The Impact of Electrode Structure on the Processes that Limit Cathode Performance

D.R. Wheeler and J.N. Harb

Department of Chemical Engineering
Brigham Young University

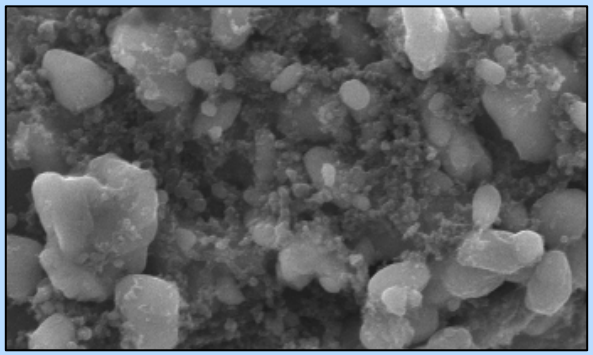
2008 DOE OVT Annual Merit Review
February 25-29, 2008
Bethesda, Maryland

Purpose

Increase battery energy density, power density, and life through improved electrode design

Better understand the influence of cathode structure on cell performance

- Porosity
- Thickness & loading
- Internal connections
- Interfaces



Benefits

- Fundamental understanding of performance-limiting processes
- Basis for optimization of cathode structure (e.g., for PHEV applications)
- Applicable to a variety of battery cathode chemistries
- Guide development of new materials and designs

Prior Review (June 2006)

Reviewer Criticisms

- Cells had poor performance, namely ASI
- Effectiveness of carbon fibers not clear
- Need to increase scientific and practical relevance of work

Response

- Cell quality has been improved through process refinement and change of materials
- Reduced emphasis on fiber work
- Modeling and experiments better address issues governing cell performance

Barriers

Batteries for PHEVs need greater energy density while maintaining power density and cycle life

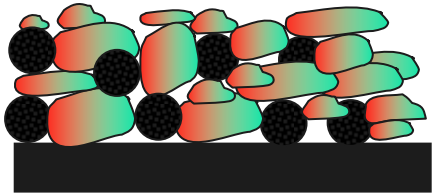
- Minimize electrode impedance

vs

- Minimize use of inert materials

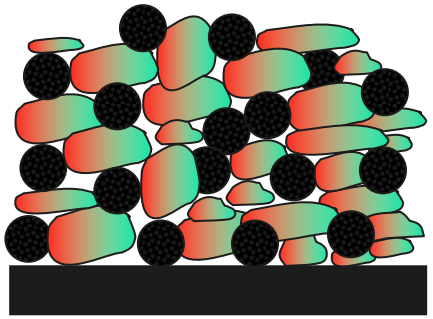
Tradeoffs in Electrode Structure

Thin



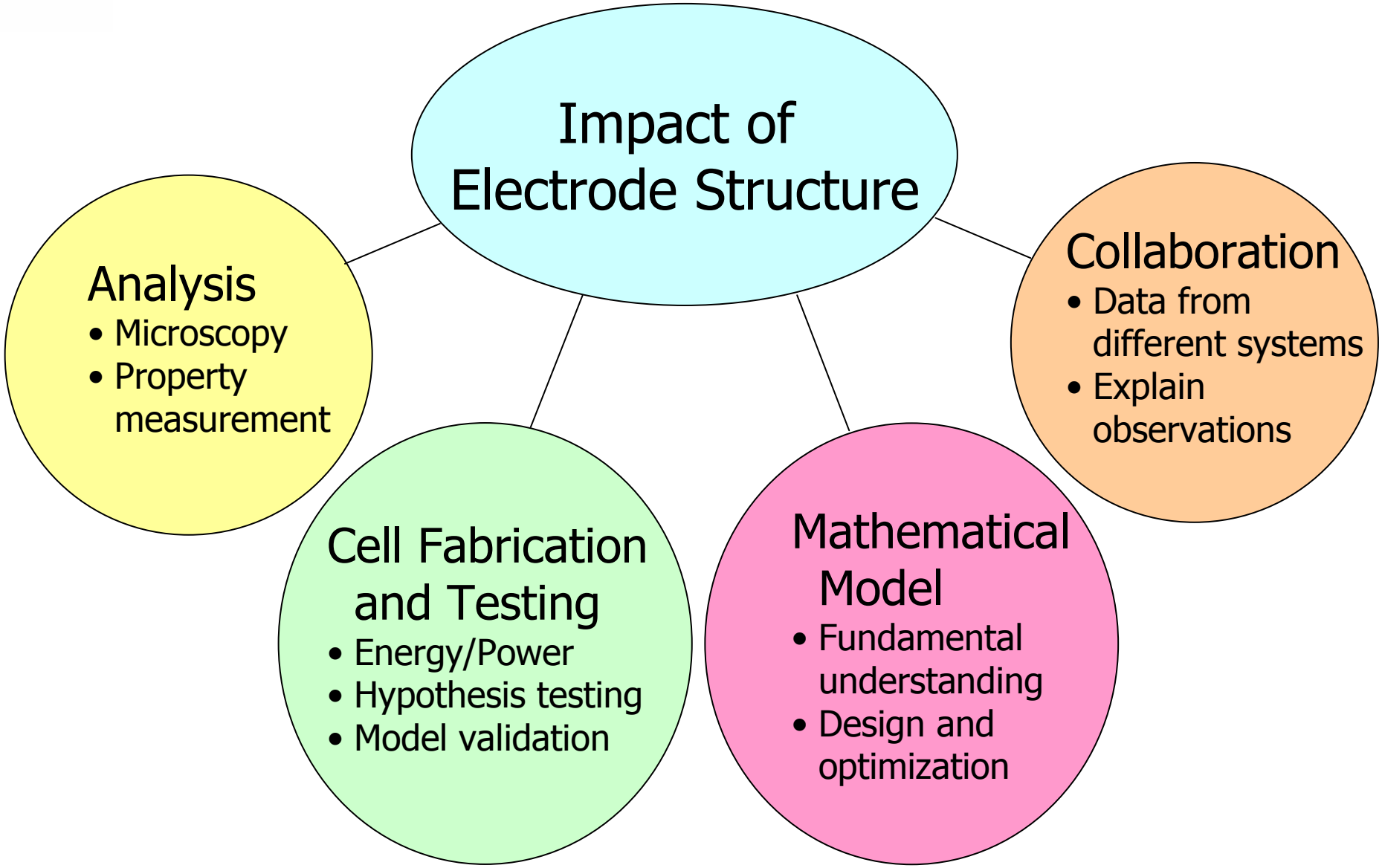
- Lower transport resistances
- Higher mass burden of inert materials (current collector + separator)

Thick



- Higher transport resistances
- Lower mass burden of inert materials (current collector + separator)

Approach

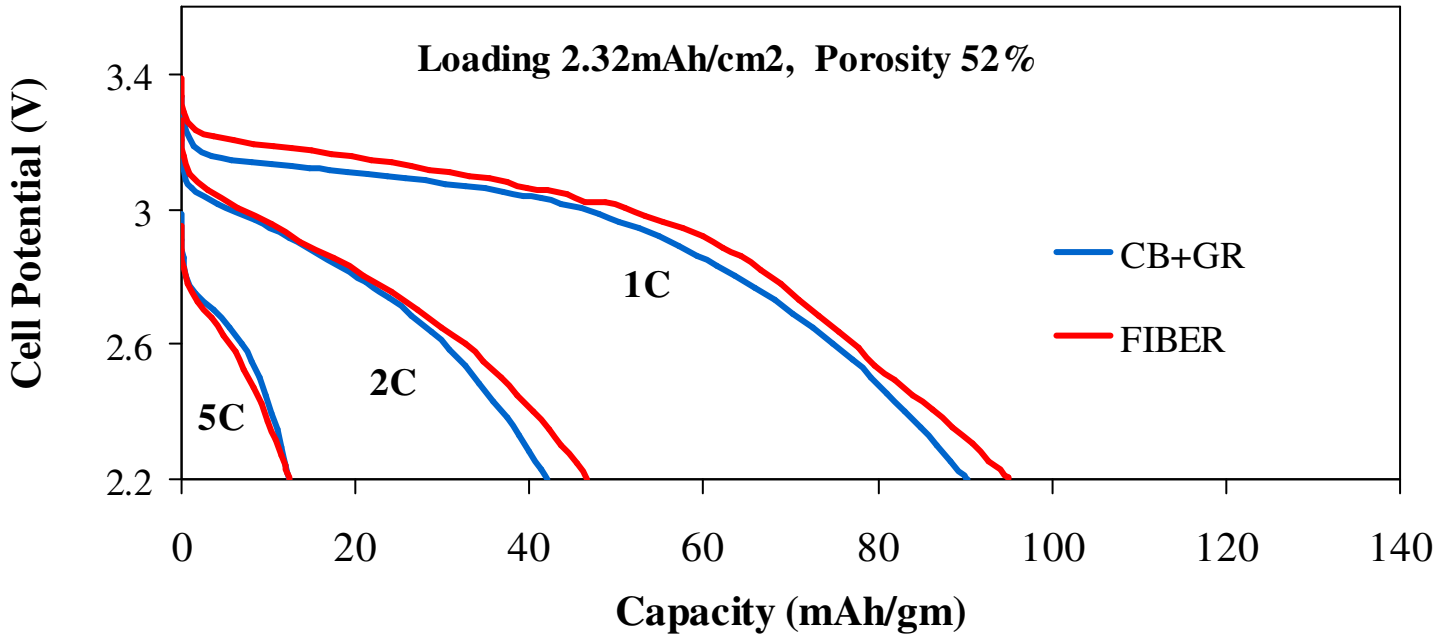

Impact of Electrode Structure
Analysis
• Microscopy
• Property measurement
Collaboration
• Data from different systems
• Explain observations
Cell Fabrication and Testing
• Energy/Power
• Hypothesis testing
• Model validation
Mathematical Model
• Fundamental understanding
• Design and optimization

Accomplishments

- Exploration and testing of PHEV optimization concepts with $LiFePO_4$ cells
- Novel experiments to assess liquid-phase impedance
- Improvement and validation of battery model to predict effects of particle sizes, electrode porosity and thickness

Effect of Fibers on Performance

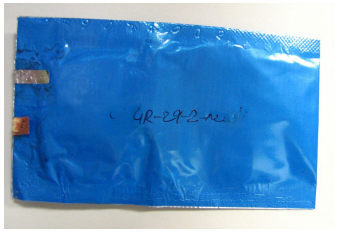
- For uncalendered electrodes, fibers can effect a significant increase in performance
- Under typical conditions, enhancement is much less



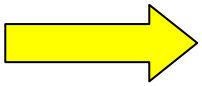
- Fibers can be a useful diagnostic tool

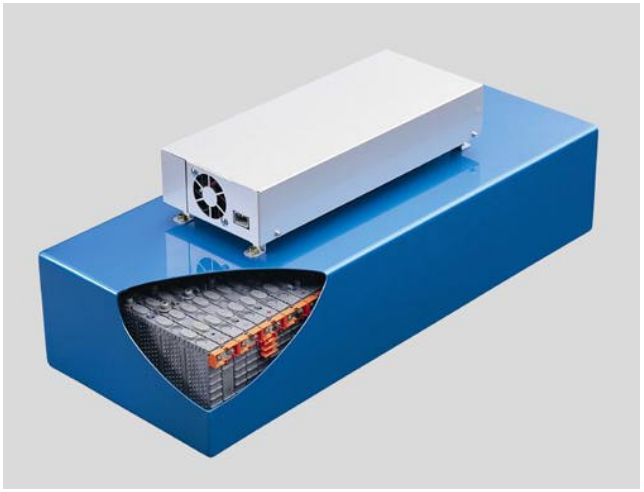
Electrode Analysis

- Determine energy and power performance of lab-scale cells as a function of loading, porosity, or other electrode parameters
- Convert lab-scale cell performance to equivalent vehicle-scale pack performance (collaboration with Paul Nelson of ANL)



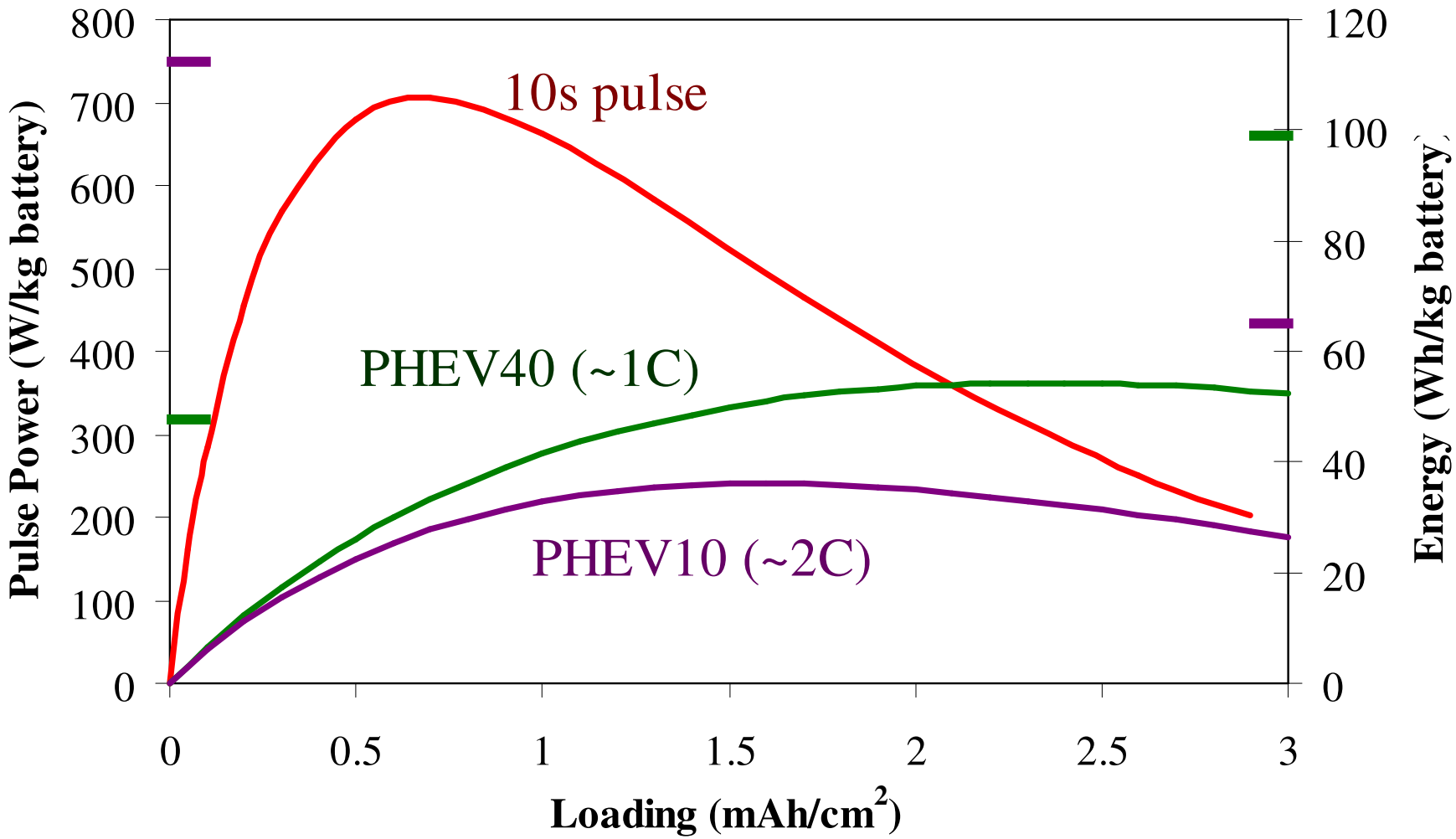
pouch cell



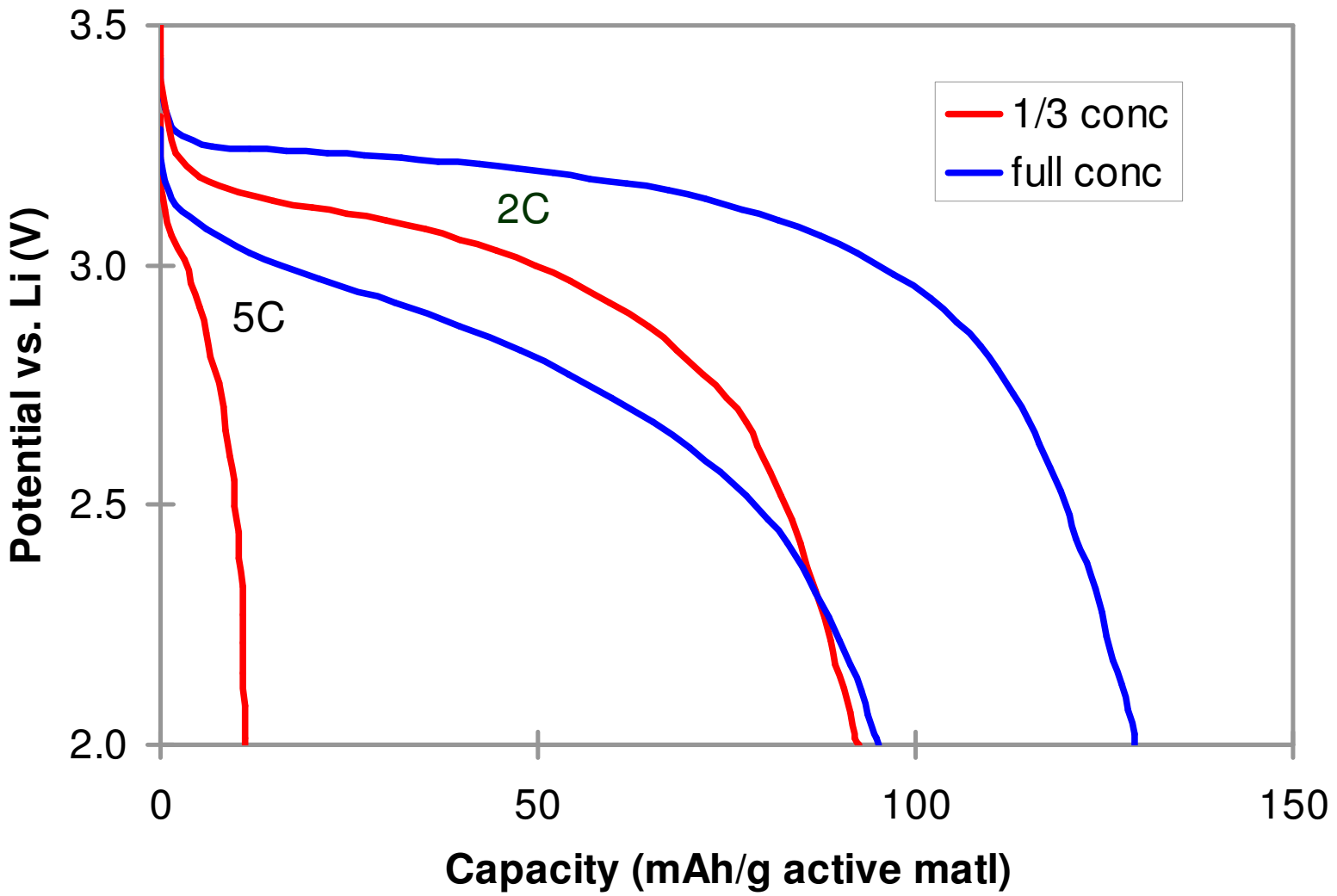


vehicle battery

Density
(large battery basis)

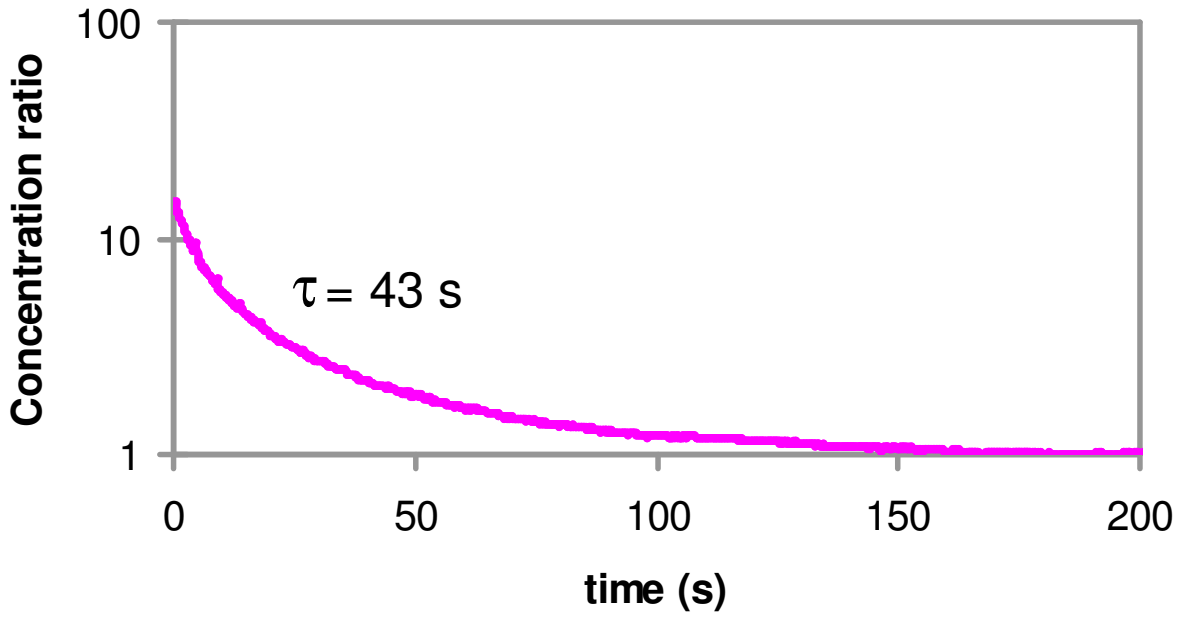


Impact of Liquid-Phase Impedance: Electrolyte Concentration



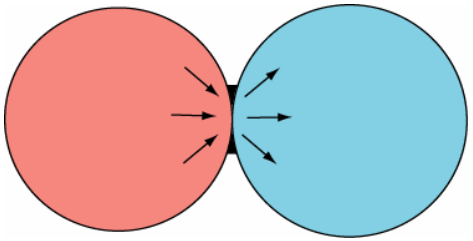
Liquid Transport Properties

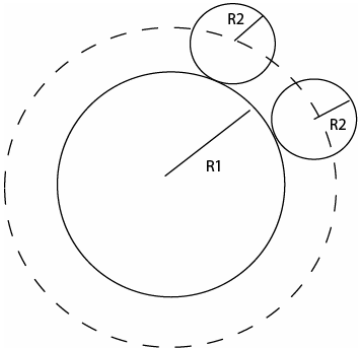
Special cell configuration used to isolate and experimentally determine effective ion transport in porous cathode (conductivity and diffusivity)



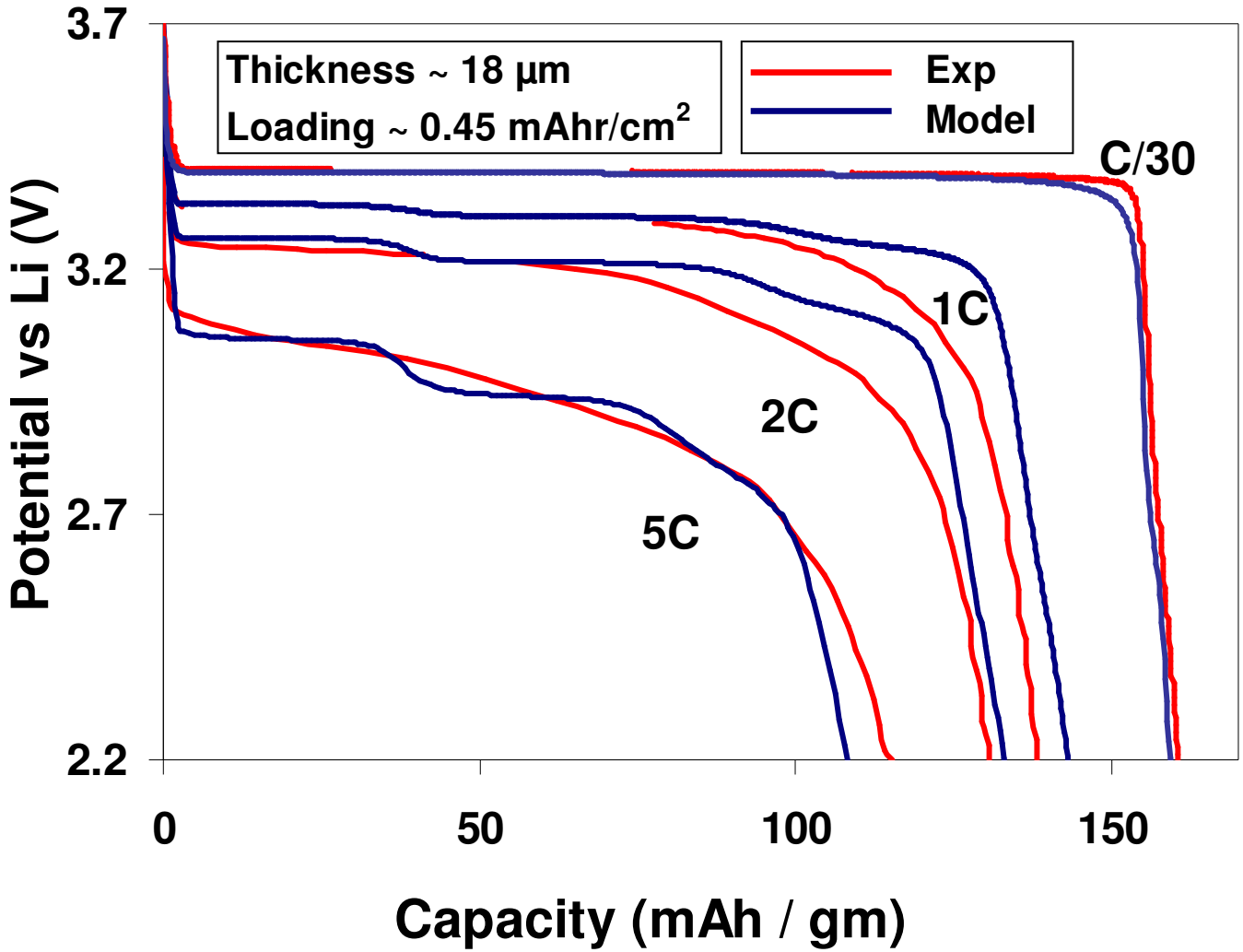
Battery Model Development

- Porous electrode theory- superposition of phases (J. Newman)
- Extensions and improvements
  - Particle-particle electronic interactions
  - Multiple particle sizes and solid phases
  - Liquid-phase transport better described
- Benefits
  - Removal of arbitrary resistances
  - Can separate influence of active material from conductive additive
  - Blended active materials possible
  - Level of detail is ideally suited to the problem of interest

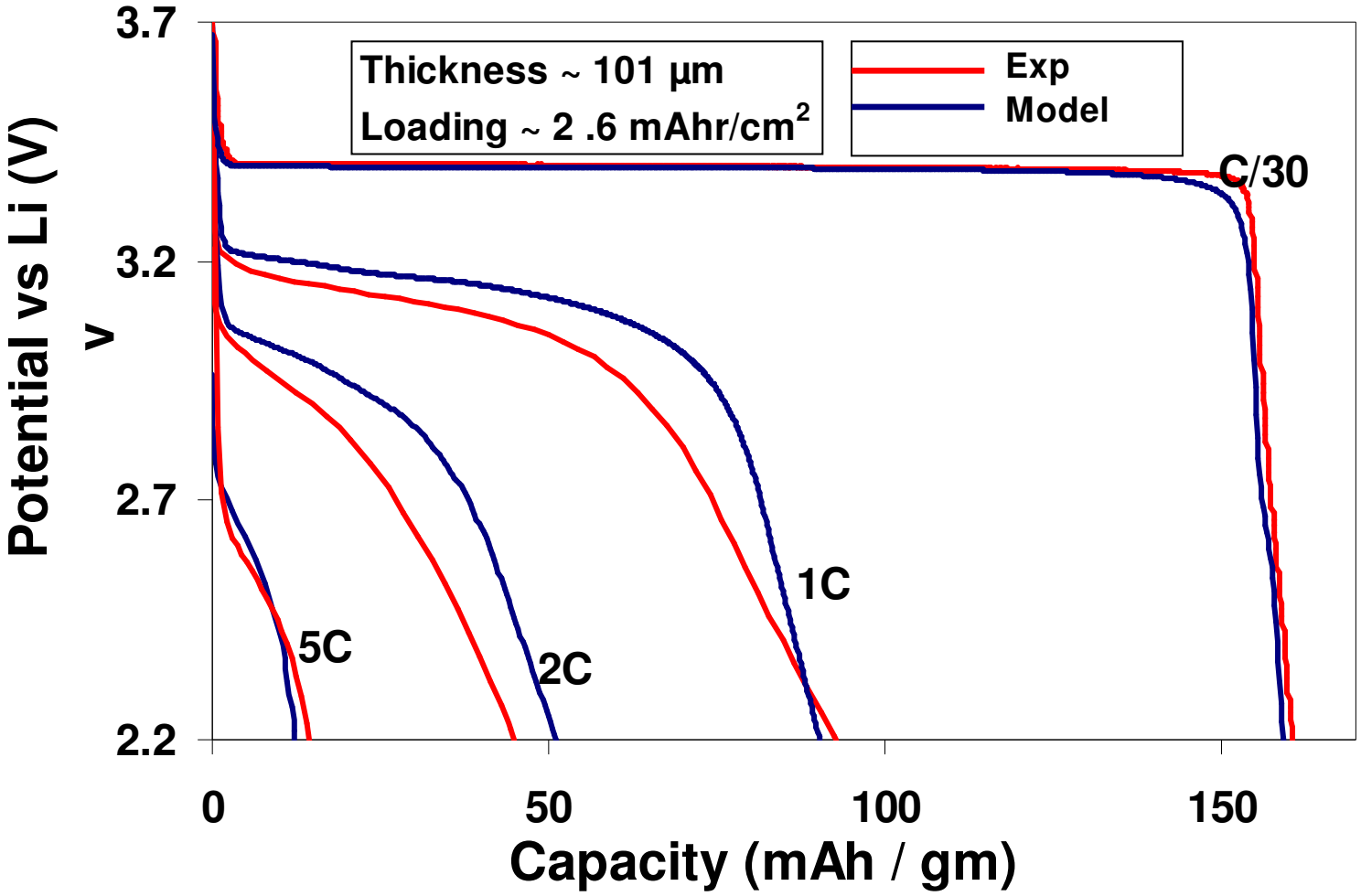




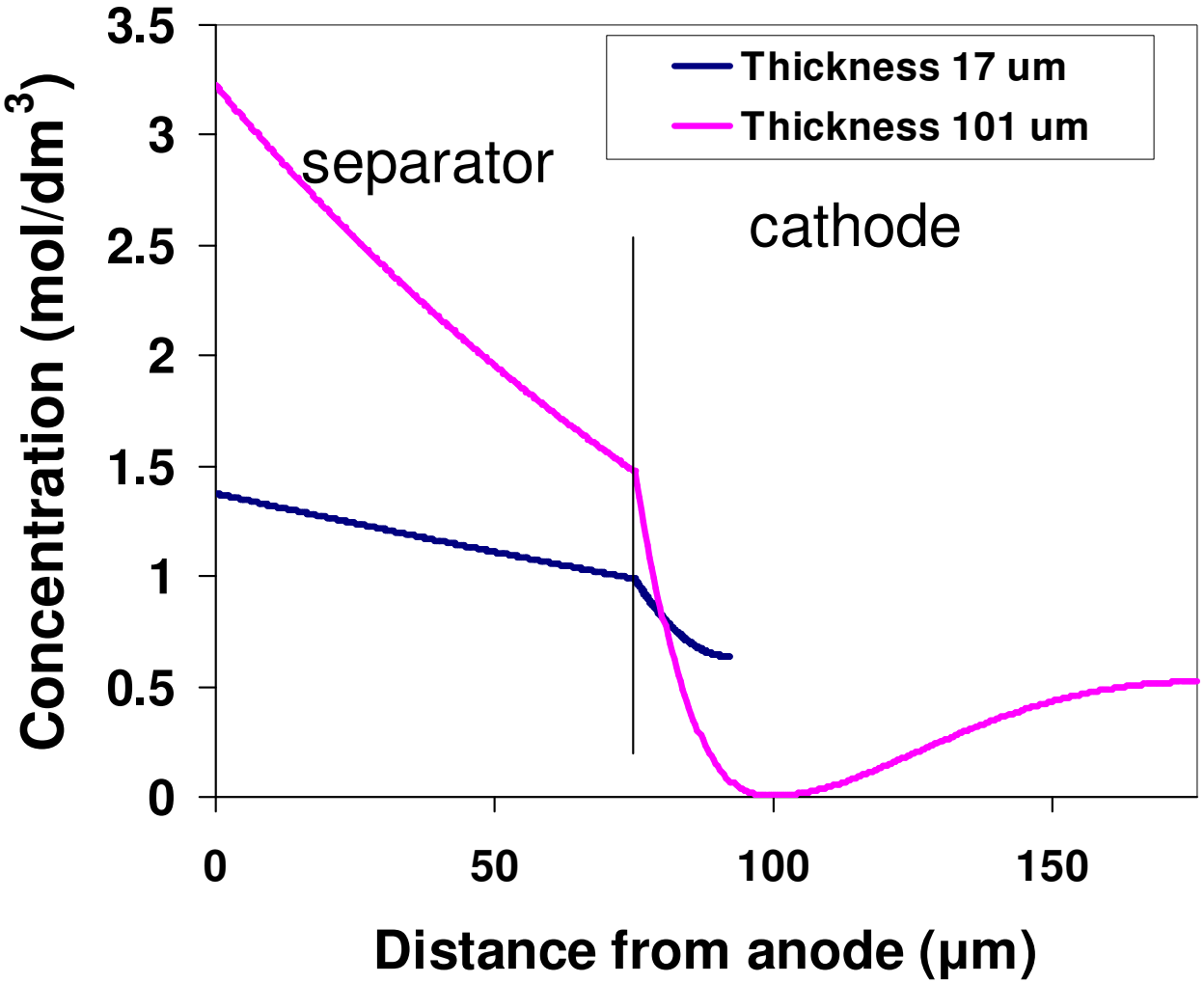
Simulation Results: Thin Cell



Simulation Results: Thick Cell



Electrolyte Concentration Depletion



Tech Transfer & Collaborations

- Collaborations with other BATT PIs including Zhaghib, Newman, Battaglia, and Srinivasan.
- Support for more applied efforts: work can suggest limitations and optimal fabrication parameters for given materials

Publications & Presentations

- D.E. Stephenson, E.M. Hartman, J. Harb, and D. Wheeler, "Modeling of particle-particle interactions in porous cathodes for lithium-ion batteries," *J. Electrochem. Soc.*, 154, A1146-A1155 (2007).
- I. Thorat, V. Mathur, J. Harb, and D. Wheeler, "Performance of carbon-fiber-containing LiFePO4 cathodes for high-power applications," *J. Power Sources* 162, 673-678 (2006).

- I. Thorat, D. Stephenson, V. Mathur, B. Walker, E. Hartman, J. Harb, and D. Wheeler, "Effect of morphology and thickness on high-rate discharge performance of porous composite cathodes," 212th Meeting of the Electrochemical Society, Washington, DC, 2007.
- D. Stephenson, I. Thorat, E. Hartman, J. Harb, and D. Wheeler, "Fundamental investigation of inter-particle contact in porous composite cathodes," 210th Meeting of the Electrochemical Society, Cancun, Mexico, 2006.

Plans for FY2009

- Collaborate with other BATT PIs to assess new battery materials such as $LiMnPO_4$
- Continue to improve physical realism of battery model for predictive use
- Develop and assess fabrication alternatives to minimize cell impedances

Summary

- We combine unique experiments with detailed battery modeling
- Tools are general and are suited to current and emerging materials
- Work leads to understanding the influence of cathode structure on cell performance for vehicle use