ABSTRACT

One of the challenges faced when using Li-ion batteries in electric vehicles is to keep the cell temperatures below a given threshold. Mathematical modeling would indeed be an efficient tool to test virtually this requirement and accelerate the battery product lifecycle. Moreover, temperature predicting models could potentially be used on-board to decrease the limitations associated with sensor based temperature feedbacks. Accordingly, we present a complete modeling procedure which was used to calculate the cell temperatures during a given electric vehicle trip. The procedure includes a simple vehicle dynamics model, an equivalent circuit battery model, and a 3D finite element thermal model. Model parameters were identified from measurements taken during constant current and pulse current discharge tests. The cell temperatures corresponding to an actual electric vehicle trip were calculated and compared with measured values. The resulting accuracy was high enough (max error 1.07 K) and suggests that designers could rely largely on similar numerical thermal simulations during the design of Li-ion battery systems for electric vehicles. Additionally, the thermal model could be used on-board in a battery management system control strategy to keep the cell temperatures within a safe window. A model reduction procedure is nevertheless needed to scale down the computational effort to the on-board capabilities.

INTRODUCTION

Li-ion batteries are currently the best candidates for energy storage systems in electric vehicles. Yet, many challenges need to be resolved, among which is keeping the temperature of the individual battery cells below a certain threshold. This is required in order to avoid an accelerated capacity fade which is caused by thermally favored side reactions. Additionally, the temperature in a large battery pack system should be as homogeneous as possible in order to guarantee similar power performance and capacity in all cells. Accurate mathematical models are indeed beneficial when it comes to resolving the temperature challenge. They can reduce dramatically the time of the battery product life cycle by allowing virtual testing of different designs and their suitability to various driving patterns. This is possible by using a vehicle model to calculate the required power from the velocity profiles of a representative driving schedule, a battery electrochemical model to calculate the voltages and currents associated with the power profiles, and a thermal model in order to calculate the temperature associated with the voltages and currents (Figure 1). The battery model is usually fed back with the temperature response in order to update its parameters since the cell electrical response is generally temperature dependent. Measured voltages and currents could also be fed directly to the thermal model (Figure 1). This could be the case for on-board models that are used to predict temperatures at different locations without the need for a large number of sensors, which is favorable in view of packaging aspects in large battery systems. Nevertheless, a prerequisite for on-board models is a high
computational efficiency which requires a model order reduction procedure.

The simplest vehicle models consist of calculating power profiles to overcome acceleration forces, drag forces, gravitational forces, and rolling resistances in a given velocity profile. Advanced vehicle simulation models include additionally detailed information about power train components, such as in the software package ADVISOR which is developed by the NREL [1] and is commonly used in the development of hybrid and electric vehicles.

Battery electrochemical models aimed for such applications consist generally of an equivalent electric circuit which replicates the dynamic current-voltage interaction. They consist of a thermodynamic static part which defines the open circuit potential (OCP) of the battery as a function of the state of charge (SOC), and a dynamic internal impedance part which characterizes the cell polarization under electric loads. Detailed equivalent circuits with inductor elements and Warburg impedance [2,3] are suitable for a wide frequency range, but would require complicated electrochemical impedance spectroscopy for the parameter identification process. On the other hand, simpler models which contain only resistors and capacitors [4,5,6] are proved suitable for vehicle application frequencies and their parameters can be identified from cell charging/discharging voltage profiles. Circuit models consisting of purely resistors could also be used [7,8], but would over-predict polarization under short duration current peaks due to the absence of transient effects.

In battery thermal models, the heat continuity equation in a cell-stack domain is solved using heat sources calculated from thermodynamic principles. In [9,10,11,12,13], a 3D domain representing explicitly the geometry of a single cell or a cell stack was used. In [14,15,16] a 2D cross section of a cell/module was analyzed assuming symmetry in one direction. In [17,18,19,20,21,22,23,24], lumped thermal models, which consider the cell as a temperature point, were utilized. When the domain exceeds by far the dimensions of a unit cell, a homogenous material was assumed whose effective thermal properties were calculated or measured [25,26]. Bernardi et. al have derived from thermodynamics principles [27] a battery heat source consisting of an irreversible term which represents Joule and Faradaic losses and an entropic term whose sign depends on the SOC and the sign of the current of the cell. While the irreversible term was always considered, the entropic term was often neglected [22,23,24,17,20,18] due to the difficulty of its characterizing test. This assumption is acceptable in hybrid vehicle applications where Joule and Faradaic losses are dominants due to the high currents and their fluctuations at a nearly constant SOC. The entropic term was also considered constant in many works [12,13,14,15,21].

In the above works, a direct connection to in-vehicle battery systems is not the case. Boundary conditions were roughly assumed and a verification with temperature measurements on the actual battery system lacked. In this work we calculated the cell temperatures corresponding to an actual electric vehicle trip and showed their comparison with on-board measurements. A simple vehicle model, an equivalent resistor-capacitor circuit model and a 3D finite element thermal model were used in the calculation procedure.

**EXPERIMENTAL**

The considered electric vehicle (EV) is a prototype developed at the FEV GmbH, and consists of 12 modules arranged in a sealed casing (Figure 2-a). Each module consists of a sealed metallic housing containing 7 serially connected Li-ion polymer pouch cells (40 Ah, 3.7 V), separated from each others by plastic frames (Figure 2-b). The EV prototype was driven in a 38.8 Km trip for 0.73 hours, and the velocity profile shown in Figure 3 was registered. The trip did not include any strong hill climbing/descending and the registered ambient temperature was 21 °C. The voltage and tab temperature of each cell were also registered. The tab temperatures are expected to be close to the inner cell temperatures, since the tabs are the extensions of the current collectors, which are good heat conducting elements.
Figure 2. a) Module arrangement in the battery pack, and b) cell stack in each module

Figure 3. Velocity profile and distance registered during the considered trip

Figure 4. Measured voltage and temperature of each cell during the considered trip

All 12 modules showed similar trends in measurements. Figure 4 shows the temperatures and voltages of each cell of modules 3, 6, 8 and 12 which could be treated as an unbiased sample the whole system. Notice the similarity in the voltage curves in the different modules which are subjected to the same boundary conditions, suggesting thus a more or less similar heat generation. Module 6 showed the strongest deviation of its maximum temperature (30.3 °C) from the average of the maximum temperatures of all modules (29.7 °C). This was a justification for us to treat a single module as representative of the whole battery pack. Nevertheless, the cells inside each module showed a more obvious inhomogeneity in temperatures. Specifically, the outer cells remained colder than the inner ones (∼ 3°C), due to their thermal contact with the module casing. The temperature scatter of all cells is not wide enough to result in different cell electrochemical responses, which was the reason why the measured voltages were similar in all cells.

MATHEMATICAL MODELING

ELECTRIC POTENTIALS AND CURRENTS

A simple vehicle model governed by the following equation was used to calculate the power profiles corresponding to the velocity profiles of Figure 3:

\[
P = \left( ma + \frac{1}{2} \rho \alpha v^2 C_d A_{front} + C_r m g \right) \times \eta_{eff} \times v + P_{aux}
\]

(1)

The vehicle parameters shown in Table 1 were used. A constant auxiliary power of 700 W was estimated for the passenger compartment's needs. Battery to wheel and wheel to battery energy losses were accounted for by using efficiency values estimated for the used vehicles.

Table 1. Vehicle parameters used in the power profile calculations

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(C_d)</td>
<td>coefficient of aerodynamic drag</td>
<td>0.325</td>
</tr>
<tr>
<td>(A_{front})</td>
<td>vehicle frontal area</td>
<td>2.42 m²</td>
</tr>
<tr>
<td>(C_r)</td>
<td>coefficient of rolling resistance</td>
<td>0.015</td>
</tr>
<tr>
<td>(m)</td>
<td>mass</td>
<td>1240 Kg</td>
</tr>
<tr>
<td>(\eta_{bw})</td>
<td>battery to wheel efficiency</td>
<td>0.8</td>
</tr>
<tr>
<td>(\eta_{wb})</td>
<td>wheel to battery efficiency</td>
<td>0.4</td>
</tr>
<tr>
<td>(P_{aux})</td>
<td>auxiliary power</td>
<td>700 W</td>
</tr>
</tbody>
</table>

In order to predict the electric potentials and currents required to meet the power profiles, an equivalent circuit model known as the RRC, was used (Figure 5). The cell OCP curves, which are required as a model input, were taken from measurements performed on the electrode active materials (negative: LiC₆, positive: LiNiCoMn) of the underlying cell [28, 29, 30, 64].
1C discharge curves at different ambient temperatures, which were provided by the manufacturer, showed a similar electrochemical performance (polarization and capacity) at 20 °C and 40 °C. As a result, one parameter set valid for the temperature range experienced in here was used (20-30°C) and was identified by fitting the model response to electric potential measurements in a test consisting of a reciprocating pulse current (20 sec) at different SOC values (Figure 6). A mathematical gradient based optimization algorithm was used in MATLAB for that purpose. The obtained parameter values were: 

$$R_1 = 5.4 \times 10^{-4} \text{ Ohms, } C = 7762 \text{ Farads and } R_2 = 1.2 \times 10^{-3} \text{ Ohms.}$$

Figure 5. Electrochemical equivalent circuit model used for electric potentials and currents calculation

Figure 6. Battery RRC model fit to pulse current test measurements

**TEMPERATURES**

Measured/calculated electric potentials and currents can be used in order to estimate the cell heat generation rate based on the equation developed by Bernardi [27]:

$$\dot{Q} = I(V - V_{OCF}) + IT \frac{\partial V_{OCF}}{\partial T}$$

The first term in the equation above is the irreversible heat source, which is always positive and dominant at high rates. The second term is the entropic reversible heat source whose sign depends on the SOC level. The cell entropic coefficient is estimated from the entropic coefficients of the underlying electrode materials which have been measured in [28]. For the cathode, a LiNiCoO$_2$ active material is assumed instead of the actual LiNiCoMn due to the lack of the actual data.

The cell was discretized into finite elements, and the above equation was applied as a spatially uniform source in the heat continuity equation at each finite element integration point. The cell core is treated as a homogenous material, and its macro effective thermal properties were measured using the procedure described in [25, 26]. A value of 930 Jkg$^{-1}$K$^{-1}$ was obtained for the specific heat capacity, while values of 1.2 Wm$^{-1}$K$^{-1}$ and 28.2 Wm$^{-1}$K$^{-1}$ were obtained for the thermal conductivity in the normal and planar direction respectively. The tabs section was explicitly modeled and the reputed values of Aluminum and Nickel were assigned for the positive and negative sides respectively. As a verification of the source term, the temperatures of a single cell during a 4.5 C discharge under natural convection conditions were simulated, and the results were in a very good agreement with thermal infra red images taken during the actual test (Figure 7). Notice how the thermal images do not show any heat localization effects caused by high current fluxes near the tabs, which justifies the choice of applying a uniform heat source.

The module model consists of the 7 cell models described above and the module housing. Natural convection boundary conditions were applied on the module housing and on the cell parts exposed to the airspace in the module. Additionally, a thermal contact resistance is applied between the outer cells and the module housing. In order to characterize the thermal behavior of the module, temperature measurements at discrete cell surface locations (Figure 8) were made during a 3.5 C discharge in ambient temperature.
which happened to be −2.0 °C. The heat transfer coefficients and contact resistances were adjusted by trial and error to the values of 5.0 W m\(^{-2}\) K\(^{-1}\) and 25.0 W m\(^{-2}\) K\(^{-1}\) respectively in order to fit the measured temperatures (Figure 8). Figure 9 shows the temperature contours at different levels of SOC in a cut section of the module. Notice how the outer cells remain colder than the inner ones, and how the temperatures are colder near the tabs, due to the flow of heat to the module airspace. In the above cell and module temperature calculations, the measured voltages were used in the heat source term.

MODEL PREDICTIONS

The above elaborated models were used to predict the battery thermal performance during the performed vehicle trip. The target power profiles, which are calculated by inserting the velocity profiles of Figure 3 in eq. 1, are fed to the RRC model to calculate the needed cell scale electric potentials and current profiles. A PID controller was used for that purpose and its proportional, integral, and derivative values were tuned by trial and error to 1, 1 and 0 respectively, to result in a maximum power error of 1.3e\(^{-04}\) W. Figure 10 shows the comparison between calculated and measured electric potentials in each battery cell. It was assumed in here that all battery cells have an identical voltage response, since the battery temperature inhomogeneity level would not lead to a non homogeneous voltage response, as backed up by the measurements in Figure 4. The average measured voltage of all cells is used in the comparison. The variation of cell SOC with time is also plotted in Figure 10. The initial SOC level was estimated to be 0.83, as hinted by the voltage value at rest before the start of the trip, which was assumed to be relaxed to the OCP of the cell. The SOC was updated using a coulombs counting algorithm. There is a reasonably good match between the measured and calculated cell voltage, with a standard deviation of 0.039 V and a maximum error of 0.13 V. The quality of the fit could be improved by using test data resulting from longer pulse currents in the calibration process, which were not available to us at the time of this work. The calculated response happens to be noisier than the measured one due to the use of a PID controller, which results in small current fluctuations. Notice how, during the times of high velocity, the voltage drops down sharply due to the high polarization of the cell. Additionally, the SOC levels obtained using the calculated currents match very well the ones obtained using the measured currents.

In order to calculate the cell temperatures during the vehicle trip, the previously calibrated finite element model was used; one time with a heating rate based on the calculated currents/voltages, and another time with a heating rate based on
measured currents/voltages. The different parts of the heat source are plotted in Figure 11 using the measured currents/voltages. Notice how the irreversible Joule's heating is always positive and dominates at times of high power requirements which started at around 930 sec (SOC $\sim 0.6$). The dominance of the Joule's heating at high power requirement is due to the simultaneous increase in electric current and its associated drop of electric potential away from the OCP, which causes a quadratic dependency on current. The large dynamic drops in electric potentials can be observed in Figure 10 and are caused by the cell polarization, which is due mainly to the electrolyte and solid active material resistance to the transport of Lithium ions.

![Figure 11. Contribution of Joule's heating and entropic heating to the total heat](image)

To the contrary, the entropic heat is not sensitive to cell polarization and depends only linearly on the applied current. Moreover, the entropic heat is negative and heat is partially absorbed until an SOC level of 0.4, after which it becomes slightly positive.

The calculated tab temperatures are plotted in Figure 12 along with the measured ones, for the outer and the middle cells. The heating trends are well captured, and a maximum error of 2.6 K and 2.0 K occurs in the middle cell when using calculated and measured currents/voltages respectively. The temperatures are generally closer to the actual ones when calculated from measured currents/voltages, due to the absence of battery modeling errors. At the beginning of the trip ($t < \sim 930$ sec), the thermal model predicted almost no heating, whereas an increase of about 1 K was registered. During the early part of the trip, the entropic heat term is considerable because of the low ohmic and reaction losses associated with low power requirements. The entropic coefficient is also positive at an early SOC stage (SOC $> 0.4$), which leads to a considerable heat being absorbed. As a result, the total generated heat is near zero, so that a noticeable increase in the tabs temperature is not the case.

![Figure 12. Comparison of measured and calculated temperatures at the tabs of a) the middle cell, and b, c) the outer cells](image)

While seeking to understand this deviation from the measured temperatures we found that the results are highly sensitive to the SOC values, which were calculated in each time increment using Coulombs counting and the available cell capacity at begin of life. It turned out to be that using in the SOC algorithm an available cell capacity, which corresponds to 88% of that at begin of life, results in a better temperature fit with a maximum error of 1.07 K near the end of the trip as shown also in Figure 12. This adjustment seems consistent given the fact that the tested battery system is not a fresh one but has been undergoing prototype testing for around 5 years, during which irreversible capacity fade occurred. Using a reduced capacity which would predict lower levels of SOC's and thus deeper levels of discharge would alter the heat generation term by altering the OCP and the entropic coefficient, which depend on the lithium ion concentration in the solid phase of the electrodes. These concentrations change with ageing due to side reactions, which consumes Lithium ions irreversibly such as the electrolyte reduction on the anode, as well as electrode cracking which isolates a portion of the electrode particles from hosting the Lithium ions. A detailed ageing analysis is not in the scope of this paper and we content ourselves with treating the actual cell capacity as an adjustable parameter to fine tune the results and account indirectly to ageing effects. In all cases, the obtained accuracy shows that Li-ion battery thermal models as presented in here could be reliable enough and used to
shorten the battery system product lifecycle as well as to make decisions in a battery management system control strategy. Nevertheless, a good calibration process at different system levels such as elaborated in this work remains a prerequisite for a high accuracy.

**SUMMARY AND CONCLUSIONS**

There are stringent temperature requirements to be fulfilled by Li-ion batteries in electric vehicle applications. Given today's urge for a rapid commercialization, mathematical simulation is highly needed in the battery design process to ensure the temperature requirements in a minimum amount of effort and time. Accordingly, we showed a methodology to calculate battery cell temperatures for a given electric vehicle's velocity profile by using a combination of a vehicle dynamics model, a battery equivalent circuit model, and a 3D FE thermal model. The considered vehicle contains a battery pack of 12 modules, each containing 7 Li-ion polymer cells (40 Ah). The vehicle model was used to calculate power requirements from a vehicle's velocity profile, which was measured during an actual vehicle trip of 38.8 Km, in addition to the temperature, the electric current and the electric potential of each cell. Drag resistances, rolling resistances, inertia and compartments power needs were accounted for. The calculated power profiles were then fed into the battery equivalent circuit model, with a PID controller ahead, to calculate the needed voltage/current profiles. The battery electric model accounts for instantaneous and transient polarization by including 2 resistances and a capacitance, whose values are identified from pulse current (20 sec) test data at 40°C. The calculated voltages were in agreement with the measured ones (SD: 0.039 V, maximum error: 0.13 V). A 3D FE transient thermal model of a cell was developed and the cell core region was assumed as a homogeneous material whose effective thermal properties are identified from thermal tests. The FE heat sources were calculated from the currents/voltages using a thermodynamic based energy balance which accounts for Joule's losses and entropy changes. The 3D model was verified by comparing the calculated surface temperatures during a constant current discharge (4.5C) with thermal images performed during a physical test and a good fit was obtained. Instead of analyzing the whole battery pack, a single module analysis was judged to be sufficient since all modules showed similar electro-thermal performances. The module thermal model described the 7 cells and the housing with natural convection boundary conditions and contact resistances. The module model was calibrated by fitting temperature measurements at discrete surface locations of the cells during a 3.5 C constant current discharge.

To predict the cell temperatures that occurred during the vehicle trip, the 3D module model was solved twice, using in each time the calculated cell current/voltages resulting from the battery model or the on-board measured cell current/voltages in the heat source term. Using calculated current/voltages, the cell tab temperatures were in agreement with the actual ones with a maximum error of 2.6 K. This suggests that a combination of validated battery and vehicle models could be used in order to estimate the heat generation associated with a given velocity profile without having to actually perform a vehicle trip. The effect of different driving patterns on heat generation could be thus better understood, so that battery systems could be optimized for various applications. A slight increase in accuracy (maximum error 2.0 K) was obtained when using measured currents/voltages in the heat sources of the model due to the absence of the battery modeling errors. While seeking to understand the reason of the deviation of the calculated temperatures, we found a large sensitivity of the cell capacity value used in the SOC update algorithm, and a value corresponding to 88% of the capacity at begin of life resulted in a better fit. We putatively related this observation to the fact that the used cells have been undergoing prototype testing for around 5 years during which a capacity fade due to ageing happened. Thus, an alteration in the solid phase lithium ion concentrations occurred, which is associated with a change in the thermodynamic variables of the heat generation equations. Reducing the cell capacity in the SOC update algorithm took indirectly cell ageing into account.

Given the achieved accuracy, the developed model could be used in a battery management system so that a model based cell temperature feedback could be taken into consideration in a control strategy that minds a safe window of operations. Nevertheless, the present computational complexity and structure should be adjusted using model reduction procedures in order to allow a production code generation, which can be deployed in the battery management system electronic control unit.

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ABBREVIATIONS

OCP
open circuit potential

PID
proportional, integrator, differential

SOC
state of charge

FE
finite element

SD
standard deviation

EV
electric vehicle

V
voltage

I
electric current

T
temperature

m
mass

a
acceleration

v
velocity

g
gravitational acceleration

ρ
density of air