NREL
NATIONAL RENEWABLE ENERGY LABORATORY

Overview of Computer-Aided Engineering of Batteries and Introduction to Multi-Scale, Multi-Dimensional Modeling of Li-Ion Batteries




P.I. - Ahmad A. Pesaran
G.-H. Kim, K. Smith,
S. Santhanagopalan, K.-J. Lee
National Renewable Energy Laboratory
May 15, 2012

Presented at the 2012 U.S. DOE Hydrogen Program and Vehicle Technologies Program Annual Merit Review & Peer Evaluation Meeting
14-18 May 2012, Arlington, Virginia

Project ID #ES117

Overview

This presentation covers two related topics: Overview CAEBAT Project and NREL battery MSMD modeling work under CAEBAT

Timeline

Project Start Date: April 2010

Project End Date: September 2014

Percent Complete: 30%

Budget

Total Project Funding:

DOE Share: $9 M

Contractor Share: $7 M

Funding Received in FY11:

$3.5 M ($2.5 M for subcontracts)

Funding for FY12:

$1.0 M expected

Barriers

- Cost and life
- Performance and safety
- Lack of validated computer-aided engineering tools for accelerating battery development cycle

Partners

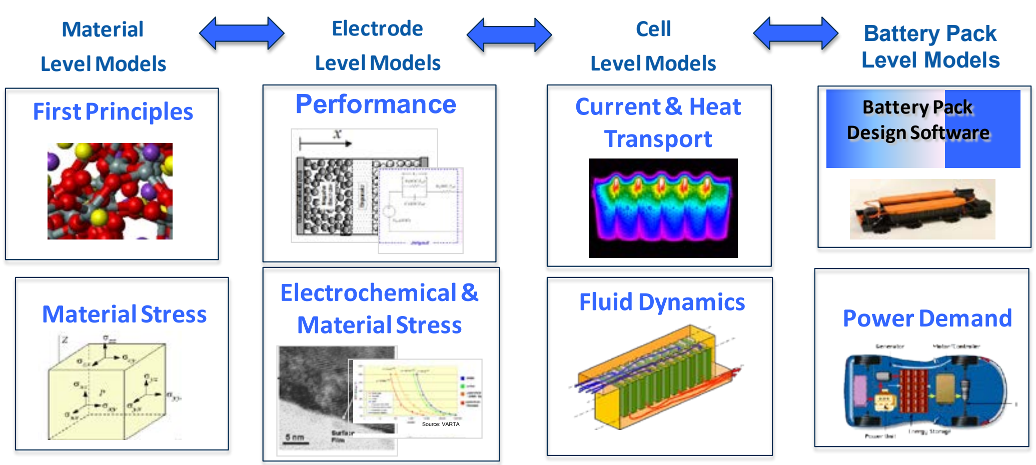
- Project lead: NREL
- ORNL, INL, CSM
- EC Power/PSU/Ford/JCI
- GM/ANSYS/ESim
- CD-adapco/Battery Design/JCI/A123Systems

Funding provided by Dave Howell of the DOE Vehicle Technologies Program. The activity is managed by Brian Cunningham of Vehicle Technologies.

Computer Aided Engineering for Electric Drive Vehicle Batteries (CAEBAT)

Relevance

- Simulation and Computer-Aided Engineering (CAE) tools are widely used to speed up the research and development cycle and reduce the number of build and break steps, particularly in the automotive industry.
- There has been a need to have several user-friendly, 3D, fully integrated, and validated CAE software tools for the battery community.
- National laboratories, industry, and universities have been developing models on cost, life, performance (electro-thermal, electrochemical) and abuse for simulating lithium-ion batteries.
- Realizing the need, DOE Vehicle Technologies initiated a project in April of 2010 to bring together these battery models to develop CAEBAT tools for designing batteries.



Objectives

- The overall objective of the CAEBAT project is to incorporate existing and new models into “validated” battery design suites/tools.

- Objectives of the past year (March 2011 to March 2012) were to:
  - Complete negotiations and enter into subcontract agreements with the three teams competitively selected in 2010.
  - Subcontractors to start technical work
  - NREL to have kickoff and quarterly meetings with subcontractors to monitor their technical performance and progress.
  - Continue developing NREL’s multi-physics electrochemical lithium-ion battery (MSMD) model, and document the approach and results in a peer-reviewed journal.

Relevance

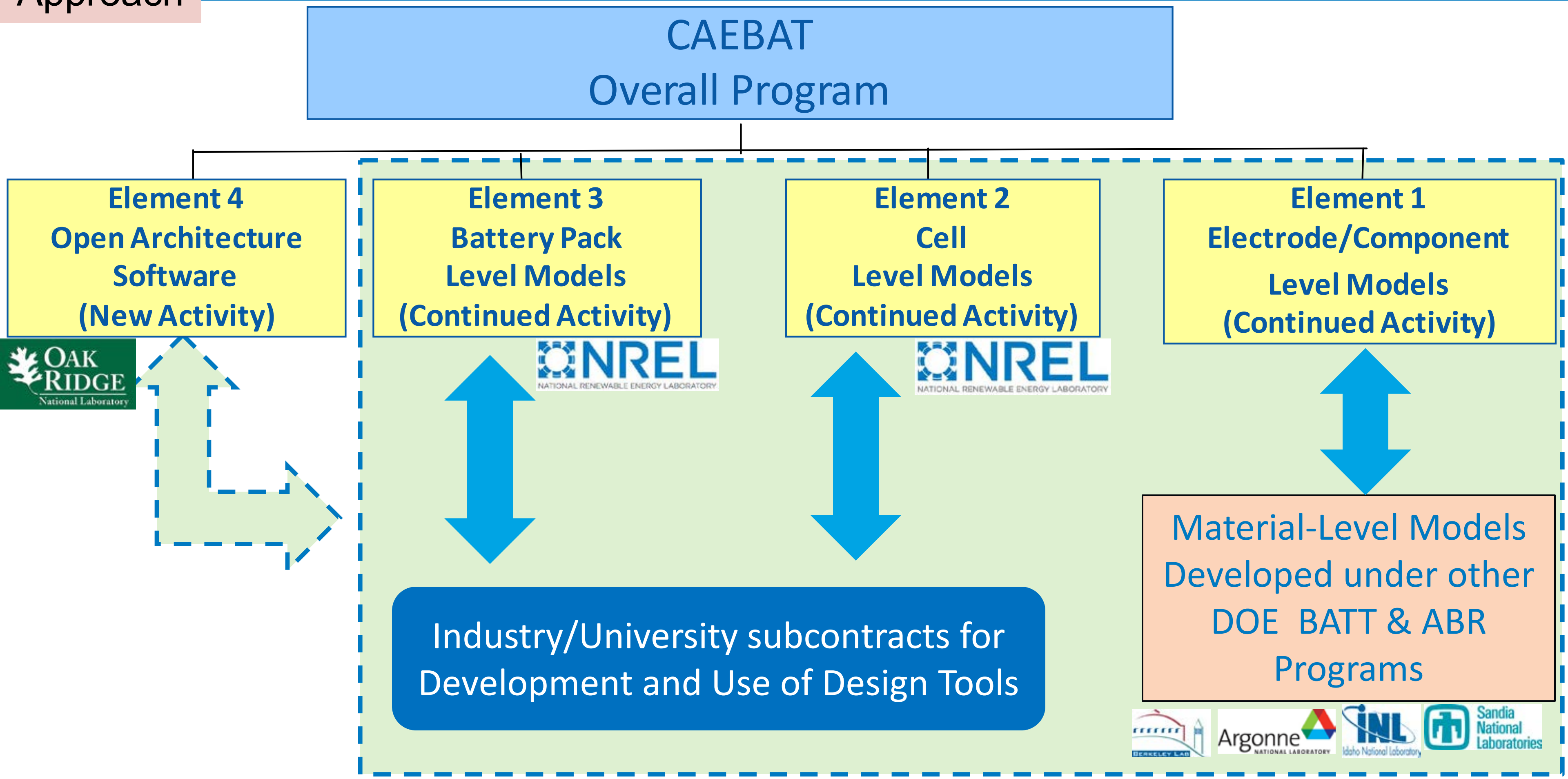
- CAEBAT objectives are relevant to the Vehicle Technologies Program's targets of:
  - PHEV battery costs of $300/kWh and life of 15 years by 2014
  - PHEV battery costs of $270/kWh and life of 10+ years life by 2017
  - EV battery costs of $150/kWh and 10 years life by 2020
- The impact of this project when CAEBAT tools are made available could be significant:
  - Shorten design cycles and optimization of batteries
  - Address the barriers of cost, performance, life, and safety of lithium-ion simultaneously, and with quantitative tools

Milestones

Date	Milestone or Go/No-Go Decision	Status
June 2011	Negotiate and place subcontracts with CAEBAT RFP awardees	Completed
July 2011	Progress review on the work for the CAEBAT-NREL program	Completed
September 2011	Document NREL's MSMD modeling approach in a peer-reviewed journal	Completed
July 2012	Document latest NREL battery models, solution methods, and codes developed under CAEBAT	On Track
September 2012	Technical Review of the three CAEBAT Subcontracts	On Track

Overall CAEBAT Strategy

Approach



- NREL to coordinate the CAEBAT project activities for DOE
- Perform battery modeling development and use (existing or new) models at National Labs
- Coordinate and exchange with other organizations doing fundamental materials modeling (such as BATT, ABR, or Basic Energy Sciences)
- Collaborate with industry and/or universities through competitive solicitations
- ORNL to develop an interface platform for interactions among all models

CAEBAT and MSMD Approach

- Develop CAEBAT software tools with industry
  - Background from FY 10 and Fall of FY11
    - We issued a competitive process (RFP) to solicit cost-shared proposals from the industry
    - After a comprehensive process, three teams were selected to develop CAEBAT software tools
  - Approach in 2011
    - Complete negotiations and enter into subcontract agreements with the three selected teams
    - Initiate CAEBAT projects and monitor technical performance and progress
    - Collaborate with ORNL on Open Architecture Software
- Perform in-house R&D to enhance and further develop NREL's existing electrochemical-thermal (MSMD) models for use by CAEBAT participants

CAEBAT Subcontracts Finalized

Accomplishments

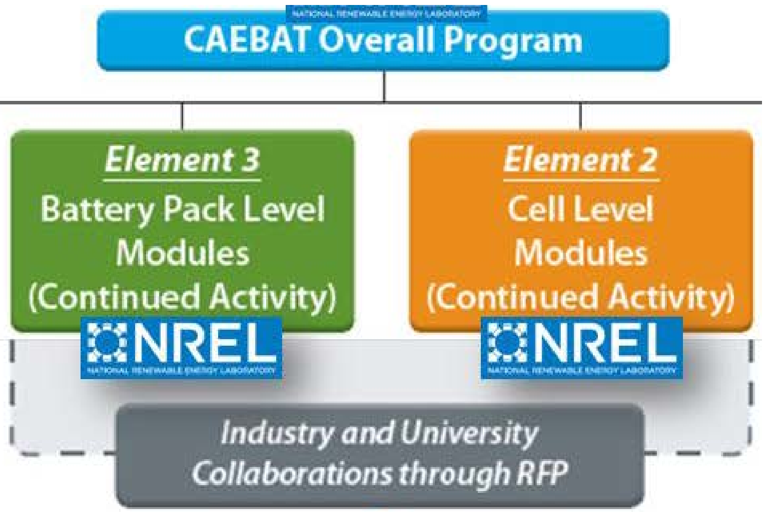
- NREL negotiated the terms and conditions with the three teams and their lower tiers, along with milestones and final budgets, assigned separate NREL technical monitors, and then signed the three subcontracts.
- Cost sharing by each of the subcontractors is 50%.
- Details: Subcontractor (partners), start date, total project budget, DOE/NREL funded amount, NREL tech monitors:
  - **EC Power** (teamed with Pennsylvania State University, Johnson Controls Inc., and Ford Motor Company); signed May 2, 2011; project budget of $3.0M; NREL subcontract budget of $1.50M, *NREL technical monitor: Shriram Santhanagopalan*
  - **General Motors** (teamed with ANSYS and ESim); subcontract signed June 1, 2011; project budget of $7.15M; NREL subcontract budget of $3.58M; *NREL technical monitor: Gi-Heon Kim*
  - **CD-adapco** (teamed with Battery Design LLC, Johnson Controls Inc. and A123 Systems); signed July 1, 2011; project budget of $2.73M; NREL subcontract budget of $1.37M; *NREL technical monitor: Kandler Smith*

CAEBAT Projects Underway

Accomplishments

- Kickoff meetings were conducted in June 2011 to review plans by each team.
- Weekly, biweekly, or monthly meetings were held to review progress and address issues.
- Quarterly progress review meetings were held at NREL, DOE, and subcontractor sites.
- Each subcontractor presented progress overview at US Drive Technical Committee Meeting.

Each subcontractor will provide objectives, approach, and accomplishments of their project in the next three presentations.

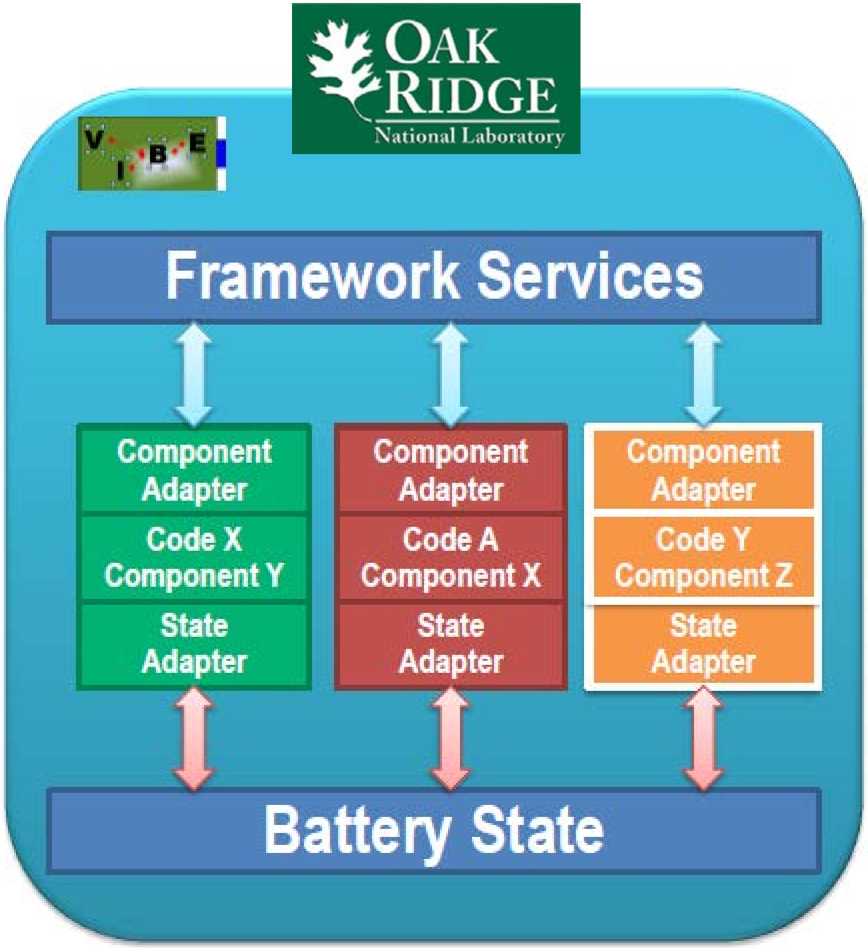


Tracking projects by monthly conference calls and face-face meetings with the three competitive teams separately.

Coordinating on Open Architecture Software

Accomplishments

- Interacted with Oak Ridge National Laboratory on the Open Architecture Software element of CAEBAT “that facilitates integrating battery modeling components within an open architecture.”
  - Participated in regular conference calls
  - Participated at ORNL’s kickoff meeting
  - Provided MSMD model for testing the integration approach
  - Provided suggestions for standardized input data and battery state



From ORNL Presentation by (S. Pannala) at the 2012 AMR

ORNL will provide the objectives, approach, and accomplishments of this project (es121) in the fourth presentations after this.

NREL Battery Modeling Under CAEBAT

Published a paper in the *Journal of the Electrochemical Society,* describing the approach and results of the NREL MSMD model, entitled "Multi-Domain Modeling of Lithium-Ion Batteries Encompassing Multi-Physics in Varied Length Scales."

Volume 158, Issue 8, pp. A955-A969 (17 June 2011)

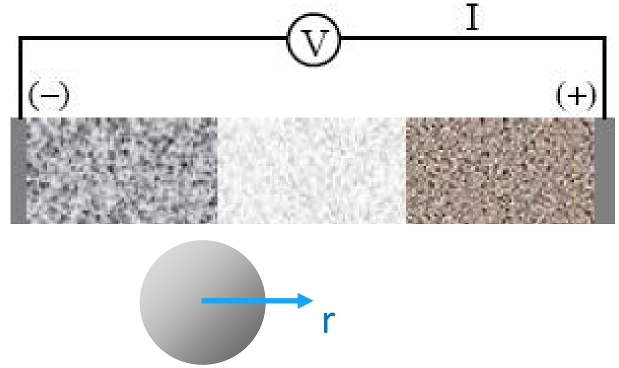
Commonly Used Porous Electrode Model

Background

Charge Transfer Kinetics at Reaction Sites

$$j^{Li} = a_s i_o \left\{ \exp\left[\frac{\alpha_a F}{RT}\eta\right] - \exp\left[-\frac{\alpha_c F}{RT}\eta\right] \right\}$$

$$i_0 = k(c_e)^{\alpha_a}(c_{s,\max} - c_{s,e})^{\alpha_a}(c_{s,e})^{\alpha_c} \qquad \eta = (\phi_s - \phi_e) - U$$



Species Conservation

$$\frac{\partial c_s}{\partial t} = \frac{D_s}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial c_s}{\partial r}\right)$$

$$\frac{\partial(\varepsilon_e c_e)}{\partial t} = \nabla \cdot \left(D_e^{eff} \nabla c_e\right) + \frac{1 - t_+^o}{F} j^{Li} - \frac{\mathbf{i}_e \cdot \nabla t_+^o}{F}$$

Charge Conservation

$$\nabla \cdot \left(\sigma^{eff} \nabla \phi_s\right) - j^{Li} = 0$$

$$\nabla \cdot \left(\kappa^{eff} \nabla \phi_e\right) + \nabla \cdot \left(\kappa_D^{eff} \nabla \ln c_e\right) + j^{Li} = 0$$

Energy Conservation

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + q'''$$

$$q''' = j^{Li}\left(\phi_s - \phi_e - U + T\frac{\partial U}{\partial T}\right) + \sigma^{eff} \nabla \phi_s \cdot \nabla \phi_s + \kappa^{eff} \nabla \phi_e \cdot \nabla \phi_e + \kappa_D^{eff} \nabla \ln c_e \cdot \nabla \phi_e$$

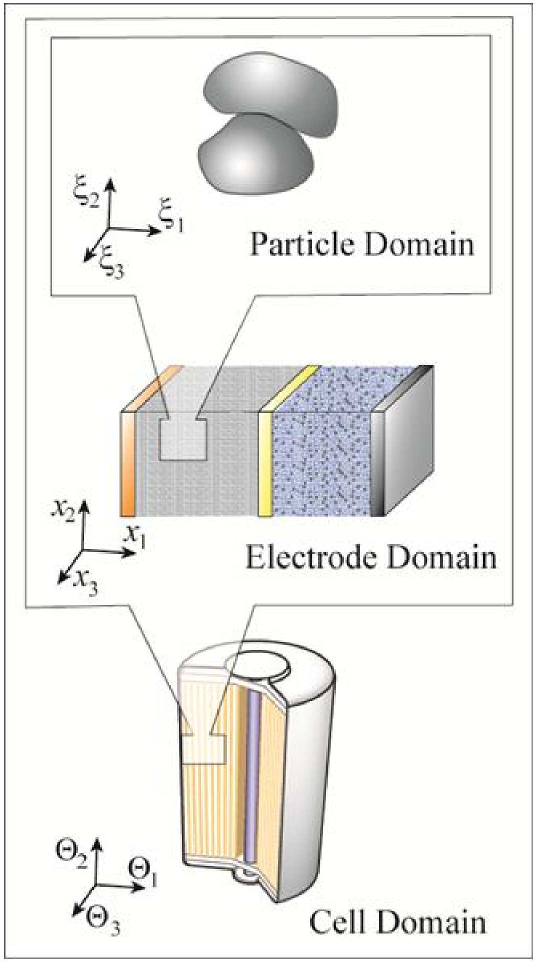
- **Pioneered by John Newman's group at the University of Berkeley (*Doyle, Fuller, and Newman 1993*)**
- Captures *lithium diffusion dynamics* and *charge transfer kinetics*
- Predicts *current/voltage response* of a battery
- Provides design guide for thermodynamics, kinetics, and transport across electrodes

- Difficult to apply in large-format batteries where *heat* and *electron current* transport critically affect the battery responses

Published NREL's MSMD Model Framework

Accomplishments

*Through the multi-year effort supported by DOE, NREL has developed a modeling framework for predictive computer simulation of LIBs known as the **Multi-Scale Multi-Dimensional (MSMD)** model that addresses the interplay among the physics in varied scales.*



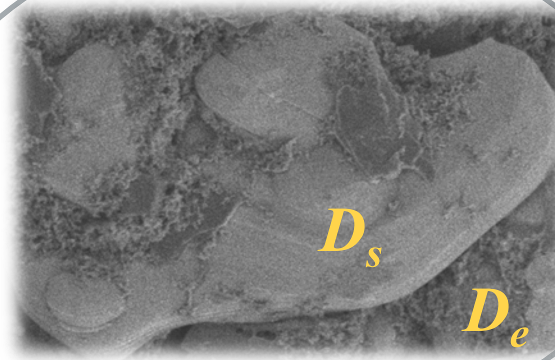
- **Introduces *multiple computational domains* for corresponding length scale physics**
- ***Decouples LIB geometries* into separate computation domains**
- ***Couples physics* using the predefined inter-domain information exchange**
- **Selectively resolves higher spatial resolution for smaller characteristic length scale physics**
- **Achieves high computational efficiency**
- **Provides flexible & expandable modularized framework**

Kim et al., "Multi-Domain Modeling of Lithium-Ion Batteries Encompassing Multi-Physics in Varied Length Scales," *J. of Electrochemical Society*, 2011, Vol. 158, No. 8, pp. A955–A969

MSMD Segregates Time & Length Scales

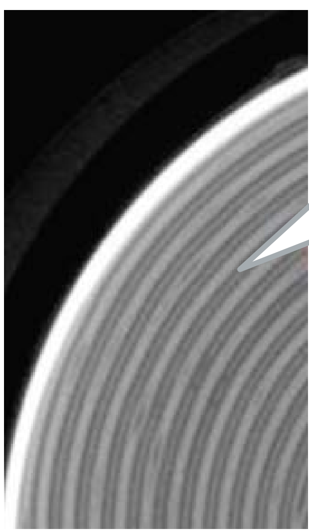
Accomplishments

- **Self-balancing nature** allows continuum approach with thermodynamic representation for sub-domain systems
- Time-scale differences in kinetic/dynamic transport processes conducive to segregation into sub-domain systems



Lithium transport is much faster in liquid electrolyte than in solid particles

e.g., $D_s \ll D_e$



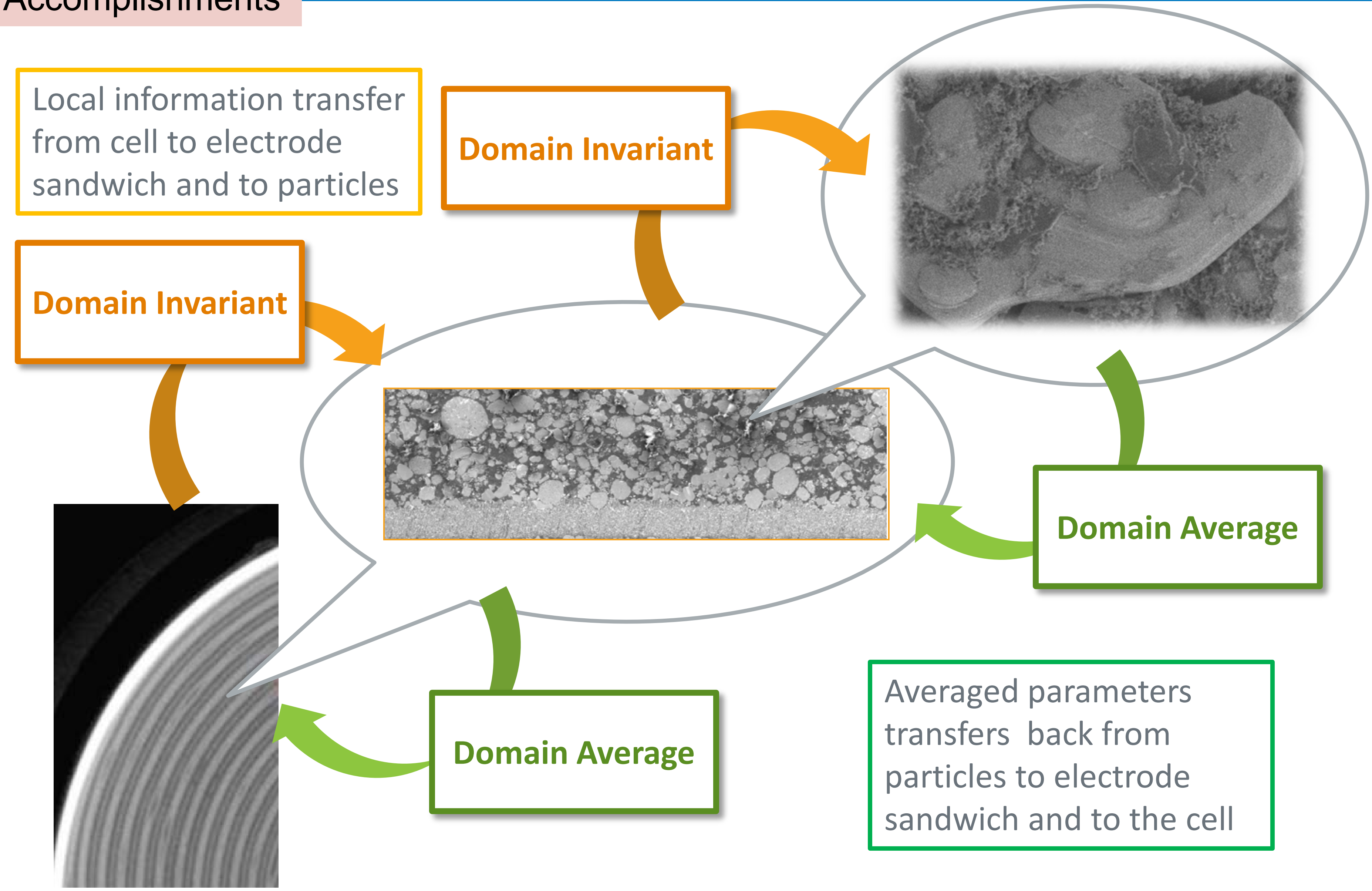
Electronic conductivity is much higher in metal current collectors than in composite electrode matrix

e.g., $\sigma_{ce} \ll \sigma_{cc}$

Kim et al., "Multi-Domain Modeling of Lithium-Ion Batteries Encompassing Multi-Physics in Varied Length Scales," *J. of Electrochemical Society*., 2011, Vol. 158, No. 8, pp. A955–A969

MSMD Decouples Geometry

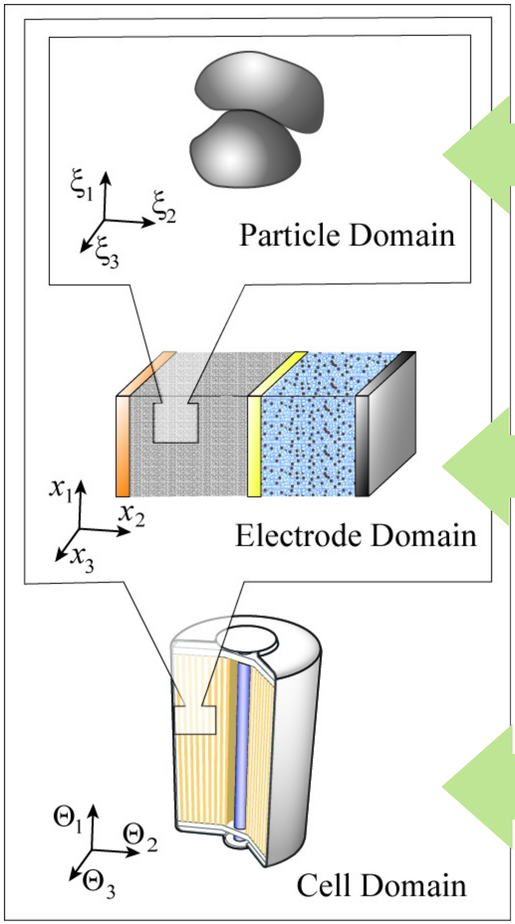
Accomplishments



MSDM Framework is Modularized

Accomplishments

Modularized hierarchical architecture of the MSMD model allows independent development of submodels for physics captured in each domain



Particle Domain Submodel Development

Solution Models & Method/Algorithms

- *2D Cylindrical particle model*
- *Reduced Order Method*

Examples

Electrode Domain Submodel Development

Solution Models & Method/Algorithms

- *1D Porous electrode model*
- *Finite Element Method*

Examples

Cell Domain Submodel Development

Solution Models & Method/Algorithms

- *3D Wound potential pair continuum model*
- ***Finite Volume Method***

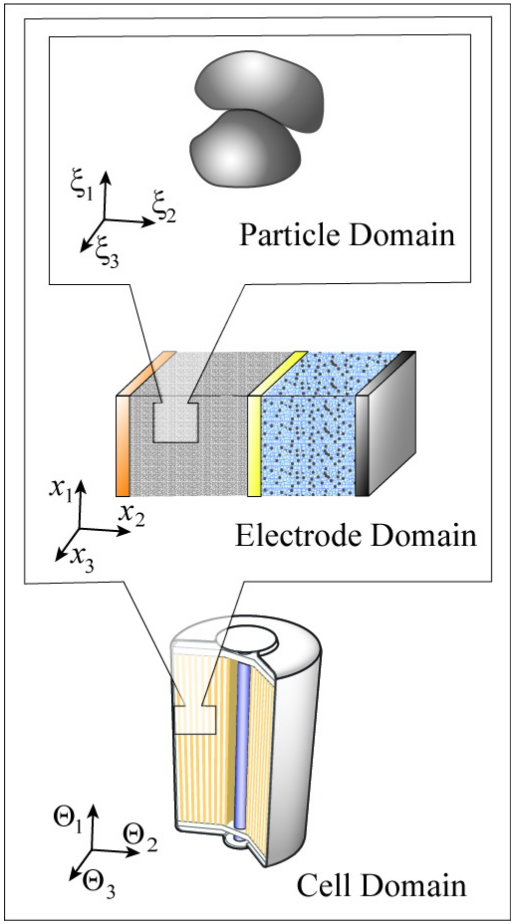
Examples

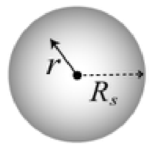
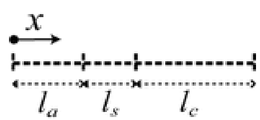
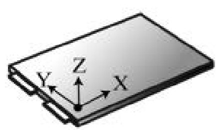
The modularized framework facilitates collaboration with experts across organizations

Application of MSMD for Predicting Cell Behavior

Large Stacked Prismatic Cell

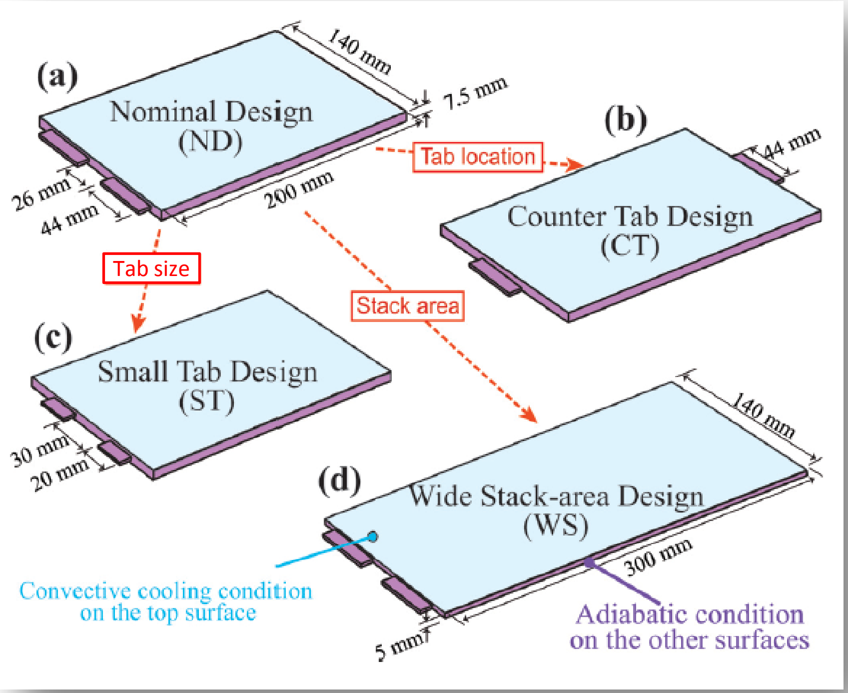
Accomplishments



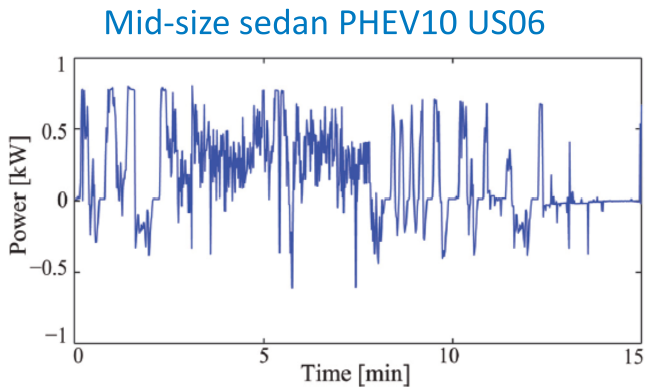
	Submodel Choice	Solution Method
Submodel in the Particle Domain		
	• *1D spherical particle model*	• *SVM (state variable method)*
Submodel in the Electrode Domain		
	• *1D porous electrode model*	• *SVM*
Submodel in the Cell Domain		
	• *3D Single Potential-Pair Continuum Model (**SPPC**)*	• *FV-LSM finite volume – linear superposition methods*

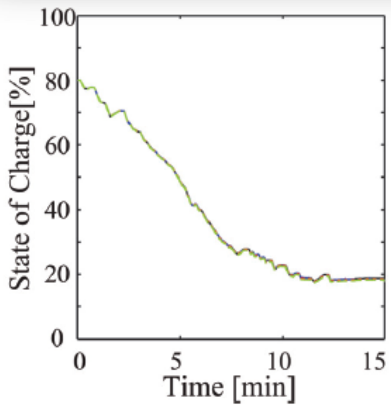
Predicted Non-Uniform Utilization in Prismatic Cells

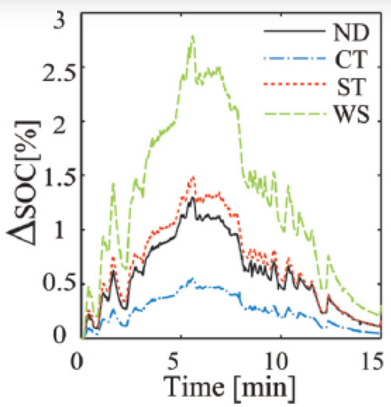
Accomplishments

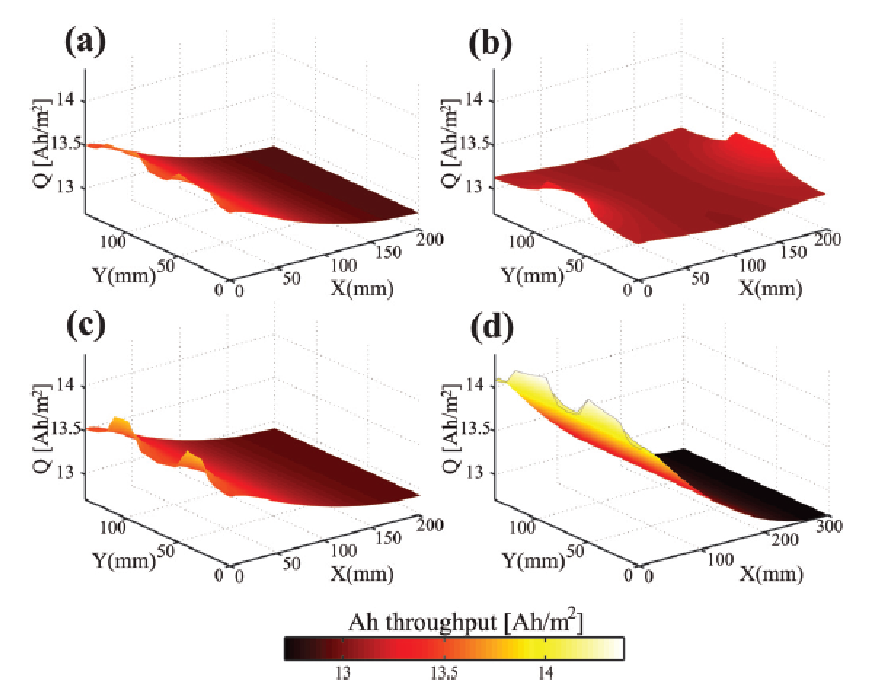


Kim et al., "Multi-Domain Modeling of Lithium-Ion Batteries Encompassing Multi-Physics in Varied Length Scales," *J. of Electrochemical Society*, 2011, Vol. 158, No. 8, pp. A955–A969





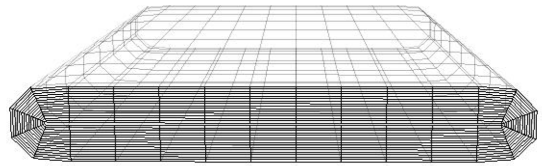




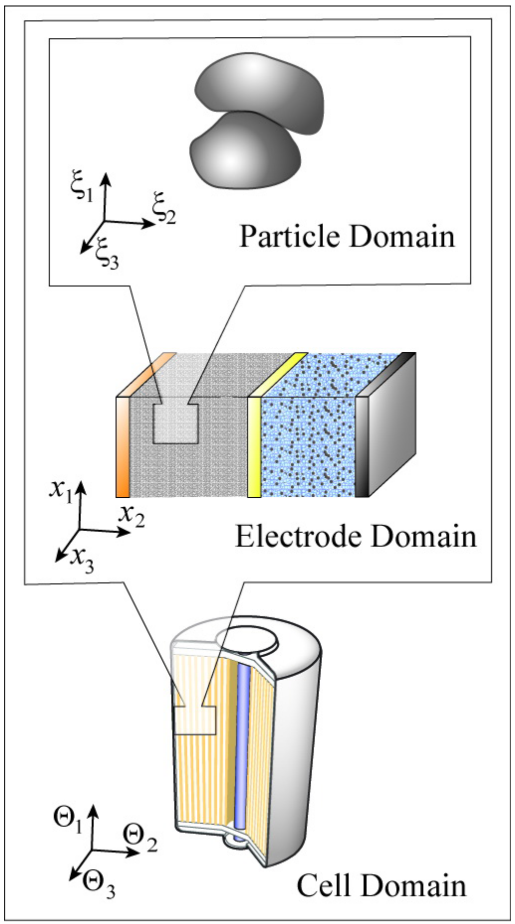
Application of MSMD for Predicting Cell Behavior

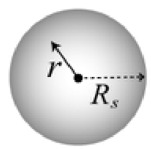
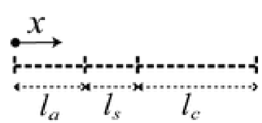
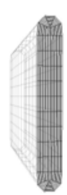
Wound Prismatic Cell

Accomplishments



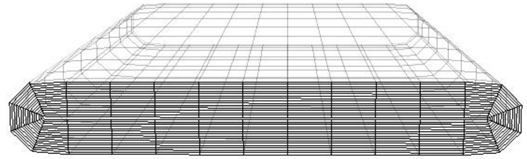
Spirally wound prismatic cell



	Submodel Choice	*Solution Method*
Submodel in the Particle Domain		
	• *1D spherical particle model*	• *SVM (state variable method)*
Submodel in the Electrode Domain		
	• *1D porous electrode model*	• *SVM*
Submodel in the Cell Domain		
	• *3D Wound Potential-Pair Continuum Model (**WPPC**)*	• *FVM (finite volume methods)*

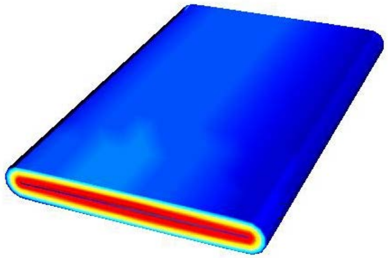
Response of a Wound Prismatic Cell

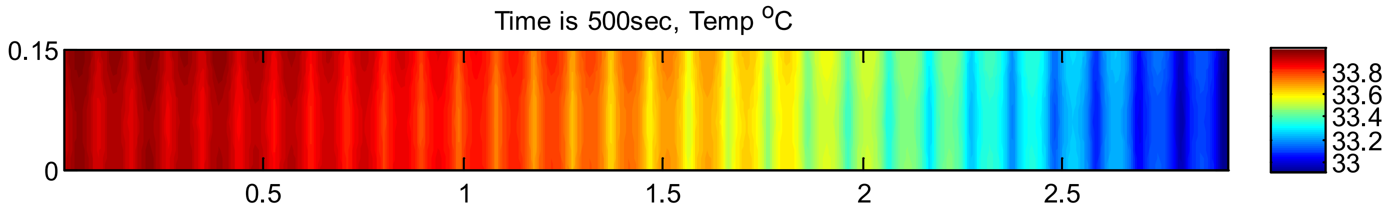
Accomplishments



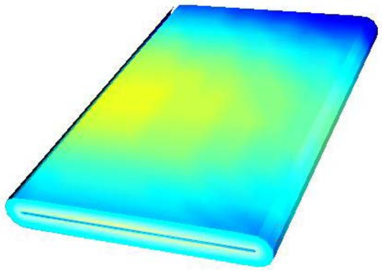
The simulation shows that non-uniform charge transfer current density and temperature distribution around the bent radius

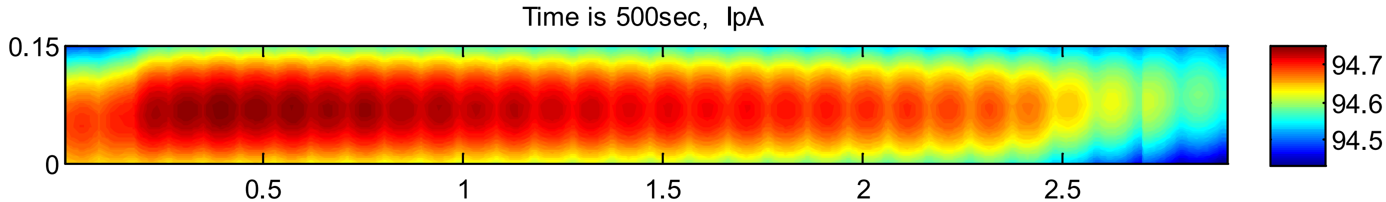
Model results after 500sec at 4C discharge of 20Ah cell with continuous tabs at surface (left images) and **unrolled** jelly roll (right images)





Temperature distribution

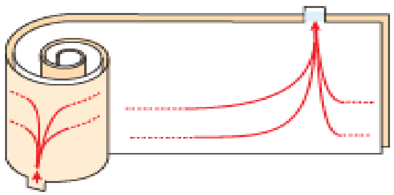




Reaction current density distribution

Thermal Response of Wound Cylindrical Cells

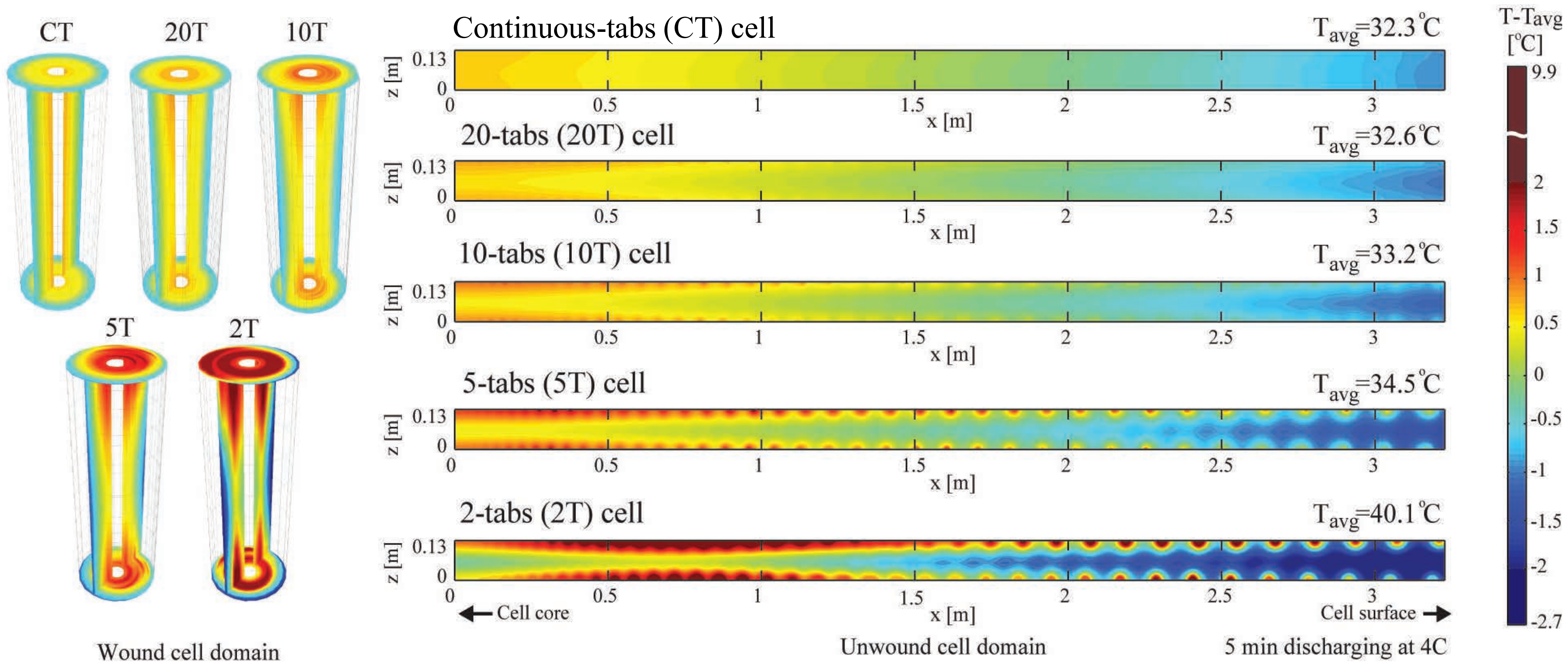
Accomplishments



Cell with discrete tabs

Impact of electrical current transport design:

- With higher number of tabs current and temperature distribution are more uniform



Temperature imbalance at 4C discharge

Kyu-Jin Lee, et al., April 2011

Collaboration and Coordination

- Coordination with other national labs under CAEBAT
  - ORNL (open architecture software)
  - INL (providing electrolyte properties to CD-adapco)
- Collaboration with CAEBAT subcontractors to develop battery CAE design tools
  - General Motors, ANSYS, E*Sim*
  - CD-adapco, Battery Design, A123 Systems, and JCI
  - EC Power, Penn State U, JCI, and Ford
- Colorado School of Mines – Published a joint paper on integrated general chemistry solver for charge transfer and side reactions in Li-ion

Proposed Future Work

- Collaborate with CAEBAT partners to develop CAEBAT tools
- Continue enhancing MSMD modeling framework
- Conduct experiments to validate NREL MSMD models
- Work with others in using MSMD models
- Collaborate with ORNL on implementing Open Architecture Software
- Review subcontractors' plans with focus on validation of cell and pack models
- Key upcoming milestones:
  - Document latest NREL battery model developments by publishing journal papers
  - Compete technical review of the three CAEBAT subcontracts
  - Review 1st version of CAEBAT subcontractors' tools for cells
- Work with collaborators and partners to promote the use of CAEBAT tools within the battery community

Publications and Presentations

- Kyu-Jin Lee, Kandler Smith, Gi-Heon Kim, *"A Three-Dimensional Thermal-Electrochemical Coupled Model for Spirally Wound Large-Format Lithium-Ion Batteries,"* presented at Space Power Workshop; Los Angeles, CA; April 18, 2011.
- A.M. Colclasure, K.A. Smith, K. A.; R.J. Kee, "Modeling Detailed Chemistry and Transport for Solid Electrolyte Interface (SEI) Films in Li-ion Batteries," *Electrochimica Acta*. Vol. 58, 30 December 2011; pp. 33-43.
- G.-H. Kim, K. Smith, K.-J. Lee, and S. Santhanagopalan, A. A. Pesaran, "Multi-Domain Modeling of Lithium-Ion Batteries Encompassing Multi-Physics in Varied Length Scales," *J. of the Electrochemical Society*, 2011, Vol. 158, No. 8, pp. A955–A969
- A. A. Pesaran, G.-H. Kim, K. Smith, K.-J. Lee, and S. Santhanagopalan, "Computer-Aided Engineering of Batteries for Designing Better Li-Ion Batteries ," presented at the Advanced Automotive Battery Conference, Orlando, Florida; February 6-8, 2012

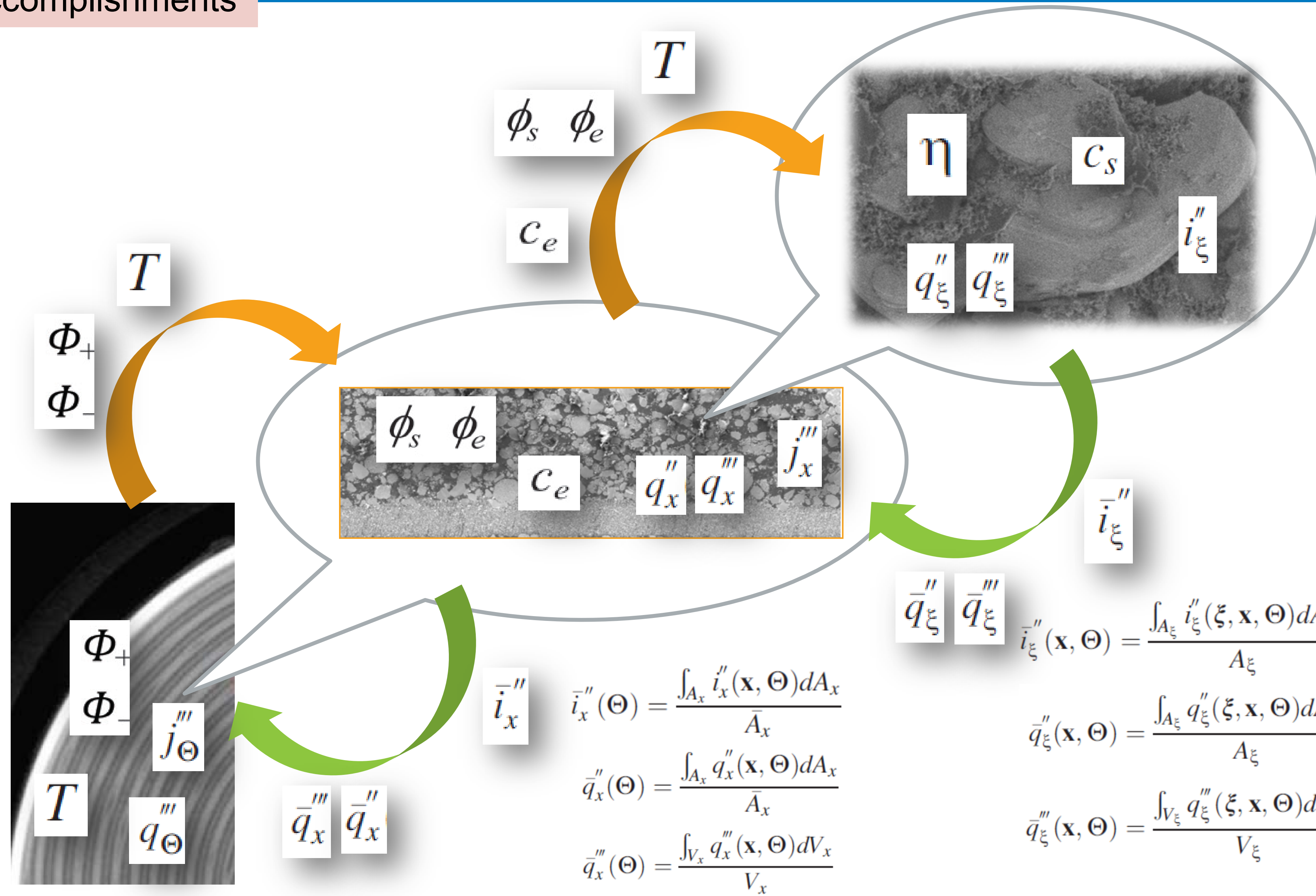
Summary

- CAEBAT activity was initiated to develop battery computer-aided engineering tools to accelerate development of batteries for electric vehicles.
- CAEBAT activities at NREL consist of two parallel paths:
  - Working with industry to develop CAEBAT tools through cost-shared subcontracts
  - NREL in-house electrochemical battery model development
- After a competitive process, NREL executed three subcontracts with three industry teams –a total of $14M with 50% cost share from industry– to develop the battery computer tools.
  - GM/ANSYS/E*sim*
  - CD-adapco/Battery Design/A123 Systems/JCI
  - EC Power/Penn State/JCI/Ford
- NREL collaborated with ORNL on CAEBAT open architecture software.
- NREL continued the development of its MSMD electrochemical/thermal modeling and published papers (for stacked prismatic, wound cylindrical, and wound prismatic configurations).
- CAEBAT project is proceeding very well and according to the plan.

Technical Back-Up Slides

MSMD Protocol for Transferring Information

Accomplishments



$$\bar{i}_x''(\Theta) = \frac{\int_{A_x} i_x''(\mathbf{x},\Theta)\,dA_x}{A_x}$$

$$\bar{q}_x''(\Theta) = \frac{\int_{A_x} q_x''(\mathbf{x},\Theta)\,dA_x}{A_x}$$

$$\bar{q}_x'''(\Theta) = \frac{\int_{V_x} q_x'''(\mathbf{x},\Theta)\,dV_x}{V_x}$$

$$\bar{i}_\xi''(\mathbf{x},\Theta) = \frac{\int_{A_\xi} i_\xi''(\xi,\mathbf{x},\Theta)\,dA_\xi}{A_\xi}$$

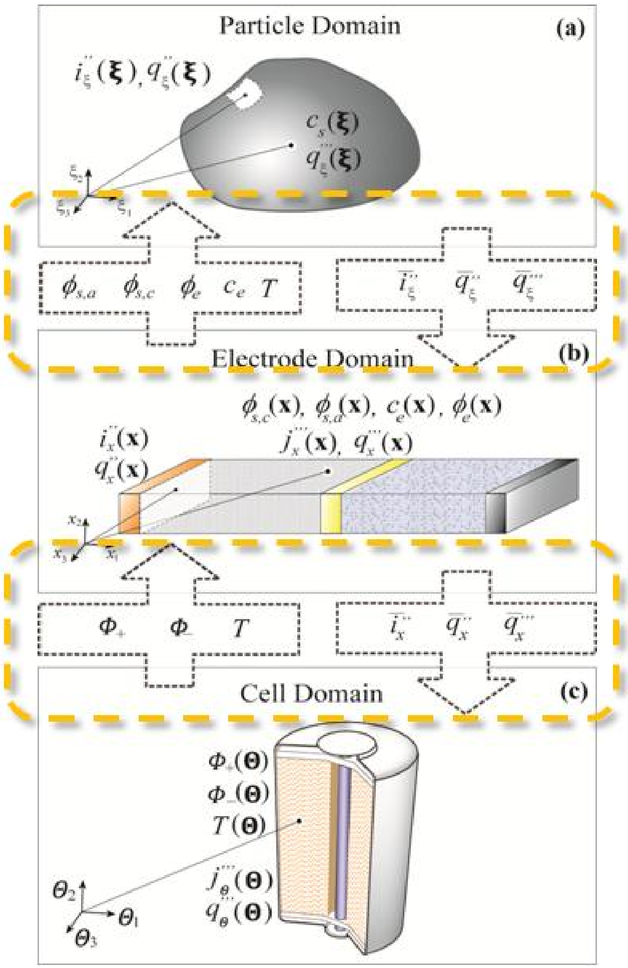
$$\bar{q}_\xi''(\mathbf{x},\Theta) = \frac{\int_{A_\xi} q_\xi''(\xi,\mathbf{x},\Theta)\,dA_\xi}{A_\xi}$$

$$\bar{q}_\xi'''(\mathbf{x},\Theta) = \frac{\int_{V_\xi} q_\xi'''(\xi,\mathbf{x},\Theta)\,dV_\xi}{V_\xi}$$

Hierarchical Architecture of MSMD

- ***Modularized flexible framework*** for multi-scale multi-physics battery modeling
- ***Expandable development platform*** providing "pre-defined but expandable communication protocol"

- Charge transfer kinetics
- Li diffusion dynamics in electrode particulates and in electrolyte
- Charge balance
- Energy conservation
- …



Particle Domain

- Charge transfer kinetics
- Li transport in active particles
- …

Electrode Domain

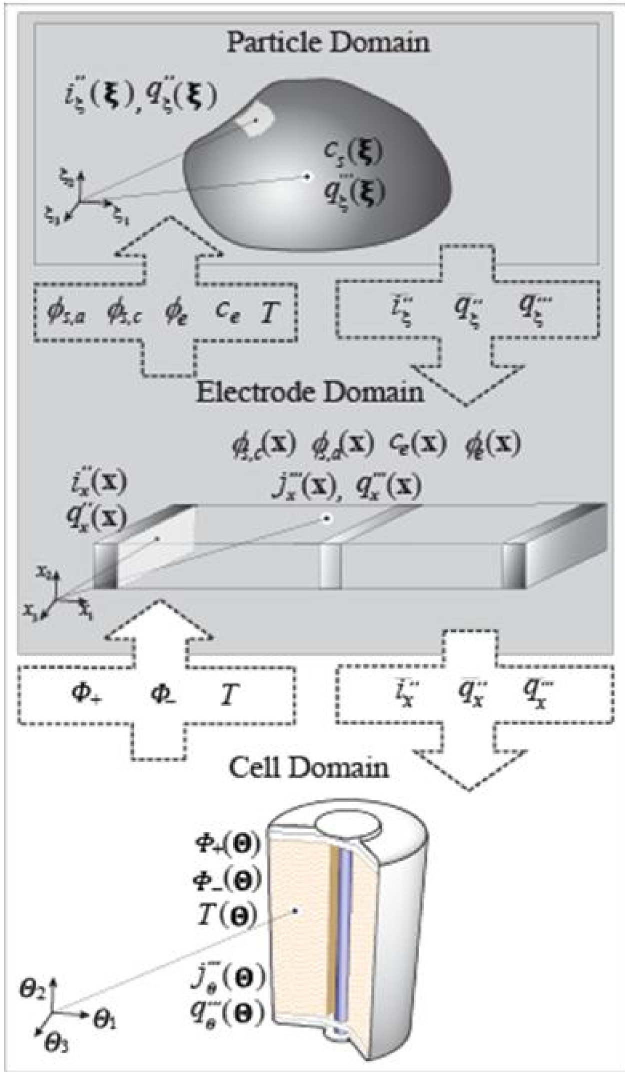
- Charge balance in solid composite electrode matrix
- Charge balance in liquid pore channels
- Li transport in electrolyte
- …

Cell Domain

- Energy conservation
- Charge conservation in current collectors
- …

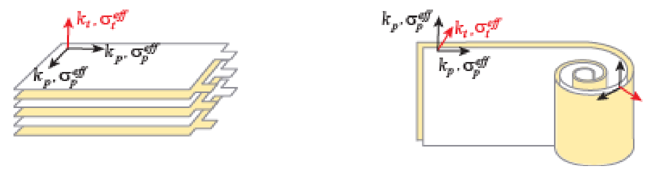
Kim et al., "Multi-Domain Modeling of Lithium-Ion Batteries Encompassing Multi-Physics in Varied Length Scales," *J. of Electrochemistry*, 2011, Vol. 158, No. 8, pp. A955–A969

NREL's Cell-Domain Models: Orthotropic Continuum Model



Cell Domain Models

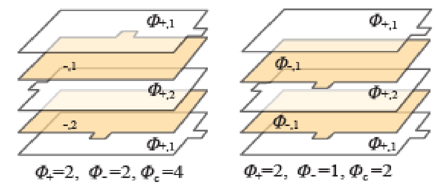
- ***SPPC (Single Potential-Pair Continuum) model:*** applicable to stack prismatic cells, tab-less wound cylindrical/(prismatic) cells:



Stacked cell

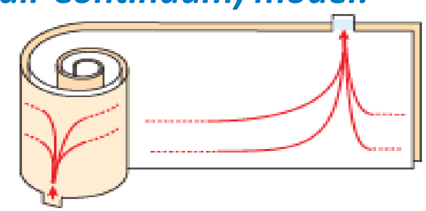
Wound cell with continuous tab

- ***MPPC (Multi Potential-Pair Continuum) model:*** applicable to alternating stacked prismatic cells:



Alternating stacked cells

- ***WPPC (Wound Potential-Pair Continuum) model:*** applicable to spirally wound cylindrical/ (prismatic) cells:



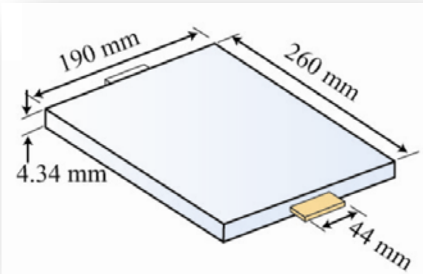
Cell with discrete tabs

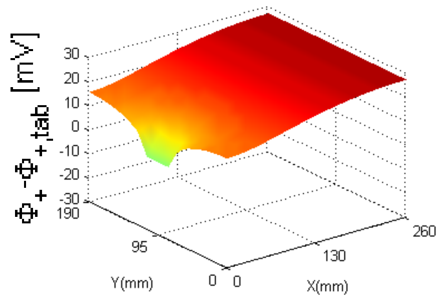
- ***Lumped model:*** applicable to small cells

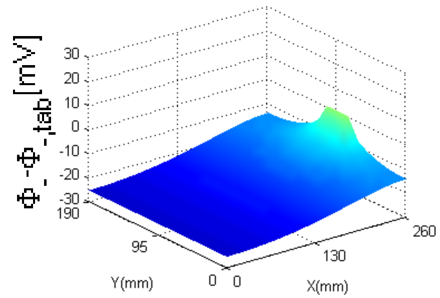
√ Discussed in this presentation

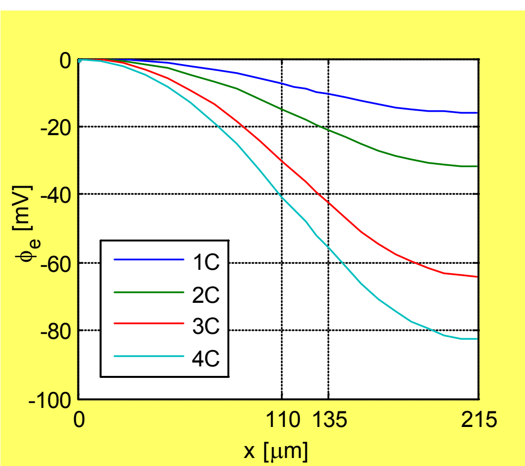
Electric Current Transport – Prismatic

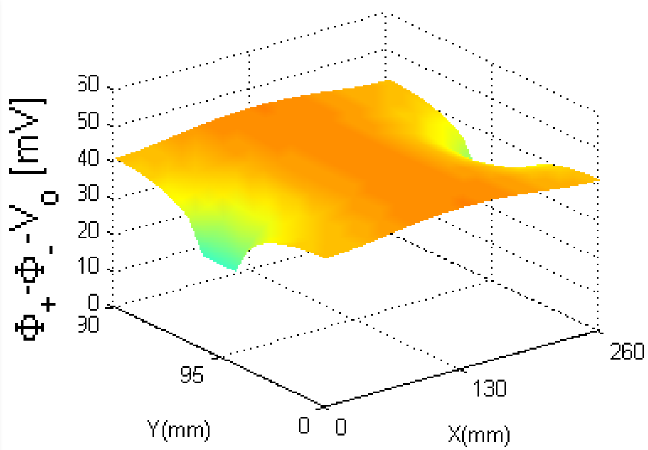
4C discharge / Single-side cooling





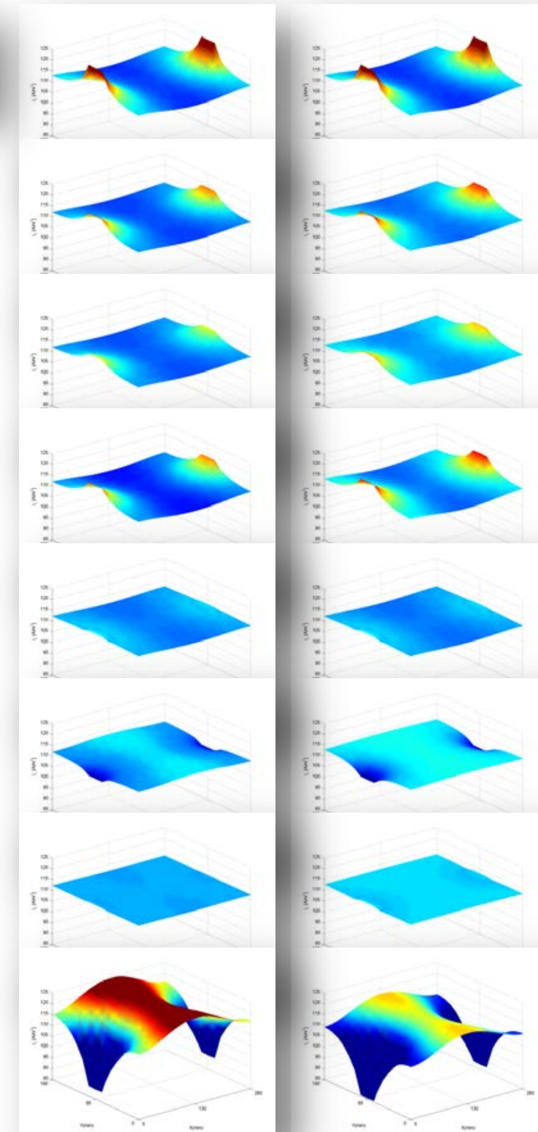






cooled top | bottom

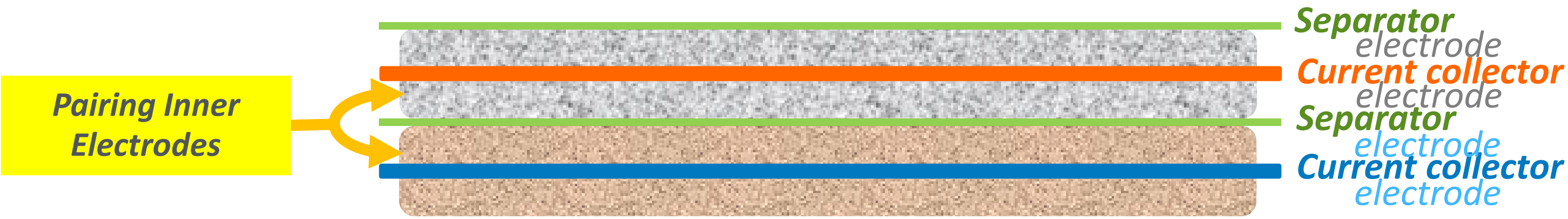
$\bar{i}_x''$



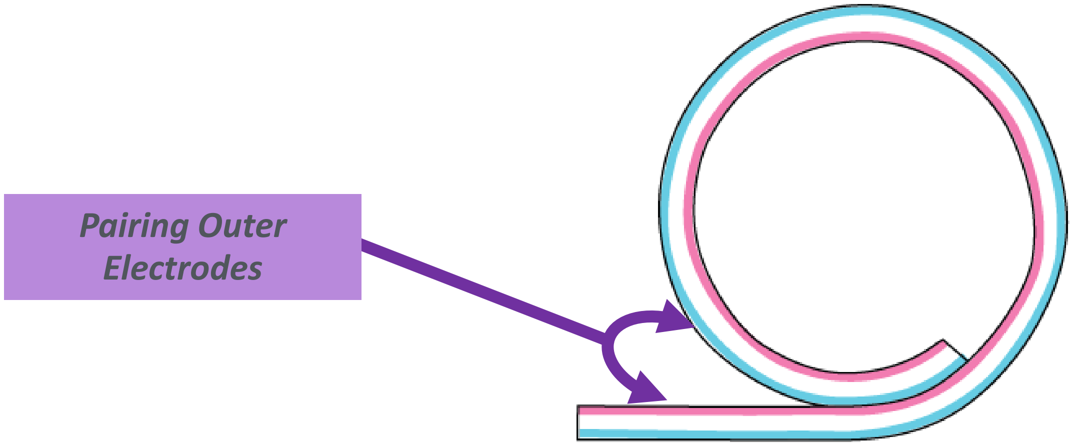
Wound Cells (Cylindrical or Prismatic)

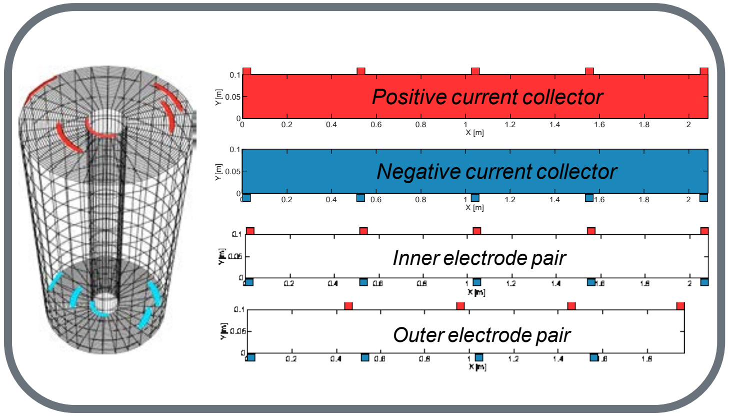
- A pair of ***wide*** current collectors
- Two electrode pairs
- Cylindrical or prismatic cells

***Stacking* : Forming the first pair between inner electrodes**

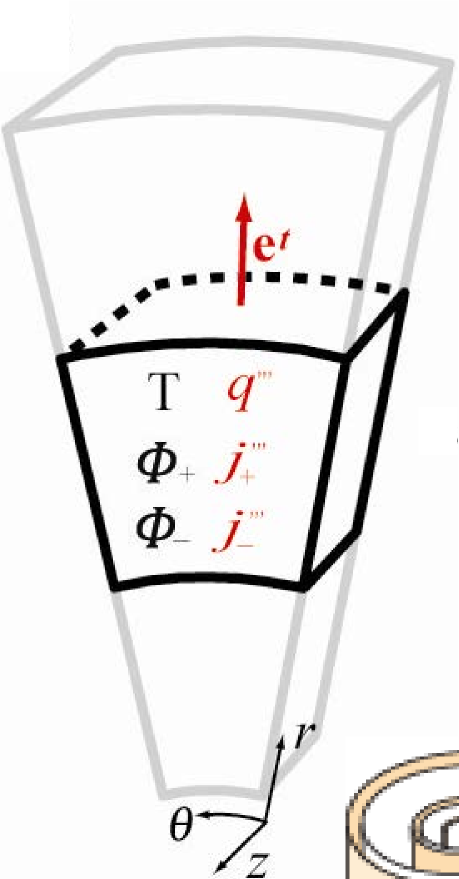


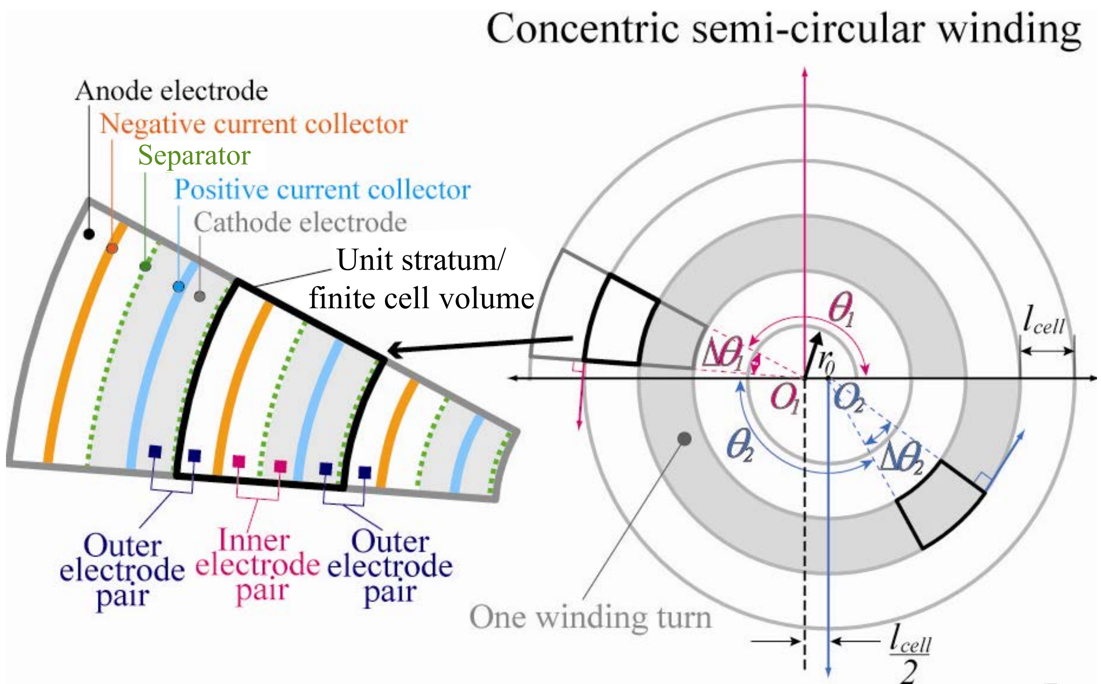
***Winding* : Forming the second pair between outer electrodes**

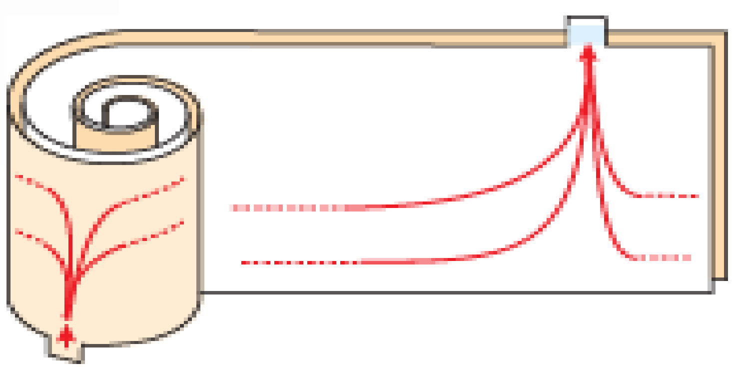




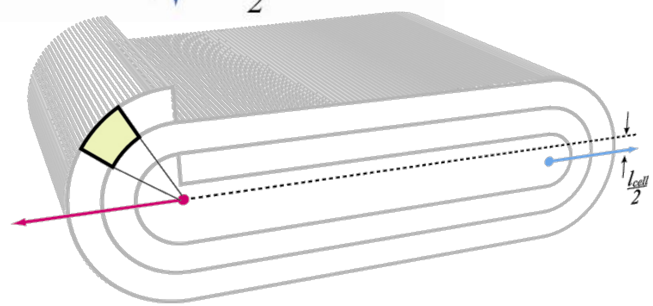
WPPC (Wound Potential-Pair Continuum)







Cell with discrete tabs

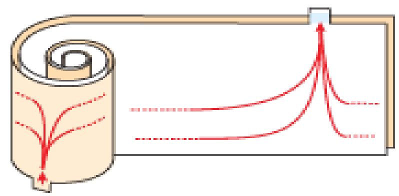


Applicable to flat wound prismatic cells

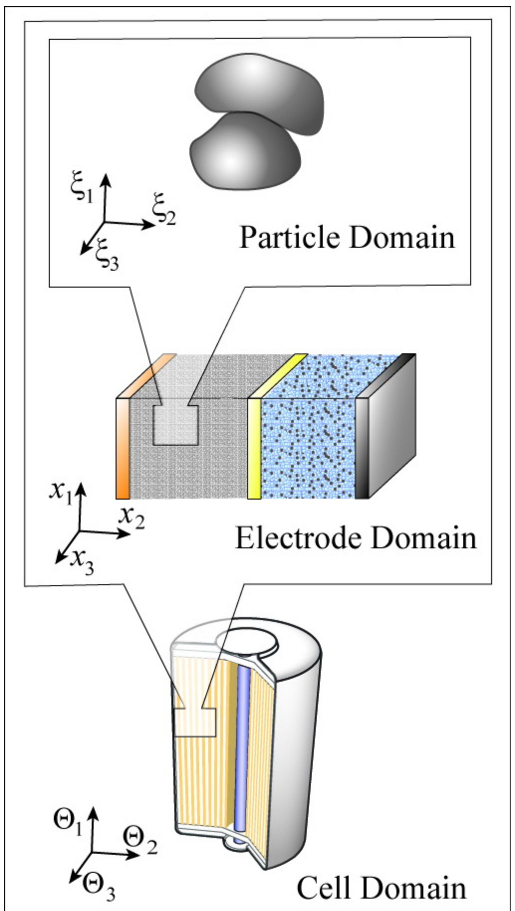
Application of MSMD for Predicting Cell Behavior

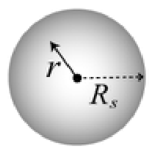
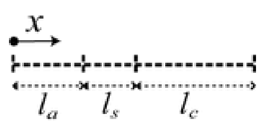
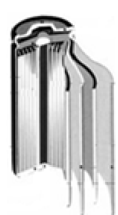
Wound Cylindrical Cell

Accomplishments



Cell with discrete tabs

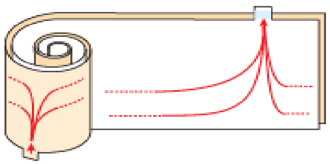


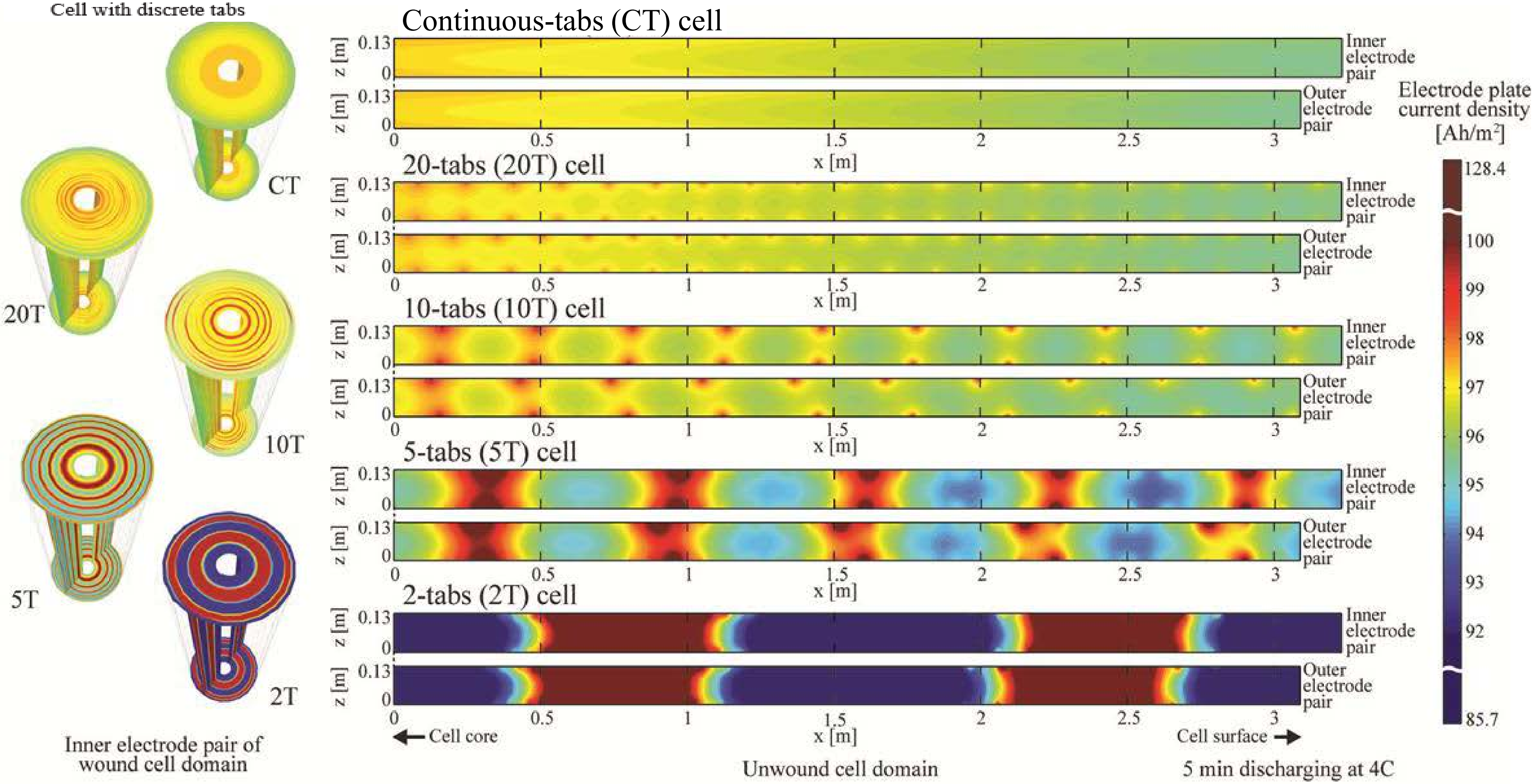
	Submodel Choice	*Solution Method*
Submodel in the Particle Domain		
	• *1D spherical particle model*	• *SVM (state variable method)*
Submodel in the Electrode Domain		
	• *1D porous electrode model*	• *SVM*
Submodel in the Cell Domain		
	• *3D Wound Potential-Pair Continuum Model (**WPPC**)*	• *FV-LSM finite volume – linear superposition methods*

Kinetics Response – Wound Cylindrical Cell

Accomplishments

Impact of electrical current transport design





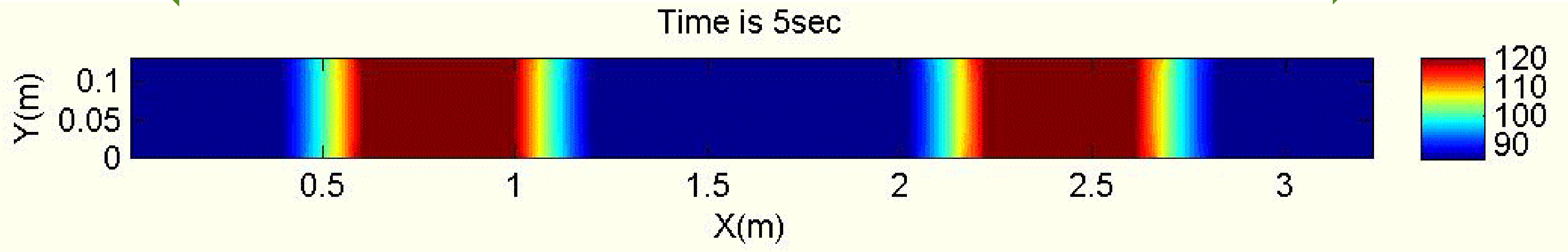
Kyu-Jin Lee, et al., April 2011

Non-uniform Kinetics during 4C Discharge cylindrical Cell

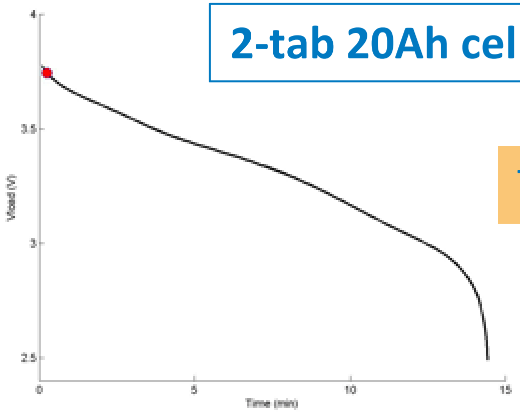
Electrode plate current density [A/m^2] at inner-electrode pair

core

surface

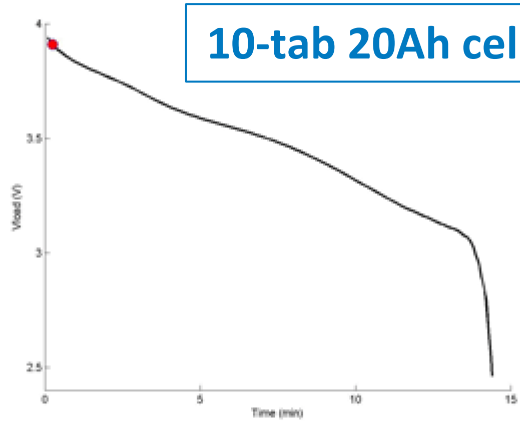


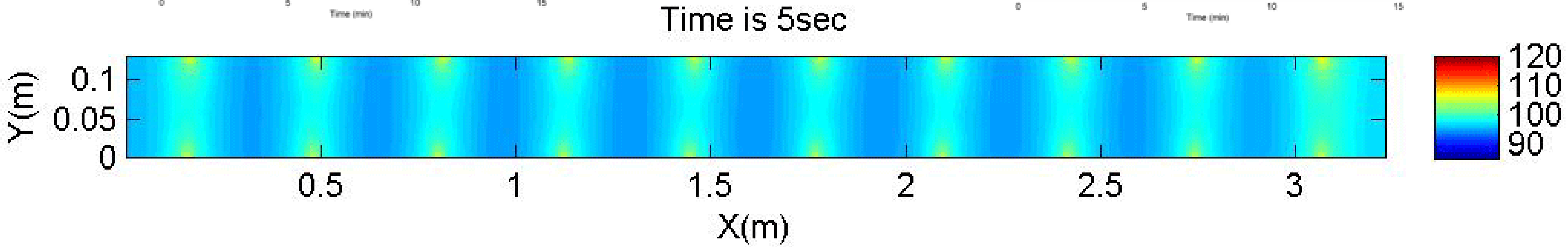
2-tab 20Ah cell



This slide has animation

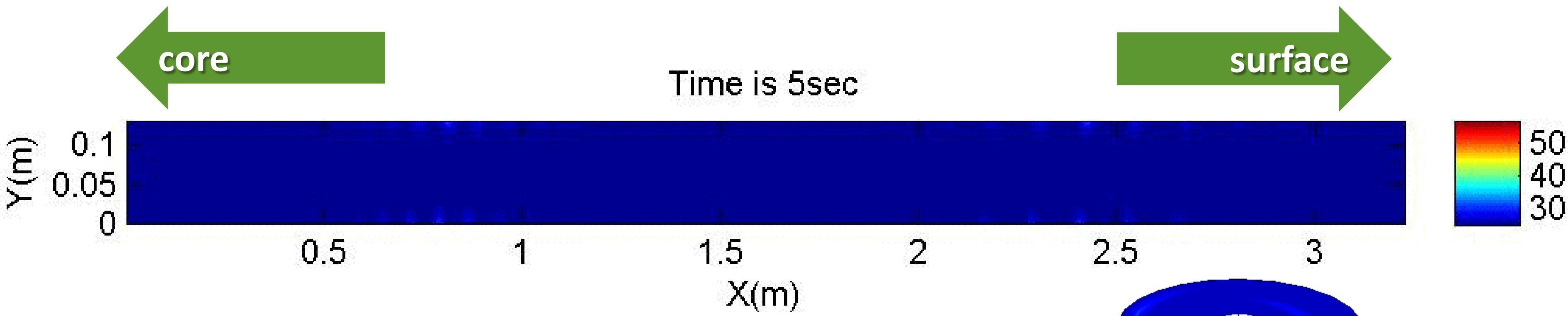
10-tab 20Ah cell

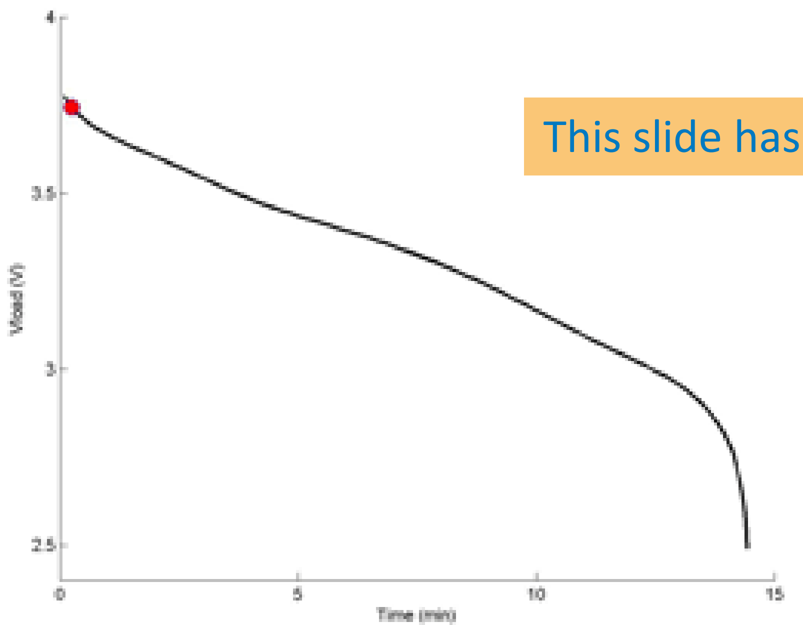




Thermal Evolution during 4C Discharge

2-Tab Design





This slide has animation