Heat Generation Modeling of a Lithium Battery: from the Cell, to the Pack on COMSOL Multiphysics

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Abstract: A thermal model to predict the heat generation during the charge and discharge of a battery pack is an essential tool to manage the thermal behavior, performance and life of the batteries. In this work, a battery cell ($LiFePO_4$) is modeled on COMSOL Multiphysics with the Batteries and Fuel Cells module. Once its heat generation known, the corresponding heat source term is used to study the temperature reached in a battery pack made of multiple cells. The thickness of the electrodes, the weight, the area, and the size of the particles were measured and implemented in the model. A 5C discharge (Ref. 2.) was then simulated. The temperature elevation (about 14°C for a single battery cell) was compared to an experiment to validate the result (Ref. 2.). The heat generation was then implemented for the simulation of the battery pack and the temperature elevation increased to 19.6°C. The models were set up with the general parameters to end up with an error of about 9% on the temperature elevation in the pack. This is a good approximation to do preliminary design in engineering.

Keywords: Lithium Battery, Discharge, Heat Generation, Temperature Elevation, Battery Pack.

1. Introduction

Lithium-Ion batteries are increasingly used in the automobile industry. The improvement of the energetic density allows a bigger autonomy for a lower weight. Lithium-Ion batteries are even used in aviation with the Efan (Fully powered by electricity airplane).
The performance and life of a battery pack is related to its temperature. To have a maximum efficiency the temperature of the pack must be within a specific range. The numerical simulation with thermal effects is a good way to develop and improve battery packs at lower cost than experimentation. It is also important to maintain safe operating temperature to avoid thermal destruction.
COMSOL Multiphysics is a finite element simulation software. It is able to couple different kind of physics by using modules such as electrical, mechanical, fluid and chemical. One of these modules is called Batteries & Fuel Cells and can simulate the heat generation of a Lithium-Ion battery. This module allows modeling the underlying electrochemical behavior in the electrodes and electrolytes. In the following, we present the modeling of the battery of the Cal Poly electric race car in order to determine the heat behavior of the battery pack in a discharge case.

2. Goals

a. Model the Electric Race Car battery cell (Fig. 1) with the Heat Transfer in Solids, and Batteries and Fuel Cells modules of Comsol.

Figure 1. Battery cell.

b. Use the heat generation found in a. to model the temperature evolution of the battery pack shown by Figure 2. with the Heat Transfer in Solids module.

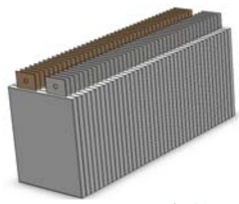

Figure 2. Battery pack (40 cells).

3. Parameters Determination

The electric car battery cell is flat and its inner layers are stacked. They are packed in a flexible and impervious aluminum enclosure. A second plastic film protects the electrodes and serves as the separator. The physical parameters required by the model, such as porosity and size of the particles, thickness of the layers, size, area, and weight of the battery were determined either by a

Scanning Electron Microscope (SEM) or by using the data given in Ref. 2.

Figure 3. Cell 104.

4. COMSOL Model of the Cell

Two Comsol Multiphysics modules are necessary to figure out the heat generation of the battery. The first, Batteries and Fuel Cells, simulates the chemical reaction between the anode, the cathode and the separator in one dimension. The second, Heat Transfer in Solids simulates the heat conduction in all the battery. The coupling between these two physics is illustrated by the Figure 4. The chemical reaction is dependent on the temperature distribution, the temperature distribution evolves due to the chemical heat generation.

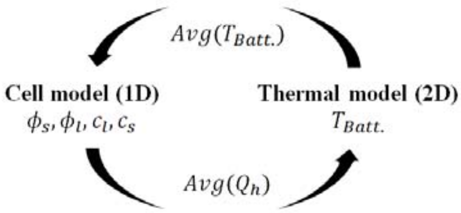

Figure 4. Coupling variables in the thermal modeling of a Li-Ion battery cell.

4.1 Step Function

To be able to simulate discharge and set zero current consecutively, it is possible to set up a step function with amplitude of one. At 5C with a capacity of 6 Ah the duration of the discharge is 720 s. After this duration the function goes to zero to let the battery cooling for 780 s.

4.2 Lithium-Ion Battery

The chemical reaction taking place in the Lithium-Ion battery may be represented by a 1D geometrical model. The Figure 5 shows the domains of this 1D model. The materials are from the left to the right: Copper, LiC_6, $LiPF_6$, $Li_yMn_2O_4$, Aluminum.

Figure 5. 1D cell representation.

4.3 Electrochemical Model Equations

The equations of the electrochemical model are too complex to be detailed in the scope of this article. A full model may be found in Ref. 1. The Comsol User's Guide for the Batteries and Fuel Cells module reminds the theory too. These equations have to be written and solved in the different parts of the cell: the negative current collector, the negative porous electrode, the separator, the positive porous electrode, the positive current collector (Fig. 5).

The negative current collector is in copper, this is a full solid material without electrolyte. The negative porous electrode is a mix of carbon, electrolyte, and lithium. The pores of the electrode are filled by electrolyte. The environment is thus liquid and solid (Ref. 1, 3). The purpose of the separator is to keep a certain distance between the two electrodes, and still let the Li ions commute. The separator is filled by electrolytes, the environment is thus liquid. The positive porous electrode is a mix of lithium manganese oxide, electrolyte, and lithium. The pores of the electrode are filled by electrolytes too. The environment is thus liquid and solid and the equations are the same as for the negative porous electrode. The positive current collector is in aluminum. This is a full solid material without electrolytes with the same modeling equations as the negative current collector.

4.4. Boundary Conditions for the Electrochemical Problem

As shown by the Figure 6., an electric ground condition is set on the negative current collector to fix the electrical potential to zero. The No Flux condition set the flux of salt ions perpendicular to the boundary to zero. On the positive current collector, the electric current density condition sets the local current density of the positive electrode to the current of the positive current collector.

Figure 6. Boundary conditions for the 1D cell.

4.5 Initial Conditions for the Electrochemical Problem

Initially the battery is empty. In the solid part of the positive electrode (on the right, Fig. 7) the potential ϕ_s is 3.6 V (the Li atoms are on the right side on Fig. 7). In the solid part of the negative electrode, the potential ϕ_s is zero. The electrolyte salt concentration c_l is set to cl_0 = 2000 mol·m^{-3} when the circuit is open. The electric potential ϕ_l in the electrolyte is - 0.1 V in all of the battery.

Figure 7. Initial conditions for the 1D cell.

4.6 Heat Transfer in the Battery Cell

The heat produced by the electrochemical reactions does not progress in the same way in each dimension. For example, the heat dissipates easier along the curves of the electrodes than perpendicular due to the anisotropy of the material. The battery is an anisotropic material because it is composed by several different layers with different properties. In all, three materials compose the battery. Their thermal capacities, heat conductivity coefficients, densities, have to be computed by specific formulas (Ref. 3).

In order to determine the temperature increase of a single cell, the standard heat transfer in solids equations are solved with the space averaged power density source term, *Q(t)*, corresponding to the heat generated by the 1D modeled electrochemical reactions. The domain for solving the heat transfer is a 2D cross-section geometry of the cell shown by the Figure 8. The chemical reactions are assumed invariant in the transverse direction of that cross section.

The term *Q(t)* is used in the heat transfer simulation of the 3D battery pack as the power density source term. It is a constant scalar field for a fixed time.

4.7 Boundary Conditions for the Heat Transfer Problem

On the outside of the steel enclosure is a convective heat flux as if the battery were surrounded by air at room temperature (Fig. 8). It is possible to figure out the average heat flux generation. The determined value of the convection coefficient is h = 6 W·m^{-2}·K^{-1}.

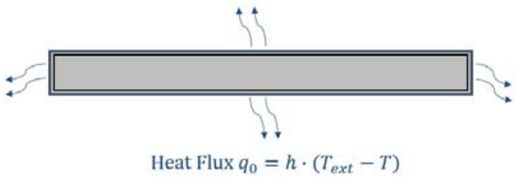

Figure 8. Boundary conditions applied to the battery cross-section.

4.8 Initial Conditions for the Heat Transfer Problem

Upmost, the totality of the battery is set at room temperature, 25°C, at the beginning of the process.

4.9 Mesh

Different levels of mesh refinement were tested from coarse to extremely fine.

5. COMSOL Model of the Battery Pack

The electric race car battery pack is composed of 40 battery cells connected together with two long screws.

Name	Expression	Description
k_t	68 W·m^{-1}·K^{-1}	Transverse thermal conductivity
k_n	1.31 W·m^{-1}·K^{-1}	Normal thermal conductivity
ρ	2548.2 kg·m^{-3}	Density
C_p	1266 J·kg^{-1} ·K^{-1}	Heat Capacity
h_e	0.1 W·m^{-2}·K^{-1}	Equivalent convection coefficient
d	0.13 mm	Thickness of the enclosure
k_{eq}	4.87 W·m^{-1}·K^{-1}	Enclosure equivalent thermal conductivity

Table 1. Parameters for the battery pack simulation.

To model the battery pack, the current collector tabs will be neglected as the closure and the two folds on each side of the battery. The physical parameters are given in Table 1.

5.1 Battery Pack Geometry

The 3D model has been drawn on SolidWorks and then imported on Comsol in ".STEP" format. It includes from 10 to 40 cells in order to see the evolution of the heat versus the length of the pack. For the sake of simplicity, Figure 9 shows a pack of ten battery cells.

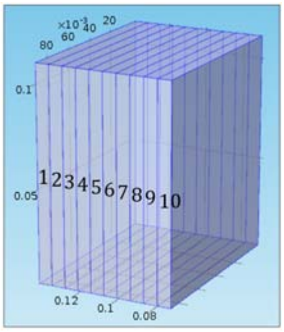

Figure 9. Pack of ten elements.

5.2 Heat Transfer Modeling of the Pack

Each battery cell is surrounded by a thin plastic film and the aluminum enclosure. The thin plastic film has a much greater thermal resistance than the aluminum. The plastic thin layer is too thin to be meshed. The plastic and aluminum layers are then replaced by a single layer with the equivalent resistivity of both layers. Between two battery cells of the pack there is single resistive layer formed by the resistive layer of the upside cell and the resistive layer of the downside cell (Fig. 10). The convective flux through this layer depends on the thermal resistivity of the layer.

The Heat Transfer in Solids equations are used to model the temperature evolution of the pack. The source term of that equation is $Q(t)$, the heat power density computed in the case of a single battery cell. On the outside of the aluminum enclosure a convective heat flux condition is set as if the battery were surrounded by air at room temperature. The equivalent convection coefficient is given in Table 1.

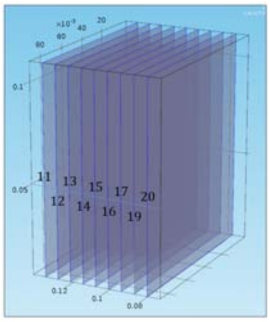

Figure 10. Thin thermally resistive layers.

The elements are initially set to the room temperature, 25°C, at the beginning of the process.

Three levels of mesh refinement were tested: coarse, fine and extremely fine.

6. Simulation Results

6.1 Computer Performance

The computer used for running the simulation has the following main features:

- Computer : DELL Optiplex 790,
- Processor : Intel(R) Core(TM) i5-2400, CPU @ 3.10 GHz 3.10 GHz,
- Installed memory (RAW): 4.00 GB,
- System type : Windows 7, 64-bit Operating System.

6.2 Single Battery Cell

The model has been run with the following mesh and solver parameters, and convergence results:

- Mesh Size : Normal,
- Time-Dependent Solver : BDF,
- Time Range : 0 - 720 seconds,
- Time Step : 5 seconds (free),
- Relative Tolerance : 0.001,
- Direct Solver : MUMPS,
- Solution Time : 78 seconds,
- LinErr : 1.3e-8,
- LinRes : 1e-12.

The results of the calculation do not vary depending on the tested mesh sizes. The maximal and minimal temperature stays constant. The differences operate in a range of a few hundredths of degrees. The particles size of the positive electrode are a tens time bigger than the battery. The default normal mesh size gives good results.

On the Figure 11., the constant green line shows the positive current at 5C discharge, the blue curve the cell potential, and the red line the temperature elevation for a free convection of the battery insulated in a foam box for a thermal convection coefficient $h = 0.1$ W·m^{-2}·K^{-1}.

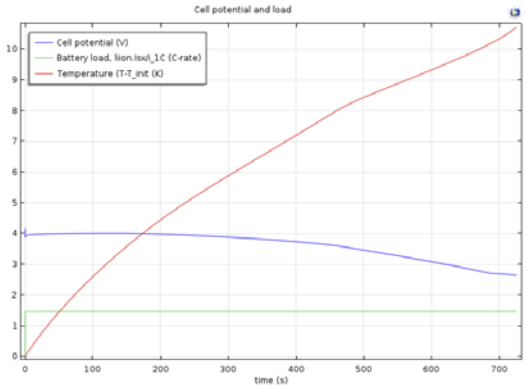

Figure 11. Temperature elevation (red), cell potential (blue), battery load 5C discharge (green).

The Figure 12. shows the electrochemically generated heat power density, $Q(t)$, in W·m^{-3}, from the Comsol model.

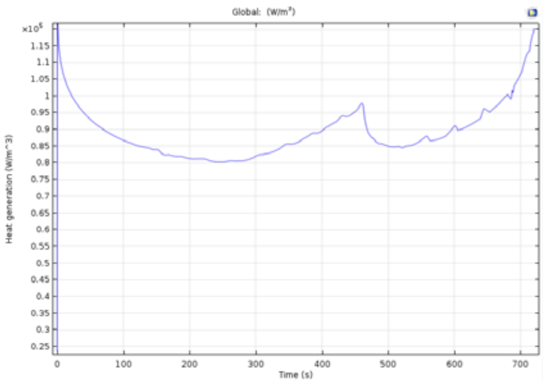

Figure 12. Heat generation found for the battery cell.

6.3 Battery Pack

The model has been run with the following mesh and solver parameters, and convergence results:

- Mesh Size : Normal,
- Time-Dependent Solver : BDF
- Time Range : 0 - 720 seconds,
- Time Step : 10 seconds (free),
- Relative Tolerance : 0.001,
- Direct Solver : MUMPS,
- Solution Time : 82 seconds,
- LinErr : 1.3e-8,
- LinRes : 1e-12.

The results do not vary significantly regarding to the used mesh sizes. The Figure 13. Shows the reached temperature distribution of the pack at the final simulation time (720 s). The minimal computed temperature is 42.9°C at the extremities of the pack and the maximum temperature is 44.6°C in the middle.

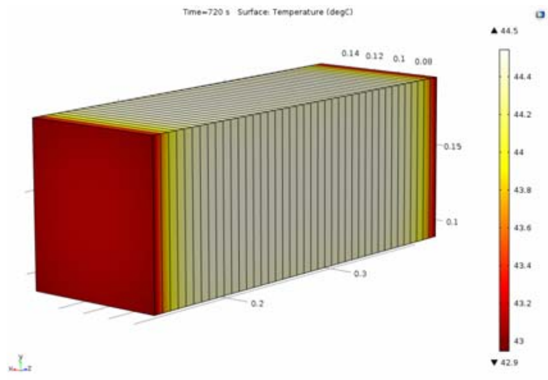

Figure 13. Pack of 40 batteries, the temperature increases from 25°C to 44.6 °C.

8. Conclusions

Our objective was to model an electric race car battery cell with the Heat Transfer in Solids and Batteries & Fuel Cells module of Comsol, and use the computed electrochemical heat generation as a heat power source term to model the temperature evolution of the battery pack. The heat generation calculated with Comsol seems very realistic (Ref. 2.). Then the battery pack maximal temperature is 44.6°C (Fig. 13) whereas the maximal temperature reached by a single battery cell is 39°C. The pack effect is a temperature elevation of only 5.6°C. Even if we consider the error to be about 9% (Ref. 2.), the temperature elevation is not too high. There will be no risk to run this battery in this pack configuration. The small pack effect comes from the anisotropy of the battery. The heat transfer is perpendicular to the length of the pack. The length has thus, no real influence on the pack effect.

The Comsol models might be improved by a better knowledge of the materials physical parameters. The companies that make the battery have their fabrication secrets, specific materials added to modify the properties of the electrodes. Thus the diffusivity and the electrical conductivity are not precisely known whereas the have a big influence on the behavior of the battery. The temperature control of the battery might also be improved by a better knowledge of the thermal convection coefficients.

9. References

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