C to -15°C [2].

High temperatures also modify Lithium-Ion cells performance and typically cause irreversible changes to them. It is frequently reported that high operating temperatures accelerate thermal aging and may shorten LIBs life [1,2,5]. High temperatures are also associated with the unwanted and dangerous phenomenon of thermal runaway, so a chain of uncontrollable exothermic reactions. When such uncontrolled heat generation exceeds the battery heat dispersion capacity, explosion may occur [6,7]. The ideal operating temperature range for LIBs is usually indicated within a temperature range of 15-35 °C, with a maximum operational temperature that may not overcome 50°C [8]. The exact operating range depends on the cells’ chemistry.

Temperature uniformity within a battery module is also a critical aspect, as temperature differences determine cells electrical imbalance and thus reduce the module efficiency. In addition, big imbalances can be
dangerous when no balancing strategy is included in the Battery Management System (BMS).

Within this framework, the formation of thermal hot spots as a possible source of thermal runaway and battery-reduced performance is a worrying scenario [9]. However, experimental characterization aimed at hot spots detection is very limited due to LIBs closed housing, small structural dimensions and tight windings [9]. Furthermore, economic limitations must be considered: the construction of different prototypes for testing different cooling strategies is expensive and usually not feasible. Hence, studies and research rely on models, which offer more versatility and possibilities.

Most of the studies on lithium-ion battery modelling use Equivalent Circuit Models (ECMs) [10–11] and electrochemical models [12–13]. ECMs are based on basic electric circuit components and are often used in real-time applications because of their mathematical simplicity. However, the structure of ECMs is usually empirical-based, the circuit components values must be identified based on an experimental charge/discharge campaign. One disadvantage of this type of model is that in several cases it is not capable to describe all the electrochemical phenomena that occur in a cell. On the other hand, electrochemistry-based battery models rely on the calculation of the terminal voltage and the SOC according to the electrochemical reaction process [9]. This type of model is not widely spread because it requires more detailed information than the ECMs, in specific technical parameters that are difficult to obtain because Li-ion cell manufacturers are not able to estimate them or do not desire to provide them. In addition to this, electrochemical model’s high computational complexity makes the electrochemistry-based models not suitable for online implementations.

In this work, a three-dimensional CFD analysis was performed, based on the ECM, to investigate the effects of different operating conditions on the thermal behaviour of a Li-ion cell. Improvements were introduced to increase the accuracy of the thermal power generation model by considering also the temperature effects on the cell. The CFD analysis was aimed to define the critical hot spots, as well as the heat generation and represents a preliminary study for the improvement of the design of a battery module embedding a cooling solution.

## 2 CFD Modelling

Ansys/Fluent platform was used to carry out the electro-thermal cell modelling. Specifically, Ansys - Fluent 2019 R1 was used. The well-established Fluent Multi-Scale Multi-Domain (MSMD) approach helps in dealing with different physics in the solution domains (anode-separator-cathode layers). When this approach is chosen the battery thermal and electrical fields are solved in the CFD domain at the battery cell’s scale using the following differential equations [14]:

\[
\nabla \cdot \left( \sigma \nabla \phi \right) = - (j_{EC} - j_{short}) \\
\nabla \cdot \left( \sigma \nabla \phi \right) = f_{EC} - j_{short}
\]

(2)

(3)

Where \( \sigma_+ \) and \( \sigma_- \) are the effective electric conductivities for the positive and negative electrodes, \( \phi_+ \) and \( \phi_- \) are phase potentials for the positive and negative electrodes [14]; \( j_{EC} \) and \( q_{EC} \) are the volumetric current transfer rate and the electrochemical reaction heat due to electrochemical reactions, respectively [14]; \( j_{short} \) and \( q_{short} \) are the current transfer rate and heat generation rate due to battery internal short-circuit, respectively [14]; in this case not needed.

The equations to calculate the source terms, \( j_{EC} \) and \( q_{EC} \), depend on the adopted submodel that, in this work, is the ECM. The Fluent ECM implementation allows to describe the cell using up to three resistors and two capacitors (Fig. 1) and it is based on the model proposed by Chen et al. [16]. In this work, an improvement over the standard model is propose: the electric circuit parameters are modified not only as a function of the SOC, but also depending on the cell temperature; this modification was implemented using look-up tables. Once the circuit has been solved, using equation 4, the source terms were calculated and distributed in the volume as shown in equations 5 and 6. The heat generation equation, equation 5, was proposed by Bernardi et al. [15].

\[
V(t) = U(SOC, T) - V_1 - V_2 - R_1(SOC, T) I(t)
\]

(4)

\[
q_{EC} = \frac{l}{Vol} \left( U - (\phi_+ - \phi_-) - \frac{dU}{dT} \right)
\]

(5)

\[
j_{EC} = \frac{l}{Vol}
\]

(6)

where \( U \) is the open circuit voltage, \( Vol \) is the cell volume and \( I \) is the total current circulating in the cell.

![Fig. 1. Equivalent electric circuit (ECM) in Ansys Fluent.](image)

The Ansys/Fluent modelling and simulation procedure was carried out following the hereby listed steps [17]:

- The 3D model of the cell was created according to the actual size of the tested cell, whose main dimensions are 300 mm (length) × 95 mm (width) × 14 mm (thickness). The dimensions for the positive and negative tabs are 47.5 mm (width) × 10 mm (length) × 2 mm (thickness). The tested cell is a pouch Li-ion cell with opposite tab, manufactured by LG CHEM. Its nominal capacity, measured capacity and nominal voltage are 60.5 Ah, 59.3 Ah and 3.70 V, respectively.
- The cell geometry was divided into three different parts, one representing the active part and two others representing the cathode and anode tabs. The thin external layer around the cell was not considered as a
separate part but the thermal conductivity of the pouch is considered in the overall thermal conductivity of the volume. It is known that the aim of this external layer is to seal and mechanically protect the cell [23-24]; the materials used for the pouch (polypropylene, aluminium and polyamides [23]) have thermal conductivities comparable to the porous electrodes; for this reason, the external layer thermal influence is usually not strongly influencing the overall thermal properties [25].

In order to solve the thermal simulation, a calculus mesh should be generated. The discretization used in this work comprises 5100 nodes and 3500 elements.

For the evaluation of the thermal power generation, the Energy and Multi-Scale Multi-Domain (MSMD) models were activated. The ECM was used for modelling the electro-thermal cell behaviour: only one RC branch was considered, so \( R_2 \) and \( C_2 \) were set equal to zero. Three different C-rates were tested (0.3C, 1C and 2C) and experimental data with different controlled external temperatures (0 °C, 25 °C, 45 °C) were used to calibrate the model parameters. The values of 2.5 V and 4.3 V were entered for the minimum and maximum stop voltages, respectively.

ECM parameters \((R_o, R_1 \text{ and } C_1)\) identification was carried out using a multiple linear regression approach. The procedure has been presented and widely described by the authors of this paper [18], but a brief explanation is given in the following lines. Pulsed discharge tests were executed at different SOC's and voltage and current were measured; the duration of the pulses was short in order to be able to consider constant SOC during this period. A multiple linear regression model was built based on equation 4, neglecting the second RC branch terms. The next step was to formulate one equation for each observation. The values of \( R_o, R_1 \) and \( C_1 \) were estimated in order to minimize the sum of the squared residuals, defined as the difference between the predicted and measured values. It is important to highlight that the open circuit voltage was identified manually before the current pulse. This procedure was repeated three times to fill the look-Up tables at the different temperatures (0°C, 25°C, 45°C), always at 1C. Table 1 reports the values of \( R_o \) obtained with this procedure; the values \( R_1 \) and \( C_1 \) are not reported for sake of conciseness.

As concerns the materials of the cell, copper was selected as the tab material. The properties of the active material were specifically set for this case. The value used for the density was 1930 kg/m³, while the thermal properties were taken from [26] where a cell with the same chemistry (NMC) was used, so the specific heat was set to 1091 J/kg.K and the thermal conductivity was set orthotropic with the following values: 31.60 W/m.K, 23.00 W/m.K, and 0.74 W/m.K for length direction (\( k_l \)), width direction (\( k_w \)) and thickness direction (\( k_y \)), respectively. The UDS diffusivity is used by Ansys in the active area instead of the electric conductivity in order to consider both materials: the collector and the electrode. To calculate the values of uds0 and uds1 equation 7 was used [14]. Where uds0 is the diffusivity of the positive side, \( \sigma \) is the electric conductivity, \( \delta \) is the thickness and the subscripts c and e are for collector and electrode respectively. A similar equation was used to estimate uds1. The electric conductivity values were taken from [19] and thus the values 1190000 S/m and 983000 S/m were obtained for uds0 and uds1, respectively.

\[
uds0 = \frac{0.5 \sigma^c \delta^c + 0.5 \sigma^e \delta^e}{\delta_{total}}
\]

The heat transfer coefficient was set to 10 W/(m²K), while the free stream temperature was set to 298 K. The convective heat transfer coefficient was evaluated according to the typical operating conditions that are present in climatic chambers were the cells are tested. A fan is typically adopted to recirculate the air and keep the temperature constant; the typical values of the flow velocity were used to assess the aforementioned values of the heat transfer coefficient.

The SIMPLE scheme was selected as solution method. The initial temperature was set to 298 K. A fixed time stepping method was used under run calculation. Time step size was defined 0.5 s and the number of time steps were determined based on the different C-rates till the complete discharge of the cell. Convergence criteria were set to absolute with a residual threshold equal to 1×10⁻⁶ for all the monitored calculation variables. The temperatures were registered at different cell positions, as shown in Fig. 2, in order to correspond to the temperatures measured during the test campaign.

| SOC [%] | T [°C] | 0 | 25 | 40 |
|--------|--------|---|----|----|
| 100    | 0.00405| 0.00186 | 0.00139|
| 80     | 0.00356| 0.00160 | 0.00131|
| 60     | 0.00352| 0.00157 | 0.00129|
| 40     | 0.00365| 0.00171 | 0.00135|
| 20     | 0.00421| 0.00187 | 0.00144|

3 Results and Discussion

3.1 Model Validation

The validation of the model consisted in the comparison of a set of experimental data with the CFD model predicted ones. A detailed comparison of the cell voltage and the cell temperature in two points (points n.7 and n.6, Fig. 2) was carried out. In specific, when the cell is completely discharged at 1C and ambient temperature of 25 °C. The results are presented in Fig. and Fig. , where the experimental and numerical data are shown together. The heat released by the cell is also
presented together with the Depth of Discharge (DOD), which is defined as SOC complement to one (the fraction of the cell capacity that has been discharged with respect to the fully charged battery). In general, a good prediction capability is shown by the model. Fig. 3 indicates that the accuracy decreases as the DOD increases. It can be affirmed that the capacitive effects were overestimated in the second half of the discharge while they were underestimated during the relaxation phase. The last aspect can be related to the fact that not enough experimental data was available to estimate the electrical model parameters in operating conditions with a SOC lower than 10%. However, it should be pointed out how this particular operating region is usually avoided in order to prolong the battery life [20, 27]. The difference of temperature can be correlated to the determination of the actual boundary conditions (heat convection coefficient); in particular it can be affirmed that the real convection coefficient in the experimental tests was not available but it was probably higher than the one used to model the heat exchange.

The Mean Squared Errors (MSEs) for the voltage and temperature were calculated considering two different ranges: the first considers the (i) starting point equals to 5 mins before the beginning of the discharge and (ii) the ending point when the DOD is equal to 0.9; the second range considers (i) the same starting point but (ii) an ending point 30 mins after the discharge has ended (relaxation phase). The voltage MSEs are equal to 0.0040 V² and 0.0077 V² respectively, while the temperature MSEs are equal to 1.33 °C² and 1.32 °C², respectively. The maximum and minimum deviations between the measured and modelled values for the voltage were 0.44 V and 2.80 x 10⁻³ V, respectively; instead for the temperature were 1.9 °C and 1.0 x 10⁻³. The electric model accuracy level is especially acceptable when the focus is the cooling system design or other thermal aspects, as in this work. However, higher accuracy can be obtained by introducing additional and more reliable data in limit conditions, as for low SOC values.

Fig. 4 shows the heat generated by the cell during the discharge phase. The highest heat generation values were obtained in both extreme DOD conditions, as confirmed by the literature [21]. These two peaks can be associated to the cell overpotentials; in other words, this means that the cell is not working at equilibrium and requires more energy than thermodynamically expected; this extra energy is eventually lost as heat. In particular, the first peak can be associated to the activation overpotential, so to the additional energy required to activate the reaction, while the second peak can be correlated with the concentration overpotential, i.e. the depletion of charge carriers on the electrode surface. This happens due to the slow diffusion of the charge carriers, which can be explained by the change in the difference in concentration of them between the electrolyte and the electrode surface. The highest thermal power is generated around 0% SOC and it was calculated around 9.1 W.

3.2 Hot spots identification

Fig. 5 shows the temperature distribution obtained at t = 9600 s (1C-rate discharge cycle). The surface hot spots of the cell are the lateral sides; the regions with lower temperature are the connectors, as shown in Fig. 5. A sectional cut at the middle of the cell is presented in Fig. 6. In this case it is possible to appreciate that the core temperature is the highest cell temperature, which confirms the importance of LIBs models to avoid thermal runaway and guarantee safety. In fact, critical temperature monitoring, such as the measurement of the core temperature, is extremely difficult. So, it should be accurately modelled.

Fig. 7 shows the difference between the hottest and coldest points within the cell in each time interval during the discharge. The maximum ΔT (1.5°C) was obtained at t = 10100 s. The temperature difference peak is shifted by 144.5 s with respect to the maximum temperature peak. From these results two main aspects can be commented: (i) the cooling system design must introduce a strategy with a higher heat exchange coefficient on the cell lateral sides and (ii) the response of the cooling system should carefully consider the thermal inertia phenomena.
The thermal performance of the cell was studied simulating its behaviour under different working and environmental conditions. The heat generated and the maximum temperature differences are presented in Tables 2 and 3. Table 2 shows the results at different C-rates, with a fixed ambient temperature of 25 °C; on the other hand, Table 3 shows the effect of temperature changes, while keeping a fixed C-rate of 1C.

Table 2. C-rate effect @25°C. CFD results.

| C-rate | Tmax (°C) | ATmax (°C) | Heatmax (W) | Energymax (kJ) |
|--------|-----------|------------|-------------|----------------|
| 0.3C   | 27.9      | 1.4        | 1.3         | 10.5           |
| 1C     | 34.8      | 1.5        | 9.1         | 27             |
| 2C     | 45.6      | 1.6        | 24.6        | 35.2           |

It can also be seen that high temperatures do not have an instantaneous impact on the performance of the cell. In particular, the heat generated and the consequential total energy remained almost constant, but a temperature above the suggested limit, higher than 50 °C, was reached. High temperatures should be avoided: they deteriorate the chemical structure of the electrodes and in some cases produce the decomposition of the electrolyte [22]; so they have a long-term impact by decreasing the cells state of health. In this specific case, it has been demonstrated that natural convection is not enough to maintain the safety conditions of a single cell. More intense cooling strategies need to be adopted.

Table 3. Temperature effect @1C. CFD results

| Ambient Temp | Tmax (°C) | ATmax (°C) | Heatmax (W) | Energymax (kJ) |
|--------------|-----------|------------|-------------|----------------|
| 0°C          | 21.0      | 1.7        | 23.5        | 40.8           |
| 25°C         | 34.8      | 1.5        | 9.1         | 27.0           |
| 45°C         | 56.1      | 2.4        | 10.7        | 27.1           |

In conclusion, these results indicate that the lateral sides of the cell represent a critical design issue: cooling efforts should consider such peculiarity, providing higher heat exchange coefficient to guarantee uniform temperature and so optimal performance.

4 Conclusion

A CFD electro-thermal model of a li-ion pouch cell was implemented in Ansys/Fluent. Through the proposed model, the geometrical temperature distribution can be evaluated and compared with available experimental results.

The model was validated using a 1C discharge cycle, which evidenced its high accuracy, except for the last 10% of DOD. The CFD analysis showed hot spots on the lateral sides of the cell. The internal heat generation revealed two peaks at the extreme values of DOD. The heat generation increases with the reduction of the temperature due to the high internal resistance of the cell. Moreover, it also increases with increasing C-rates because of the internal ohmic losses. The obtained results show how an undesired peak temperature, above 158% respectively. Electric vehicles limitations and reduced performance in cold weather are well known. The energy released should be used to uniformly heat the battery until the optimum working conditions are reached. A special attention must be addressed to the heat distribution in order to decrease the difference of temperature within the cell and then also within the module.

3.3 Ambient temperature and C-rates effects

The thermal performance of the cell was studied simulating its behaviour under different working and environmental conditions. The heat generated and the maximum temperature differences are presented in Tables 2 and 3. Table 2 shows the results at different C-rates, with a fixed ambient temperature of 25 °C; on the other hand, Table 3 shows the effect of temperature changes, while keeping a fixed C-rate of 1C.

Table 2 indicates that the heat generated increased with the C-rate and, as a consequence, also the total heat that need to be dissipated. This result can be explained underlining the relationship between the heat generation and the current (see equation 5).

Table 3 shows how the energy and power dissipated increased considerably at low ambient temperature because of the increase of the battery internal resistance. The case of 0 °C shows a relevant increase of total energy and heat dissipated of 51% and
50 °C (which is the maximum recommended temperature by the manufacturers), could arise in hot spots when the cell is exposed to high external temperature (above 45 °C). Hence, natural convection is not enough to maintain the cell in the allowed temperature ranges. A proper cooling strategy needs to be implemented to provide the quantified (more than 10.7 W) cooling load. This confirms the importance of LIBs modelling to monitor temperature distribution, avoid thermal runaway and guarantee safety.

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