Multi-domain Simulation of a Lithium Polymer Battery

Transient thermal and thermoelectric simulation of a lithium polymer battery intended for use in implantable medical devices

In the field of medical devices, consumer electronics and other electronics, batteries are of prime importance and are a driving force in design. Of particular importance is battery thermal management and the constraints these impose on the rest of the product. As one of the driving thermal forces, it is important to take into account the complex, multiphysical electrochemical effects of the electrode. In this test case, a detailed battery geometry is analyzed under a progression of thermal analyses. As a result, the transient thermal performance of the battery was fully characterized.

The Model
A detailed battery geometry was created from schematics for an electrochemical cell intended for implantation in medical devices. The major features of this design are a coiled electrochemical core, 2 layers of insulation, electrical and thermal isolation in the headspace and the feedthrough pin encased in an insulating member.

The case is made out of a medical grade titanium alloy. Insulating material is Ethylene tetrafluoroethylene (ETFE) with a Niobium feedthrough pin. A insulating member made out of CABAL-12 glass encases part of the feedthrough pin. Two nickel electrode tabs project up from the electrode core to form the circuit elements, with the cathode tab connected to the feedthrough pin and the anode tab connected by a weld bracket to the grounded battery cover.

Figure 1 – Exploded view of battery

For the electrode physics, the behavior of a fully realized electrode can conveniently and effectively be modeled with an empirical approach. The driving parameters of an empirical model will depend on the type of simulation and the analysis objectives. For a
thermal analysis, the two major sources of heat in the battery will be enthalpy change from the electrochemical reaction and ohmic heating in the charge conducting components. The rate of enthalpy change is represented in each simulation and the ohmic heating representation will depend on the simulation type.

The rate of enthalpy change is dependent on both the State of Charge (SOC) of the battery and on the temperature:

$$\Delta S = F \frac{\partial V_o}{\partial T}$$

Experimental data for this relation is available (Okamoto, et al., 2007) and related to the added heat generation of the electrical core:

$$Q_S = -\frac{T_{cell} \Delta S \cdot I}{F}$$

In the simulation a linear discharge is assumed and the Degree of Discharge (DOD) is proportional to time. The total discharge time is 6000 s at a constant current of 1 A.

The 38°C at the model boundaries represent test conditions assuming implantation in the human body.

**Thermal Analysis (CFX)**

The battery geometry was created in a CAD package and imported into Design Modeler through its respective CAD connection module. The Fill feature in Design Modeler was used to create bodies for the internal air gaps present in the battery. The model was meshed in Ansys meshing with CFD physics preferences.

The thermal analysis was set up in Ansys CFX v12. In particular, the expression language user interface of CFX allowed easy creation and setup of the time and temperature dependent heat generation properties. The density, specific heat and thermal conductivity were specified for all the materials in the analysis.

**Results**

Contour plots of temperature and heat flux are presented below at 50% SOC. The thermal performance of the battery overall was demonstrated to be fairly robust, as the surface temperature deviated from the environmental conditions.
by less than a few degrees. Over the time course of the transient analysis, the maximum temperature trended upward until stabilizing at just above 39 (°C) at 50% SOC.

The electrode core is enclosed in two insulating layers, ETFE liner and titanium alloy case. To better present the thermal performance of the individual components, a cross section of the temperature gradient is presented, also at 50% SOC. In this figure the insulating layers can clearly be distinguished by the high temperature gradients. The insulation can be seen to provide some thermal isolation, though the range of temperatures is small.

The primary purpose of the ETFE liner is to electrically insulate the battery core but since the core itself was only modeled thermally, it is not possible to evaluate the performance of the liner in this regard.

**Thermoelectric Analysis**

The previous thermal analysis in CFX represented ohmic heating through a component in the empirical equations, which may not fully capture this effect for this simulation setup. The original empirical equations were of a distinct battery design and the joule heating component was calculated from the internal resistance of that design. An thermoelectric analysis in Ansys Workbench, with electric material properties defined could better capture the ohmic heating effects and give insight into the electrical performance of the cell. The time and temperature dependant equations were implemented with Ansys Parametric Design Language (APDL) snippets.

The geometry was meshed separately for Ansys simulation v12 and a thermal –electric analysis was initiated. The heat generation in the core was implemented in APDL scripting and the thermal boundary conditions were replicated from CFX. Electric boundary conditions were specified for a 1 A constant discharge.

**Comparison with CFX Thermal**

The thermoelectric simulation shows some agreement with the CFX results, with divergence on the maximum surface temperature at the end of discharge. This discrepancy is likely due to implementation
differences. Surface temperature contours are shown for a mid and full DOD. When the enthalpy heat generation loss is low, as it is for the middle state of discharge, the ohmic and enthalpic heat sources have a near equivalent effect on the surface temperature, which is not the case at the end state of discharge. These results suggest that ohmic heating in the headspace is not a dominating heat generation source, which indicates that the heat generation results in the CFX simulation are a suitable approximation for bulk thermal analysis.

**Feed-Through Pin**

A critical area of the battery is the feedthrough pin, along which the positive cathode current is transmitted from the lithium polymer electrode, through various layers of insulation to project from the battery case as an external lead. The total current density of the cathode tab/feedthrough pin connection is shown.

**Electrical Throughput/Characteristics**

The voltage distribution of the insulation layers and feedthrough pin is shown. The feedthrough pin is encased in an insulating member as it projects through the grounded battery cover. The insulating member is made of CABAL-12, a highly electrically isolating material, as can be seen by the high voltage difference across it. It should be noted that the resistivity of CABAL-12 in this analysis was reduced by 8 orders of magnitude in order to achieve convergence of the simulation. There was still, however, a difference of 10 orders of magnitude between it and the Niobium of the feedthrough pin.

All other insulation is made of ETFE. The headspace insulator here is shown to provide good insulation through a combination of the high resistivity of the material and isolating air gaps.

**Ground Integrity**

The electrical analysis also shows the functioning of the circuit ground. In the design the anode electrode tab projects from the battery core, through the insulation, and is connected by a nickel weld bracket to the
batter cover, providing the ground voltage for the overall circuit.

The surface of the battery developed current from the ground connection, as is shown. This can be considered to be something of a ‘leakage’ as the potential of the ground component may vary more than expected. Also, the ground of the circuit on the battery case is exposed to environmental factors and a change the electrical properties of the environment could contaminate the ground, hurting overall efficiency of the battery.

**Conclusion**

A battery design with empirical electrode properties is prepared and a thermal analysis is performed. This preliminary shows a safe temperature distribution but raises questions about the electrical layout of the components. A more detailed electrical simulation or a refinement to the design should be considered in order for the design to be suitable for use in a medical device.

---

**Figure 8 - Total Current Density on case surface**

**References**


Ozen Engineering Inc is an engineering services company located in Sunnyvale, CA and providing consulting, software sales, training and support.

Visit: [www.ozeninc.com](http://www.ozeninc.com), email info@ozeninc.com or call (408) 739-4884 for more information.

©2009 Ozen Engineering Inc