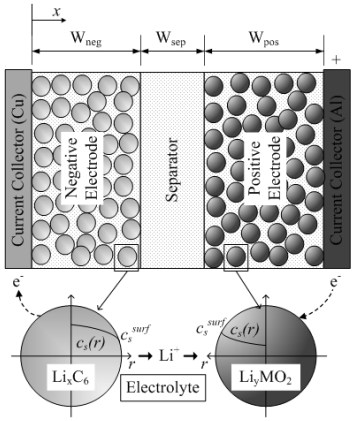
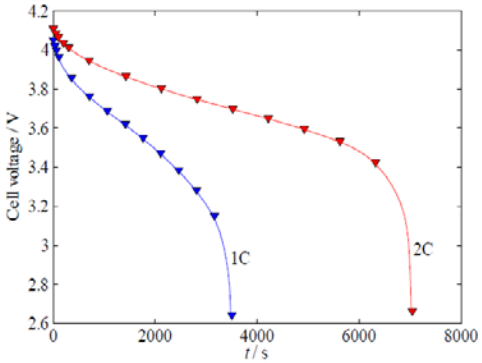
Modeling of Transport Phenomena in Electrochemical Energy Systems

Lithium-Ion batteries

Modeling of transport phenomena in Lithium-Ion batteries enables us to determine their performance as well as aid in their design. Also, new battery architectures and new materials could be investigated using the model.



Schematic of a Li-Ion cell



Discharge curve: Full model (symbols) vs. reduced model (line)

The mathematical model comprises the governing transient conservation of charge, species and energy in the solid and electrolyte phases. A Li-Ion cell with Li_xC_6 negative electrode and $LiMn_2O_4$ positive electrode is investigated.

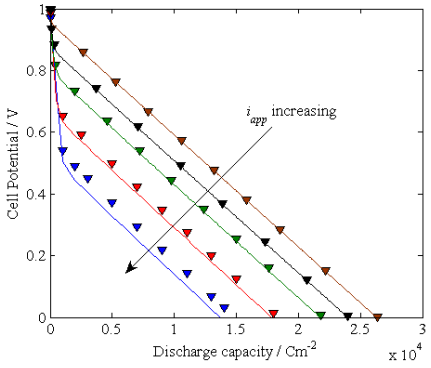
In order to improve the computational cost, model reductions are carried out using approximate solutions for solid phase diffusion of Lithium. The reduced model results agrees well with that of the full model for various discharge rates.

Work is under way to investigate a passive thermal management system for a high power battery pack.

Electrochemical capacitors

Electrochemical capacitors that store energy by mechanism of double-layer as well as faradaic process due to redox reactions are called pseudocapacitors. They are used as high power devices in energy storage systems.

Batteries and electrochemical capacitors exhibit electrochemical similarities. The model of a pseudocapacitor considers the double-layer process in addition to that of a battery model. A pseudocapacitor with RuO_2/carbon composite electrode is modeled by considering the transient conservation of charge and species in the solid and electrolyte phases.



Discharge curve: Full model (symbols) vs. reduced model (line)

The model is reduced to minimize the computational time. The reduced model predictions agrees well with the full model predictions.

Work is underway to include the conservation of energy in the model as well as to build a stack model using the reduced model as the basic building block.

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