Validation of a new simulation tool for the analysis of electrochemical and thermal performance of lithium ion batteries.

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ABSTRACT: With the increasing focus on the use of lithium ion batteries for traction applications the ability to simulate electrochemical and thermal performance of such batteries is of great interest. This paper details a multi-length scale approach which is used to simulate a single lithium ion pouch cell and compare against some previously published experimental work. This approach is then extended and used as a building block to a much more complex simulation using multiple cells within a battery pack. This technology also simulates the cooling system performance and the inherent coupled behavior of the battery’s operation and its thermal environment.

KEY WORDS: Lithium-ion battery, thermal response, Simulation, Battery simulation, Computer Aided Engineering

1. Introduction

In November 2009 CD-adapco and Battery Design LLC announced a partnership to produce a design tool which would simulate lithium ion batteries and the surrounding thermal environment created by a battery module or pack installation. CD-adapco’s computer aided engineering tool, STAR-CCM+, has been enhanced to include this battery simulation technology. It is now possible to predict flow, thermal and electrochemistry quantities within this one code and as such demonstrate the effects of design changes on the closely coupled relationship between a battery module’s load and performance and its surrounding environment. This paper details one of the fundamental battery thermal and electrochemical behavioral models as well as showing an application of such a model within a larger real world application. The tool was developed with large format lithium ion cells in mind and as such the battery cell is not modeled as a lumped or single model but rather a discretisation is applied to each battery cell’s active region capturing internal gradients.

2. Simulation Architecture

2.1. Overview

STAR-CCM+’s new feature, the Battery Simulation Module (BSM), can be used to simulate the electrochemical and thermal behavior of a complete electrical vehicle battery pack. It is possible to setup a Conjugate Heat Transfer analysis in STAR-CCM+ to optimize the thermal management of such a device.

In order to assess this new feature, a fundamental study of the implemented battery model has been carried out, this studied only a single battery cell in isolation and compares this to previously published experimental results.

Firstly, the battery cell properties of the studied cell will be described, and then the simulation settings and operating conditions will be presented. Finally, the computed results will be compared to the experimental data found in [1].

3. Battery Cell Model Details

3.1. Modeling the Electrochemistry Behaviour

A lithium ion polymer battery (LIPB) consists of a Li[NiCoMn]O2 positive electrode with an aluminum collector, a graphitic negative electrode with a copper collector and an electronically non-conductive separator between the two electrodes and electrolyte with lithium salts. A pouch cell is then a repeating unit of these three elements, which is why it is called also a “stack plate”. The distance between the parallel plate electrodes, alternatively called the separator thickness, is relatively thin such that the current flow between the electrodes would be perpendicular to the electrodes plane. For this study the three layer unit is repeated 7 times, which makes the battery cell ~0.5mm thick.

The battery cell as it is defined in [1] has the following dimensions and properties:
The battery cell has a capacity of 26 Ahr. Its voltage trace when loaded with a constant discharge varies with the discharge rate (C rates) applied to it. The following graphs summaries the different Voltage discharge behavior against C rates [1]:

Figure 2 Experimental discharge curves at discharge rates ranging from 1 to 5 C for the LIPB nominal capacities.

The battery is modelled in BSM using the NTG (Newman, Tiedemann, Gu) model. This is one of three numerical battery models available to the user, the others being an equivalent circuit model [6] or a detailed electrochemistry model based on the methodology of [7] & [8]. The remainder of this study will use the NTG model to demonstrate the methodology however the same solution architecture applies to other numerical battery models.

The current density \( J \) is a function of the potential difference between the positive and negative electrodes. This functional form depends on the characteristics of the electrodes which are expressed in the NTG model using polynomials:

\[
U = a_0 + a_1 DoD + a_2 DoD^2 + a_3 DoD^3 \tag{3}
\]

\[
Y = a_4 + a_5 DoD + a_6 DoD^2 \tag{4}
\]

\[
Q = I \cdot (U - V_{cell}) \tag{5}
\]

\( V_{cell} \) = working cell voltage

\( DoD \) = Depth of Discharge (fraction)

\( J \) = Current Density, A/m²

\( I \) = Current, A

\( Q \) = Heat Generation, W

\( Y \) and \( U \) are fitting parameters. They are expressed as a function of the depth of discharge (DOD). In this study the same TBM file is used for the 3 different cases, therefore the coefficients \( a_0 \) to \( a_6 \) have been determined through a regression process in order to account for the effect of a different loads applied to the battery cell.

All the fitting data can be found in the TBM file used in this study (see appendix) and the regression process is detailed in the BDS software tool.

3.2. Modeling the Thermal Behaviour

The thermal modelling procedure to calculate the temperature distribution on the electrodes is managed by STAR-CCM+. The Energy Equation is defined analytically, considering some simplification for this particular case, as follows:

\[
\rho \cdot C_p \cdot \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( k_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( k_y \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( k_z \frac{\partial T}{\partial z} \right) + q - q_{conv} \tag{6}
\]

Where \( \rho \) is the density (kg/m³), \( C_p \) the volume averaged specific heat capacity at constant pressure (J/kg.K), \( T \) is the temperature (K), \( k_x \), \( k_y \) and \( k_z \) are the effective thermal conductivity along the \( x \), \( y \) and \( z \) directions respectively (W/m.K), \( q \) the heat generation rate per unit volume (W/m³), and \( q_{conv} \) is the heat dissipation rate (W/m³) through the surfaces of the battery by convection.

The heat generation rate \( q \) is calculated with STAR-CCM+ electrochemical solver based on the battery cell specifications contained within the .tbm file, and is passed to the energy equation. The heat dissipation rate \( q_{conv} \) is computed by STAR-CCM+. It is dependent on the heat transfer coefficient \( h \). The latter is defined for a wall placed in a natural convection flow for which values can be found in [3]. It is worth noting this simplification is due to the limited data available to replicate the experiment, in real world examples STAR-CCM+ will compute the heat transfer rate based on local flow rate or conduction conditions.

The effect of the discharge rate on the battery is studied next. Apart from the fact that the battery will discharge slower or faster depending to the load applied, this varying load will affect the temperature variation in the cell, which is of particular interest in this case. Indeed, it is a critical parameter to control, as the overall performances and life time of the battery cell are very sensitive to the ambient and working temperatures.
In the experiment, the effect of a constant discharge is measured on three different cases:

<table>
<thead>
<tr>
<th>Case</th>
<th>C rate</th>
<th>Equivalent discharge current (A)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case1</td>
<td>1</td>
<td>26</td>
</tr>
<tr>
<td>Case2</td>
<td>3</td>
<td>78</td>
</tr>
<tr>
<td>Case3</td>
<td>5</td>
<td>130</td>
</tr>
</tbody>
</table>

The battery cell is placed in an adiabatic oven at room temperature. There is no use of a ventilation system to control the oven temperature. Therefore, the main physical phenomenon observed in the oven is natural convection. There are no details concerning the temperature measurements in the experiment except the use of an infrared camera. However the latter seems to also be used for temperature distribution images. Thermocouples placed at relevant locations would be more appropriate but this has not been mentioned in the experiment description in [1].

3.3. Simulation settings and Boundary Conditions

Once the .tbm file has been imported in STAR-CCM+, the built-in CAD generator creates a single battery cell part. It is actually composed of 5 distinct CAD parts, they are:
- The Positive Electrode Tab Root
- The Positive Electrode Tab Stem
- The Negative Electrode Tab Root
- The Negative Electrode Tab Stem
- The Stack Plate

The root has the shape of a tent and idealises the location where all the electrode’s collector plates of the same polarity are pinched together. The tab is then connected on top of the root to allow a connection with any other conductive parts such as the battery cells’ post. The Stack plate CAD part represents the assembly of positive and negative electrode layers stacked with the separators plates as shown in figure 3. The individual electrode layers are not resolved in the 3D model however the numerical battery cell model does account for these parts.

3.4. Discretisation of the Battery Cell

A single battery cell is generated using BSM (see figure 4). The mesh is generated with STAR-CCM+'s dedicated battery mesher which meshes the roots and tabs using the thin mesher model and the stack plate region using regular hexahedral blocks. The Stack mesh is a Cartesian mesh as it also defines the network of sub-battery models used by the electrical solver. The Stack resolution is arbitrarily set with 15 finite volume cells on the x and y directions and 1 finite volume cell on the z directions. This leads to the battery model being applied to each of the 225 finite volumes and these are connected in an electrical matrix. 1 finite volume cell is sufficient in the z direction as the battery cell is so thin that it is assumed temperature is uniformly distributed in that thin direction. For tab roots and stems, a finite volume cell size of 2 mm for the surface mesh is applied. In the thin part of the tabs, 2 thin layers are used for the resolution in the z direction.

3.5. Operating Conditions

As said above, the physics of the surrounding air in the oven is a natural convection phenomenon. This can be modelled using convective walls as an external boundary condition on the outer surface of the battery cell. Therefore, there is no need to mesh and solve the surrounding air in this validation case. A heat transfer coefficient (HTC) is provided, and is set as a constant value throughout the simulation (see table 3). The value is chosen appropriately for natural convection flows as described in [3], in which HTC has been evaluated into a range of values going from $6 \text{ W/m}^2\cdot\text{K}$ to $45 \text{ W/m}^2\cdot\text{K}$.

<table>
<thead>
<tr>
<th>Case</th>
<th>Heat Transfer Coefficient (W/m$^2\cdot$K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case1 – 1C</td>
<td>10</td>
</tr>
<tr>
<td>Case2 – 3C</td>
<td>25</td>
</tr>
<tr>
<td>Case3 – 5C</td>
<td>30</td>
</tr>
</tbody>
</table>

Finally the choice of the ambient temperature is set as to be 25.0°C, as described in the experiment [1].
3.6. Solver Settings

The time step size is set to 5s. The number of inner iterations per time step, a numerical quantity used by STAR-CCM+, is set to 10 iterations per time steps.

The simulation stopping criteria are defined as the time when the battery cells becomes flat, i.e. SOC = 0% (see table 4). Therefore the simulations are run for the periods listed in table 4.

Table 4 Solution Time

<table>
<thead>
<tr>
<th>Solution Time (s)</th>
<th>Case1</th>
<th>Case2</th>
<th>Case3</th>
</tr>
</thead>
<tbody>
<tr>
<td>3600</td>
<td>1200</td>
<td>720</td>
<td></td>
</tr>
</tbody>
</table>

4. Results and Discussion

The cases were run on a single processor using a desktop machine:
- OS: Linux 2.6.31.12-0.1
- CPU type: Intel(R) Xeon(R) CPU E5440 @ 2.83Ghz

4.1. Temperature Probes and Distribution

Minimum and maximum temperatures were reported in [1] throughout the Stack region. In STAR-CCM+, the maximum and minimum temperatures within the stack region are recorded for each time step.

The computed maximum temperatures are in very good agreement with the experimental measurements (figure 5). As the load increases, it can be seen that the increase in battery heat temperature is accurately calculated.

4.2. The electrical Behavior

As described above, the NTG model uses polynomials to fit the voltage of the battery cell through various discharge conditions. Being limited on the order of the polynomial at a third order, the voltage discharge curve leads to the following graph in which discrepancies are observed in comparison to the experimental data (see figure 8).

However, this fitting is acceptable and leads to good results.
5. Model Extensions

The NTG model has been presented using a 3rd order polynomial fitting process for isothermal discharge curves. The results presented a good fit to the integral values and also the spatial results and gradients taken from [1]. After concluding this process the cell model has been extended to include the effects of temperature on the battery’s performance.

The previously presented equation (4) is then modified to include temperature dependence.

\[
Y = (a_4 + a_5 \cdot \text{DoD} + a_6 \cdot \text{DoD}^2) e^{\frac{E_a}{R} \left( \frac{1}{T_{\text{ref}}} - \frac{1}{T} \right)}
\]  

Equation (6) contains an Arrhenius term to account for the change in reaction rate within the battery. This means that the fitting process is extended to include an activation energy term. This extends the fitting data to include a range of discharge curves at different ambient temperatures. As before the coefficients \(a_0\) to \(a_6\) have been determined as well as the \(E_a\) value and these are stored in the TBM file representing the battery. The model has also been extended to make possible the use of higher order coefficients within the polynomials to capture the non linear behavior, up to 6th order polynomials are now provided for.

6. Battery Module and Pack Simulations

Having validated the approach, as shown above, and enhanced the method to include temperature dependence, STAR-CCM+ is used to predict a string of battery cells operating as a module. This is an extension of the above method and Figure 10 shows one such model. This contains a string of 8 battery cells connected together using appropriate posts and straps, which complete the thermal and electrical network. A temperature dependent set of model coefficients are then applied to each battery cell, each of which is further discretised in to a matrix of 15 * 15 sub-battery elements as defined in section 3.4. Moreover these battery cells are surrounded by a computational mesh which models the convective cooling of the air surrounding these cells using a finite volume method as part of STAR-CCM+. This means that the convection and conduction of heat from the battery cell source is resolved and ultimately the quality of the thermal environment that the battery cells are subject to within and application is predicted.

![Figure 9: Voltage discharge against Capacity at 3C rate. Computations at 3 different temperatures, 15°C, 25°C, and 45°C](image)

![Figure 10: A 8 Cell module showing the battery cell’s temperature as well as tab and connector temperatures](image)

During such a coupled simulation the average temperature of the battery cells is monitored and then the uniformity of these average temperatures can be evaluated. This uniformity has a direct effect on the battery lifetime and should be seen as a measure of the effectiveness of the cooling system installation. Figure 11 shows this average temperature trace for each battery cell after 10 minutes of simulation. It can be seen that even after 10 minutes of gentle discharge there is a spread developing of average cell temperature which would lead to different discharge performance. Indeed the importance of capturing the 3D thermal path as well as the electrical path, because it is a major form of heat transfer, is shown as the tabs; particularly the positive can be at elevated temperatures. These tabs then act as a heat source into the battery cell or a conductor of heat from one cell to another.

This kind of 3 dimensional study deserves extensive discussion and will be the subject of another paper which builds on the methodology presented in this paper. This short discussion is included as a taste of future work in this field. Indeed the software architecture will be used with other, more complex, battery models.

![Figure 11: Average temperature results of each battery cell within an 8 battery cell module.](image)

7. Conclusions

The paper has presented an approach to model the electrochemical and thermal performance of an individual battery cell, and also compared with previously presented experimental results. This approach has then been applied to a short module and again electrochemical and thermal results presented. Through this study the method has captured the important coupled phenomena between a battery cell’s electrochemical performance and that of the surrounding thermal environment. This technique provides enhanced results and is available within the flagship CAE environment STAR-CCM+ making this coupled analysis within
reach of the modern day simulation practitioner. An example of which is available in [9]

References

[11] Kawase, M - Development of thermal numerical modeling of large format Li-ion battery for space application, 9th Space conference, ESCP (2011)