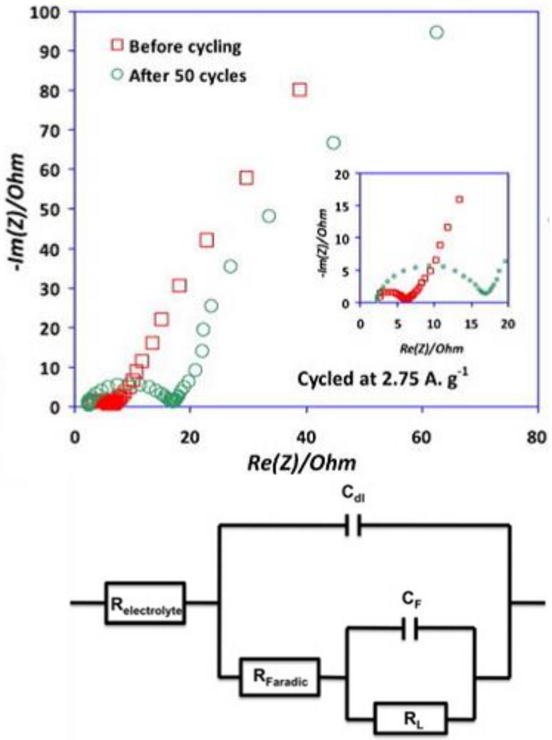
Multiphysics Simulation Story: Highly Accurate Li-ion Battery Simulation

French Atomic and Alternative Energy Commission (CEA), FRANCE

Mikael Cugnet

The Challenge

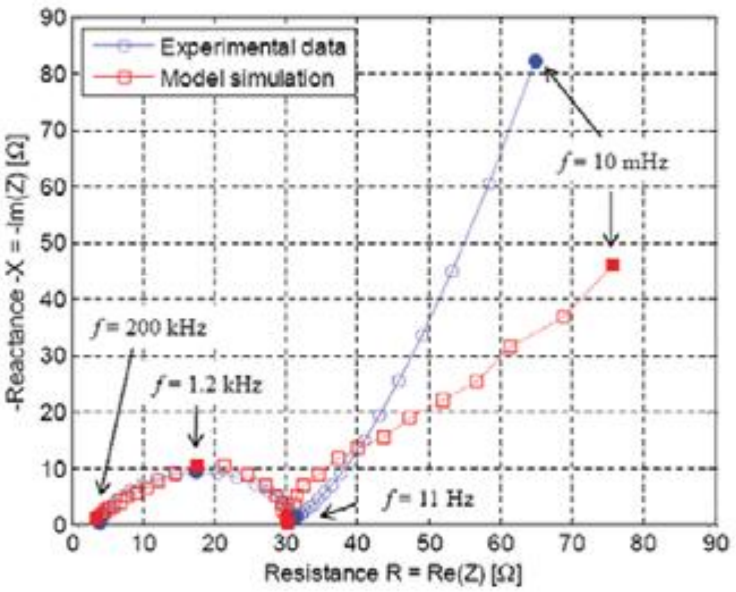
- Battery management systems (BMSs) are designed to protect the battery and predict their charge level through using circuit models derived from electrochemical impedance spectroscopy (EIS)
  - EIS allows construction of an equivalent circuit model (ECM) that consists of resistances and capacitors connected both in series and in parallel, and determine a battery's internal resistance, which in turn dictates how much energy it can deliver
- Yet, ECMs do not provide any information about important cell properties like the electrode active material resistance, the reaction rate, the specific capacitance, and the diffusion coefficient



Using Electrochemical Impedance Spectroscopy, battery impedance is measured at a range of frequencies in the milliHertz to kiloHertz range. From this impedance plot (top), it is possible to construct an equivalent circuit model (bottom).

The Solution

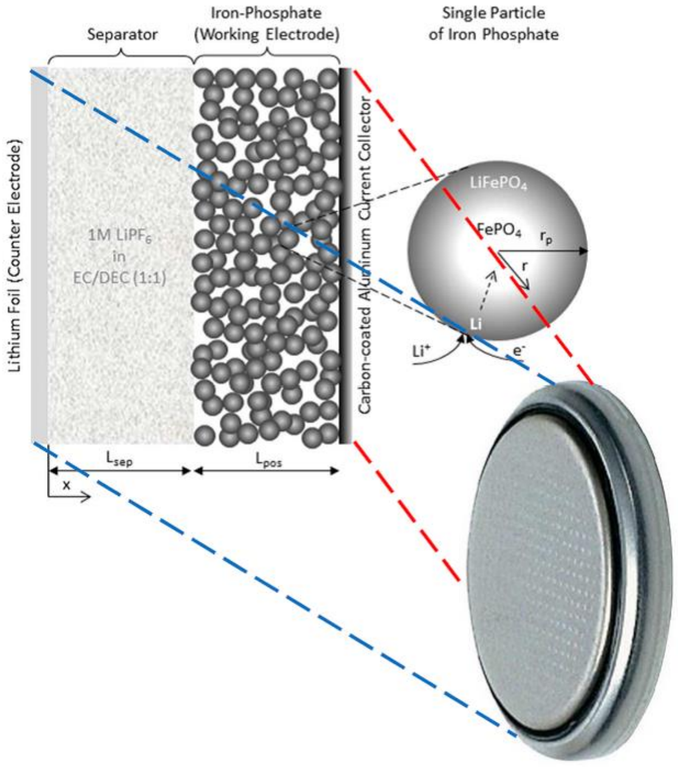
- Researchers turned to multiphysics simulation to get a deeper understanding of what is going on inside the cells
- Rather than work with an equivalent circuit model, the researchers decided to create a physics-based model of a $LiFePO_4$/Li half cell
- Researchers could clearly see that in their half cell:
    - The active material used in the electrode has poor electronic conductivity
    - The capacitive behavior of the cell is far from being negligible at frequencies higher than 10 Hz
- They concluded that an electric double layer needs to be included within the model to simulate the experimental results, and thus in subsequent models of the battery



Including an Electric Double Layer allowed for a perfect agreement between simulation results at high frequencies.

The Simulation

- Equations governing battery behavior were included in COMSOL Multiphysics:
  - The electrical double layer (EDL) was modeled using the corresponding feature available in COMSOL
  - Full control of all parameters allowed researchers to achieve an understanding of the battery
- The simulation consists of two coupled 1D models:
  - The first model represents the macroscopic level and is made up of two domains: the working electrode, plus the separator between the iron-phosphate electrode and the lithium foil, which also serves as the counter-electrode
  - The second model represents the microscopic level, which has only one domain and models a spherical particle of iron phosphate, the main component of the working electrode's active material
  - LiveLink™ for MATLAB® was used to run the model for each frequency and process the results to achieve the full impedance spectrum of the half-cell



Modeling of the half cell at macroscopic (left) and microscopic (right) level.