National Aeronautics and Space Administration

Towards the Development of a First Principles Multiphysics Lithium-ion Battery Operational Model to Assist JPL Mission Power Assessment Tools

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Program: Spontaneous Concept

Background:

- The success of lithium-ion (Li-ion) batteries is well known in planetary space missions e.g., for their successful use in MER, MSL, Juno, GRAIL etc. The performance of a Li-ion battery is determined by the processes involving intercalation and de-intercalation of lithium ions into and from the electrodes, and their diffusion in the electrolyte and by the processes of charge transfer at the electrodes-electrolyte interfaces (Figure 1).
- The process of degradation (ageing) in a complex system like Li-ion battery leads to capacity / power fade.
- Currently, JPL's Multi-mission Power Analysis Tool (MMPAT), which is being used in several JPL missions, have been created from the performance database and will be better served with an elegant model such as we proposed here.

Project Objective:

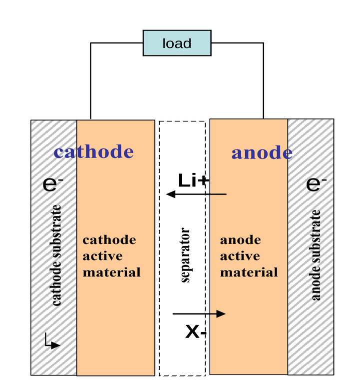
We propose to develop an operational multiphysics model for lithium-lion batteries, based on a first principles approach that will be more comprehensive and expandable, and will be a valuable asset for power management on spacecraft, especially when combined with a power analysis tool such as MMPAT.

FY19 Results:

- Developed a first principles multiphysics Li-ion battery model that includes capacity fade using commercial COMSOL Multiphysics software.
- The validation of the first principle Li-ion battery operational model was done for the 8 Ah (10 Ahr nameplate capacity) MER prototype laboratory cells.
- Good validation is obtained comparing the modeling and experimental results for discharge characterization curves. Comparison of the discharge curves at T=23°C at C/5 (1.6A) loads for upto 2000 cycles, each cycle corresponds to ~12-14.5hrs.

Benefits to NASA and JPL:

We have shown good validation of the multiphysics first principle Li-ion battery model for the MER prototype Li-ion cells for capacity fade. This model could be further extended to chemistries used in MSL/M2020 Li-ion batteries. This operational model would be a valuable tool in combination with JPL's Multi-mission Power Analysis Tool (MMPAT), to predict the life and performance under different conditions (temperature, loads) for a given mission objectives.



Material / ionic charge balance

$$\nabla \cdot \left\{ -\kappa_2^{eff} \nabla \phi_2 + \frac{2RT\kappa_2^{eff}}{F}\left[1 + \frac{\partial \ln f}{\partial \ln c_s}\right][1 - t_+]\nabla(\ln c_s) \right\} = S_a j_{loc}$$

$$\varepsilon \frac{dc_s}{dt} + \nabla \cdot \left\{ -D_2^{eff}\nabla c_s - \frac{i_2}{F}(1 - t_+) \right\} = 0$$

D_2^{eff}: diffusion coefficient | c_s: salt concentration
i_2: current density | T: temperature
F: Faraday's constant | f: ionic activity coefficient
K_2^{eff}: conductivity | ϕ_2: solution phase potential

Electrode kinetics

$$j_{loc} = i_0 \left\{ \exp\left(\frac{\eta F}{RT}\right) - \exp\left(\frac{(-\eta)F}{RT}\right) \right\}$$

η = f (electrode and electrolyte phase potentials)
i_o: exchange current density
j : lithium ion flux

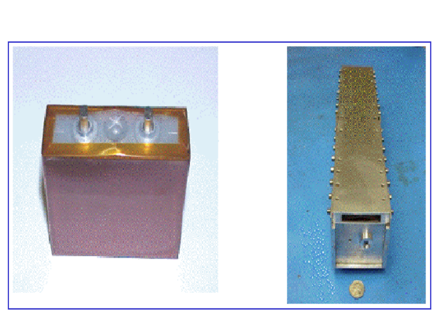
Current balance

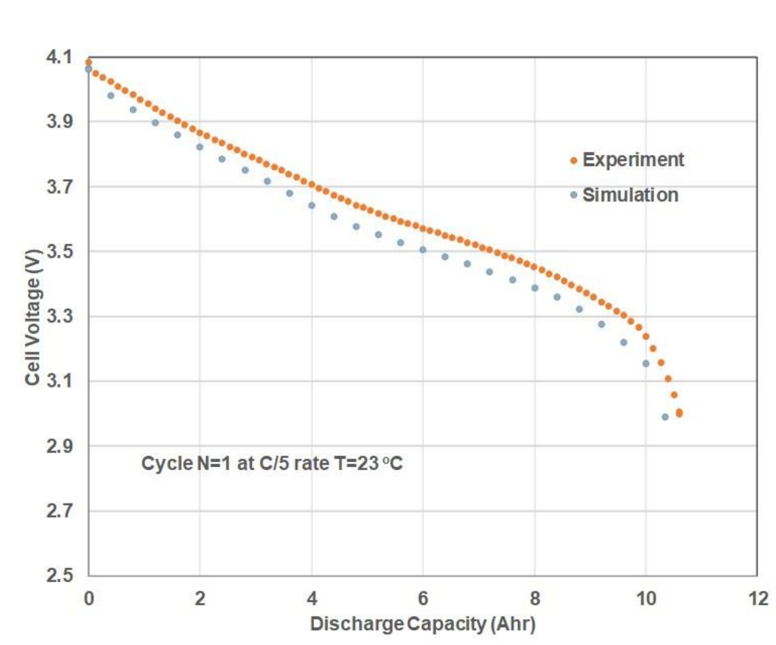
$$\nabla \cdot (-\kappa_1 \nabla \phi_1) = -S_a j_{loc}$$

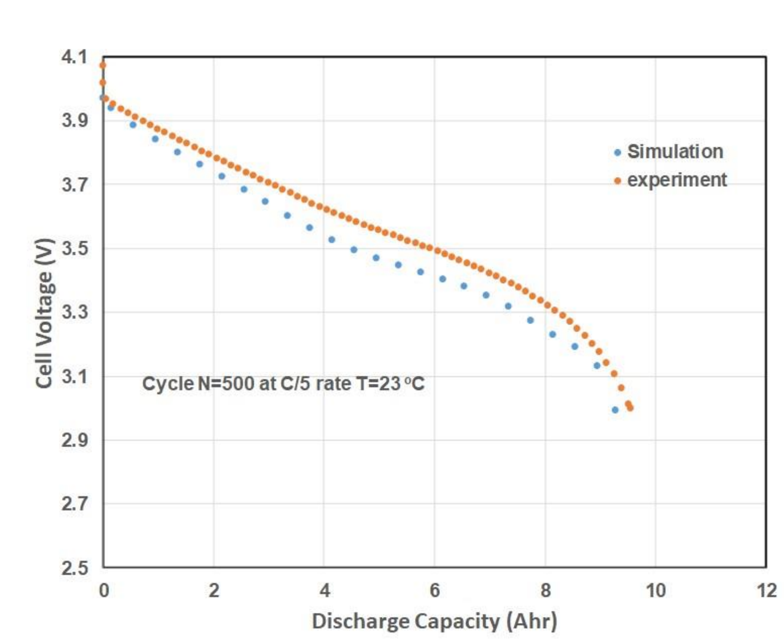
K_1: electronic conductivity of electrode
S_a: specific surface area
ϕ_1: electrode potential

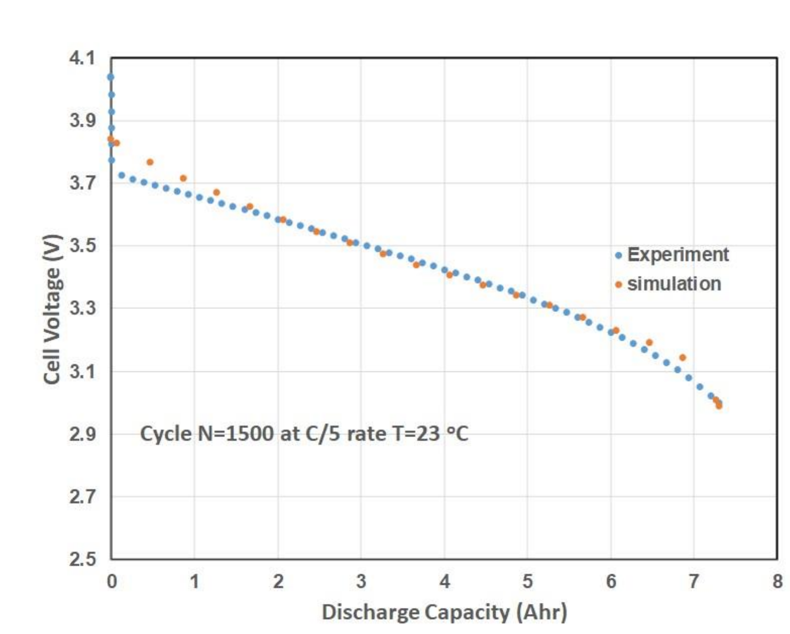
1 cycle = 12-14.5 hrs

MER prototype laboratory cells
8 Ah (10 Ahr nameplate capacity)

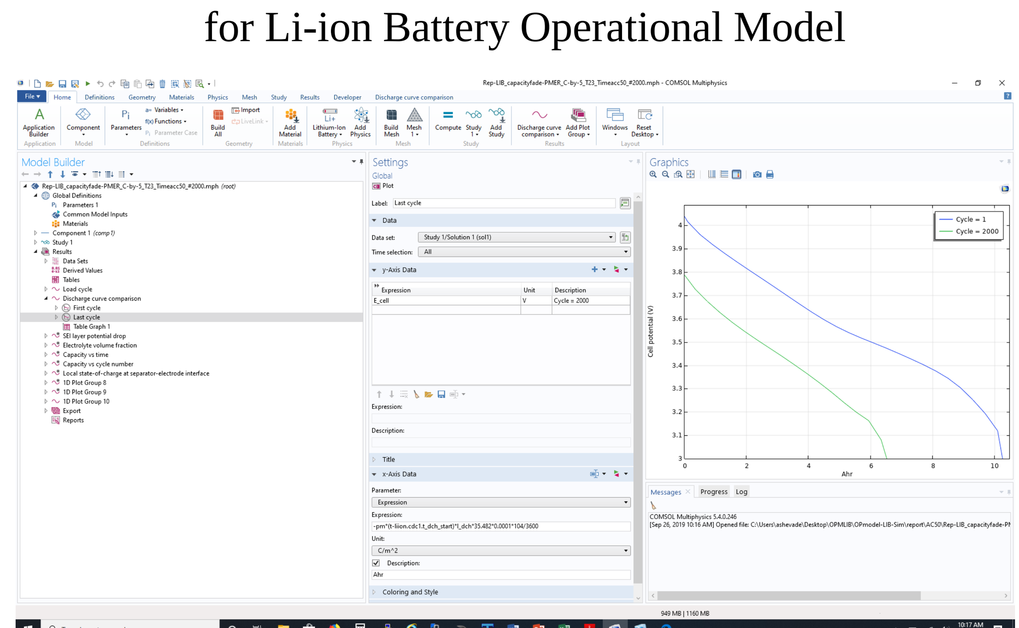


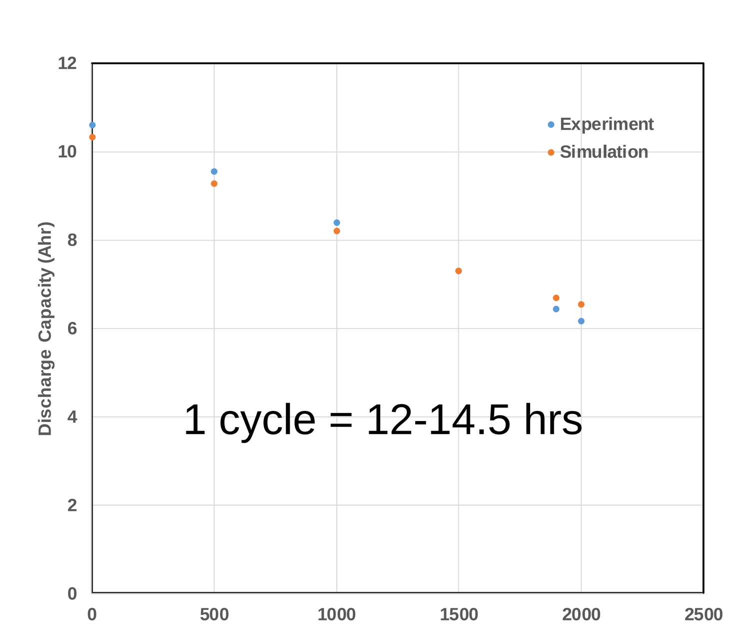






Commercial COMSOL Multiphysics Software Platform GUI for Li-ion Battery Operational Model





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