3D Thermal and 1D Electro-Thermal Model Coupling Framework for Lithium-Ion Battery Cells in Automotive Industry Platforms

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Abstract—This article represents modeling steps for Lithium-ion cells to achieve accurate temperature distribution pattern, while maintaining lowest computational burden. A 1D electro-thermal model based on equivalent circuit approach is implemented to output the electrical characteristics as a function of temperature, current, and SoC. Temperature calculation tasks are done through 3D thermal model using volumetric heat input. A model order reduction approach is applied to the 3D model for coupling compatibility and preparing the models for integration into vehicles’ powertrain. Results in commercial automotive industry simulation platforms, and validation tests demonstrate model precision and the feasibility of the presented approach.

Index Terms—battery characterization, battery modeling, CFD, model order reduction, thermal modeling.

I. INTRODUCTION

Having the significant increase in widespread Lithium-ion batteries’ applications from consumer electronics to automotive and grid storage, a deep knowledge of battery behavior is necessary to study, analyze, and optimize their utilization. On the other hand, most battery management systems (BMS), ensure the safe operation and estimate the state of an entire storage unit using model-based algorithms targeted at each individual cell within multi-cell packs or modules [1].

Various types of modeling approaches are introduced within the literature to predict and simulate non-linear battery behavior in time and frequency domains [2]. Electrical models merely rely on electric parameters of a battery cell (e.g. voltage and current), while a thermal model, either developed in one dimension or three dimensions, outputs cell temperature under operation. In case the battery potential is simulated based on chemical reactions, the model would be an electro-chemical type [3]. Combinations of these methods are also used in particular electro-thermal modeling due to dependency of represented variables to each other.

A major challenge for developing the beforementioned model types, is the unavailability of parameters’ values not provided by the manufacturers, or the diversity of these parameters under various operational conditions which makes their availability almost impossible. To overcome this challenge, a set of standardized or custom characterization tests are performed on cells under various operating conditions (e.g. multi-point charge/discharge C-rates), and different environmental conditions (e.g. ambient temperature) to extract required model parameters [4].

For specific applications, particularly electric vehicles’ powertrain simulations, both electrical and thermal parameters of batteries are essential. On the other hand, cooling or heating systems are usually an essential attachment to batteries in which their design requires a high level of precision in temperature distribution pattern through the cell models [5]. Thus, often electrical, and 3D or 1D thermal models are coupled together to achieve highest accuracy [6]. Such model coupling in simulation platforms requires synchronization of run-times among several e-components of a power train [7]. A trade-off between model accuracy, complexity, and CPU time to real-time ratio is considered for providing a smooth and errorless simulation.

In this article, a 23 Ah prismatic cell is selected for characterization and an equivalent RC circuit model is considered for electrical modeling. Thermal behavior of the cell is modeled within 3D computational fluid dynamics (CFD) simulations. To facilitate model coupling and to overcome running time synchronization challenges, the 3D model is converted into a 1D lumped-element network and then coupled with the 1D electro-thermal model. This approach considerably increases co-simulation running speed without sacrificing battery model accuracy. In the next section, an overview of equivalent circuit electro-thermal modeling followed by characterization of the cell are presented. Section III covers the 3D modeling aspects and its validation. The reduced order modeling (ROM) and coupling of 1D and 3D models to achieve overall battery model are discussed in Section IV and lastly, Section V concludes the article.

II. 1D ELECTRO-THERMAL MODEL

The electrical behavior of battery cells and supercapacitors are commonly modeled by equivalent circuits (EC) in various forms and degrees of complexity [8]. Fig.1 demonstrates an nth-order EC. The open circuit voltage (OCV) of the cell
is assumed as an ideal DC voltage source, connected to an Ohmic resistance $R_0$, and followed by multiple $RC$ loops for simulating battery polarization effect [9]. For this work, two branches are considered having $R_1$, $R_2$, $C_1$, and $C_2$. The Kirchhoffs Voltage Law (KVL) gives the battery terminal voltage $V_{bat}$ as

$$V_{bat} = OCV - R_0I_{bat} - V_{p1} - V_{p2}$$

(1)

where $I_{bat}$ is the charge/discharge current, and $V_{p1}$ and $V_{p2}$ are voltage drops across each $RC$ branch. All the beforementioned parameters are a function of instantaneous $I_{bat}$ (also referred to as C-rate), cell temperature $T_{bat}$, state of charge (SoC), and number of cycles the battery has undergone i.e. aged. The latter is not in the scope of this article. A diverse set of characterization tests are performed on the cell to extract the required parameters for the EC model which makes this modeling process an empirical approach.

Discharge capacity, OCV, and hybrid pulse power characterization (HPPC) tests are performed on the cell in various temperature points and C-rates as described in the following. Required parameters are extracted from these tests and they are stored as look-up tables within the model. To derive parameter values among and outside testing points, interpolation and extrapolation methods are used to have a continues parameterization of the cell.

A. Discharge Capacity Test

Since the amount of energy could be stored in a battery is dependent on its temperature, this test aims at maximum battery capacity consideration as a function of C-rate and temperature of the cell. As demonstrated in Fig. 2, the test profile consists of six full discharge cycles in C-rates ranging from $C/3$ to $8C$, while it is observed that the amount of energy (in Ah) extracted from the cell under each discharge rate is different. Equal resting periods for battery relaxation are considered between consecutive charge and discharge cycles. The same profile is repeatedly applied to the cell in several cell and ambient temperature points.

B. OCV Test

This test aims at extracting the OCV parameter of the cell as a function of SoC and temperature. As demonstrated in Fig. 3, the test profile is divided into two parts of charging and discharging. Initially, the cell is pre-charged to 100% SoC and the tester begins to discharge it in multiple steps of 5% depth of discharge (DoD) under 1C discharge rate. Between each two consecutive discharges, the cell is given some resting period to stabilize, and the stable voltage value is logged as OCV at that corresponding SoC. Once the cell is fully discharged in multiple steps, reverse procedure is applied to charge the cell up until it gets fully charged again. Same test is conducted in multiple cell and ambient temperatures and eventually, look-up tables of OCV vs. SoC are generated to be implemented into the EC model.

C. HPPC Test

The aim of this test is to extract $R_0$, $R_n$, and $C_n$ values of the $RC$ loop(s) under different charge/discharge C-rates, temperatures, and SoCs. Therefore, a pulse train composed of 12 pulses ranging from $\pm C/3$ to $\pm 8C$ is defined as a test profile and is applied to the cell. Fig. 4(a) demonstrates the voltage response of the tested cell where after every 5% DoD discharge, the pulse train shown in Fig. 4(b) is applied until the cell is fully discharged. Parameters are extracted as in the zoomed voltage curve in response to a 2C charge pulse in Fig. 4(c). The instantaneous $\frac{dv}{dt}$ is considered caused by the ohmic resistance $R_0$, and the sloped part is considered to be caused by the polarization effects interpreted as $V_{p1}$ and $V_{p2}$. Polarization resistances and capacitances are then calculated through $RC$ loops’ time constants $\tau_1$ and $\tau_2$ measurements. A summarized demonstration of the 1D modeling steps is
shown on Fig. 5 where the blue (dotted) loop represents the experimental procedure on the cell. The beforementioned test profiles are defined offline in the host computer, and fed into the battery testers (PEC ACT0550 in this case). Each Li-ion cell is connected to one of the cycler channels capable of current, voltage, and temperature logging fed back into the host computer. Cells undergo each test in controlled temperature chambers set for all pre-defined temperature points. Then, the data processing stage is performed (red solid arrows on the figure) commenced with extracting the parameters. This task is done either in MATLAB or built-in parametrisation wizard in AVL CRUISE M. Once all the required look-up tables are achieved, they are implemented into the battery module within CRUISE M. Interpolation and extrapolation techniques are used to achieve consistent data series of the parameters within/outside the testing points. To estimate the instantaneous SoC(t), common coulomb counting method is utilized as

$$\text{SoC}(t) = \text{SoC}(t_0) - \frac{1}{C} \int_{t_0}^{t} I_{bat}(t) dt$$  \hspace{1cm} (2)$$

where \( \text{SoC}(t_0) \) is the initial SoC of the cell (at \( t = t_0 \)) derived from the OCV vs. SoC results, \( C \) stands for cell capacity in (Ah), and \( I_{bat}(t) \) is the instantaneous current value derived from or injected into the cell. The other parameter signal extracted from the model shall be total Ohmic power loss caused by internal resistances of the cell which is calculated by

$$P_{\text{loss}} = (R_0 + R_1 + R_2)I_{bat}^2.$$  \hspace{1cm} (3)$$

For validation of model’s electrical response, battery model terminal voltage \( V_{bat} \) is compared against experimental lab measurements of the cell voltage under the World-wide harmonized Light duty Test Cycle (WLTC) profile as demonstrated in terms of cell current in Fig. 6. The comparison of the voltage graphs confirms the validity of the model in following the measured values in constant and dynamic parts. Also, the error graph shows less than 3% deviation during the entire 1800s cycle run, which is considered acceptable. It shall be noted that high spikes visible on the experimental measured voltage graph (and consequently on the error graph) are caused by the battery tester and not coming from the cell itself.

### III. 3D THERMAL MODEL

AVL FIRE M platform is used for implementation of cell’s CFD simulations. The power loss is calculated in the 1D electro-thermal model within (3) and it is applied to the multi-domain cell as a volumetric heat input.
The initial step towards 3D model development is the cell geometry design and domain specifications. As in Fig.7(a), the geometry is divided into four domains of inner-cell material with thermal specifications derived from manufacturer, two plus/minus tabs in Aluminum material, and cell casing around the inner-domain which is also assigned as Aluminum. The heat input is applied to the inner-cell domain since it is supposed to include the electro-chemical reactions and to generate the power loss.

For this cell, the polygon-shaped meshing is conducted in FIRE M with two boundary mesh layers on the edges of each domain. The thickness of each layer is considered to be 1mm and in total, 11083 mesh-cells are generated as shown on Fig.7(b). The cell is in natural convection heat transfer with ambient in all directions. Further simulation setting parameters are listed in Table I.

The 3D cell model is validated by conducting a 0% to 100% charging test in 4C rate. The cell is located in a 25°C climate chamber and it has given enough time for temperature stabilization. The tabs are welded to copper contacts to make an interface with plugs coming from the tester. Constant-current of 92A has been injected for 900s and during the test, the cell has been monitored with a thermal camera. It shall be noted that the constant-voltage phase of standard battery charging has been avoided in this validation test. The last frame captured with the camera is illustrated on Fig.8 which represents temperature distribution at $t = 900s$. The similar 4C charge rate is conducted in the CFD simulation as well. The comparison between simulation and experimental results shown in Fig.8 confirms the validity and accuracy of the implemented model in terms of both temperature distribution pattern throughout the cell, and temperature raise values. The results confirm the necessity of performing 3D modeling since for this cell, there is a temperature deviation among sides of the cell, and middle parts. This could be a point of interest for specific purposes (e.g. designing an optimal cooling system).

IV. 1D-3D MODEL COUPLING

As described, 3D thermal modeling brings the advantages of temperature monitoring in any point of the cell geometry, and very precise temperature values. But it comes with the price of high computation burden leading to lengthy run-times. A 3D to 1D model order reduction approach by generating a lumped-element network out of the CFD model, is introduced in [10] and applied to the model developed in this study. Therefore, the reduced order model (ROM) is transferred from FIRE M to CRUISE M making it compatible for coupling with the 1D electro-thermal model.

Fig.9 demonstrates the reduced order model generated for the cell which is composed of the four solid domains explained before, and representing the material and physical characteristics assigned to each domain, and domain interface blocks containing heat exchange parameters between connected domains. The volumetric heat input which is applied to inner-cell domain in here is transformed into a heat generator block and connected to the corresponding solid domain block. All parameters are modifiable and could be adjusted for dynamic and transient simulations in 1D making them possible for online simulations, coupled with the 1D model. One major advantage of this approach is that each domain delivers...
its specific temperature value. Meaning that the temperature distribution differentiation feature has not been lost after 3D to 1D order reduction.

The overall Li-ion cell model composed of the three sub-models presented in this work, their integration and input/output (I/O) signals are presented in Fig.10. The 3D model is simulated in FIRE M in an offline mode to generate the reduced order lumped-element network. It requires ambient temperature $T_{amb}$, initial cell temperature $T_{ini}$, and power loss $P_{loss}$ signals during a steady load profile extracted from the 1D electro-thermal model as inputs. This process is done once, and the rest of the simulations could be run in CRUISE M. The reduced order model block is responsible for accurate battery temperature $T_{bat}$ generation which is fed back into the 1D model. This block requires $P_{loss}$ and $T_{ini}$ signals for that purpose. The electrical characteristics of the cell (e.g. terminal voltage $V_{bat}$, SoC, etc.) are outputed by the 1D electro-thermal model. The inputs for this block are initialization signals $T_{ini}$ and SoC$_{ini}$, and the battery current $I_{bat}$ which could be a constant or dynamic load profile.

Similar to the 3D model, the final 1D coupled model performance is validated against measured battery surface temperature values logged by thermocouples. Two charging test scenarios have been conducted on the cell at 4C and 8C rates. Hence, constant-current of 92A and 184A have been injected for 900s and 450s, respectively. Again, it shall be noted that the constant-voltage phase of standard battery charging has been avoided in these validation tests. In the simulations, temperature of the cell-casing domain is logged instead of the inner-cell material to provide a fair comparison with the experiments where the sensors are installed on the casing. The results are demonstrated in Fig.11 where the model outputs have accurately followed the experimental measurements with negligible deviation or error.

V. CONCLUSIONS

A framework for comprehensive electrical and thermal characterization and modeling of Li-ion batteries for automotive applications is presented within this article. To take advantage of high accuracy of 3D CFD simulations, the temperature calculation tasks are shifted to a 3D thermal model. This approach significantly impacts model run-times and makes it almost impossible for coupling within other powertrain e-component models. Therefore, the thermal model order has been reduced to 1D, while the accuracy is maintained and the resulted model could be coupled with the electrical part by exchanging temperature and power loss signals. While this study is performed on a single cell, the presented approach could be up-scaled up to multi-cell configurations i.e. in series or parallel for modules or packs modeling. Lastly, the fast and precise models provide the ability to differentiate between temperature values on each part or side of the cell geometry in 1D level.

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