Energy Storage R&D

Computer-Aided Engineering for Electric Drive Vehicle Batteries (CAEBAT)

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Overview

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

Timeline

- Project start date: April 2010
- Project end date: Sept 2014
- Percent complete: 15%

Barriers – Batteries

- Cost and life
- Performance and safety
- Slow prototype-driven design cycles for materials, cells and packs
- Lack of validated battery computer-aided engineering tools suitable for non-expert use

Budget

- Funding received in
  - FY10: $3.5M ($3.0M for subcontracts)
  - FY11: expected $3.5M ($2.5M for subcontracts)

Partners

- ORNL
- LBNL
- ANL
- SNL
- INL
- LLNL
- Colorado School of Mines

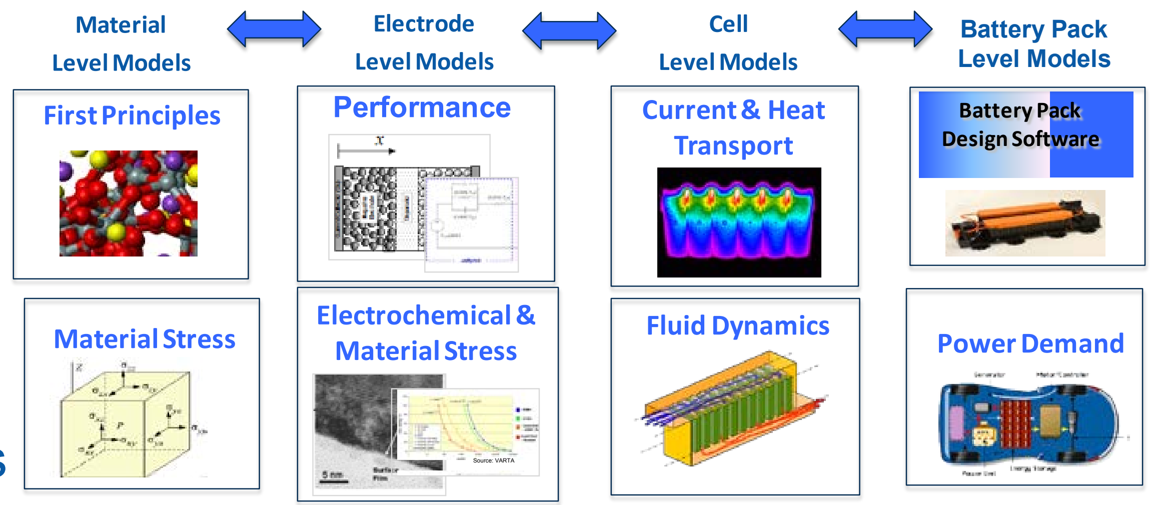
Funding provided by Dave Howell, Office of Vehicle Technologies (VT).
Activity managed by Brian Cunningham, Vehicle Technologies Program.

Relevance – Need for Better Design Tools

- Computer-aided engineering (CAE) tools are widely used in many industries to speed up the product development cycle and reduce the number of build-and-break steps.
- In fact, use of CAE tools has enabled automakers to reduce product development cost and time while improving the safety, comfort, and durability of the components and the vehicles they produce.
- However, there are no <u>mature</u> CAE tools for the design and commercial development of electric drive vehicle batteries.
- Although there are a number of battery models in academia, national labs, and industry, they either
  - Include relevant physics details, but neglect engineering complexities, or
  - Include relevant macroscopic geometry and system conditions, but use too many simplifications in fundamental physics
- There are a number of custom battery codes available; however, they all require expert users.

Computer Aided Engineering for Electric Drive Vehicle Batteries (CAEBAT)

Relevance

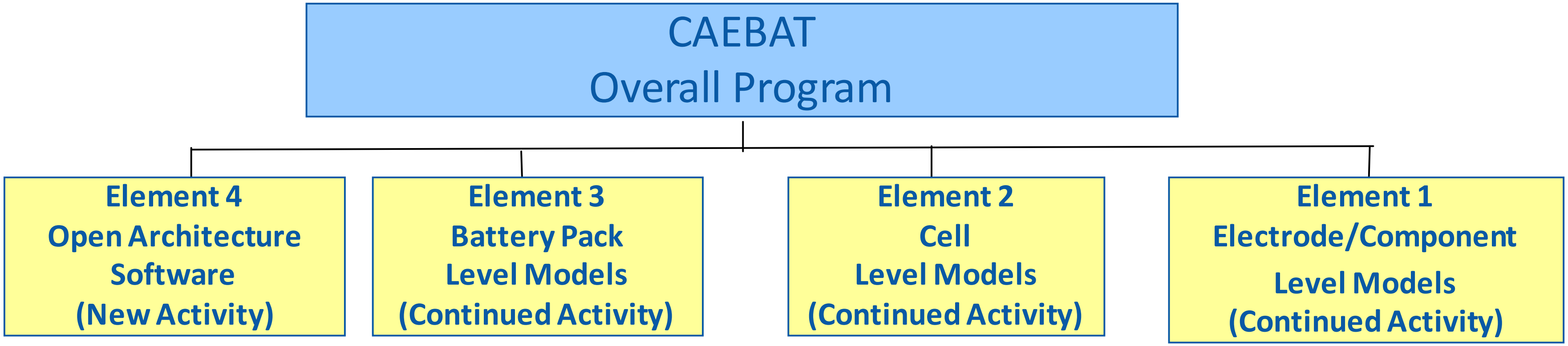


- Battery CAE capabilities need to be further developed to accelerate the development of batteries.
- In previous years, under DOE funding, national laboratories and universities have developed several tools for electrothermal, electrochemical, and abuse reaction modeling of lithium-ion batteries.
- The concern has been that they were not all integrated and additional tools were needed.
- In April of 2010, the DOE VT Energy Storage Program initiated the multi-year CAEBAT activity to develop design tools and an open architecture software framework that will enable disparate models to interface with each other.

Objectives – DOE CAEBAT Program

Relevance

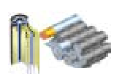
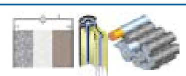
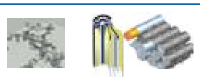
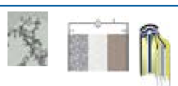
- The objective of CAEBAT is to incorporate existing and new models into design suites/tools with the goal of shortening design cycles and optimizing batteries (cells and packs) for improved performance, safety, long life, and low cost.
  - The software suite will include material properties, electrode design, pack design for thermal management purposes, load profiles, and aging data as input, and could greatly speed up the design of new batteries and provide critical guidance to developers.



Objectives – NREL CAEBAT Tasks

Relevance

- As project coordinator, NREL supports DOE in establishing the CAEBAT programmatic activities and objectives.
  - Provide input/documents for the CAEBAT project plan
  - Coordinate activities among national laboratories
  - Support industry and universities through a competitive process to develop battery CAE software tools
- Enhance and further develop NREL's existing electrochemical, thermal, abuse reaction, and internal short circuit models for use by CAEBAT participants

Model	Length Scale μm --- mm ---- m	Geometry	Physics / Application
Electro-thermal (FEA) & Fluid-dynamics (CFD)		1-D, 2-D, & 3-D	• Electrical, thermal & fluid flow • Performance, detailed cooling design • Commercial software (restrictive assumptions)
Electrochemical-thermal ("MSMD")		1-D, 2-D & 3-D	• Electrochemical, electrical & thermal • Performance, design
Electrochemical-thermal-degradation ("MSMD-life")		1-D, 2-D & 3-D	• Electrochemical, electrical & thermal • Cycling- & thermal-induced degradation • Performance, design, life prediction
Thermal abuse reaction kinetics		Thermal network, 2-D & 3-D	• Chemical & thermal • Safety evaluation
Internal short circuit		3-D	• Chemical, electrical, electrochem. & thermal • Safety evaluation

List of NREL Milestones

Title	Due Date	Status
Draft Scope of Work for the CAEBAT program	June 2010	Completed
Issue Request for Proposals (RFP), review proposals and select industry awardees	December 2010	Completed
Negotiate and place subcontracts with CAEBAT RFP awardees	June 2011 (Rescheduled)	On Track
Progress review on the work for the CAEBAT-NREL program	July 2011 (Rescheduled)	On Track

Approach/Strategy

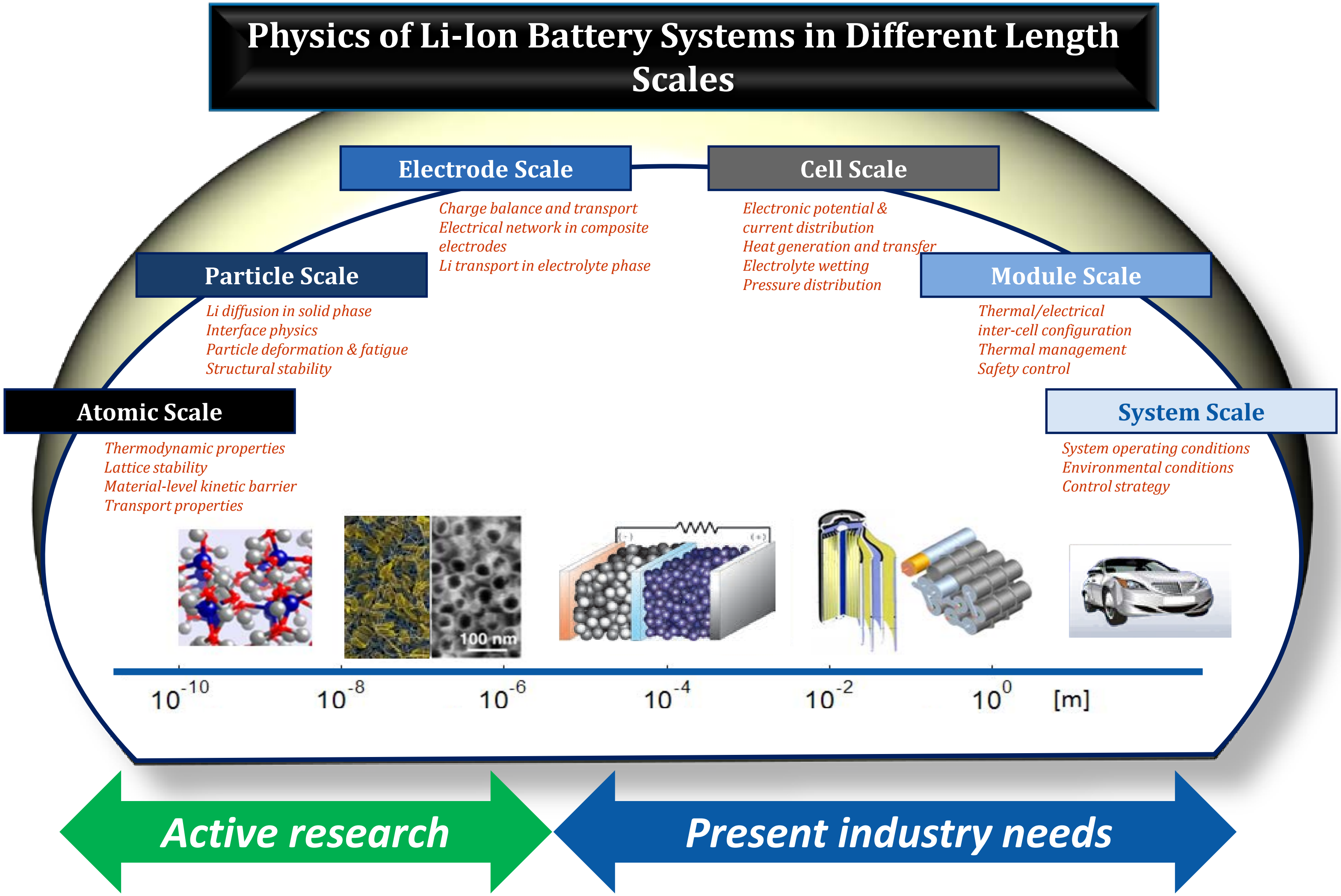
- Based on DOE's guidance, work with battery community & stakeholders (battery developers, car manufacturers, national laboratories, universities, software companies, etc.) to further refine the scope of the CAEBAT activity:
  - Interact with other national laboratories to understand the capability of existing battery models and other computational capabilities.
  - Interact with industry and universities to understand the scope of their capabilities and eventual needs.
  - Provide input/documents to DOE for defining the CAEBAT project plan.
- Through competitive process, solicit cost-shared proposals from the industry and identify teams to develop battery CAE software tools.
- Perform in-house R&D to enhance and further develop NREL's existing electrochemical, thermal, abuse reaction, and internal short circuit models for use by CAEBAT participants.

Overall CAEBAT Project

Technical Accomplishments/Progress

Accomplishments

With input from stakeholders, we identified *various physics across a wide range of length and time scales* that must be addressed, particularly at the pack/vehicle scale.



Identified Community's Expectation for Battery CAE Tools

- **Address Multi-Scale Physics Interactions**: Integrate different scale battery physics in a computationally efficient manner
- **Flexible**: Provide a modularized multi-physics platform to enable user the choice from multiple sub-model options with various physical/computational complexities
- **Expandable**: Provide an expandable framework to "add new physics of interest" or to "drop physics of low significance or indifference"
- **Validated:** Ensure that the correct equations are solved by performing carefully designed experiments
- **Verified:** The equations are solved accurately

Interacted with Six Other National Laboratories

Accomplishments

- Battery modeling experts from Argonne National Lab (ANL), Sandia National Lab (SNL), Idaho National Lab (INL), and Oak Ridge National Lab (ORNL) visited NREL
- NREL battery researchers visited Lawrence Berkeley National Lab (LBNL), Lawrence Livermore National Lab (LLNL), and ORNL
- The capabilities and potential roles for each lab were identified
- Each lab provided input for the CAEBAT project planning document
- Based on DOE's guidance:
  - ORNL was funded in FY10 and FY11 to lead Element 4 to develop an open architecture software
  - Other labs were directed to continue any battery modeling work under their existing Advanced Battery Research (ABR) and Batteries for Advanced Transportation Technologies (BATT) Programs

Updated DOE CAEBAT Program Elements

Accomplishments

CAEBAT Program

- **Element 4: Create Open Architecture Software**
  - Platform Selection
  - Interface Definitions
  - Input-Output Formats
- **Element 3: Develop Pack Models**
  - CAD Design Layout
  - Thermal Models
  - Fluid Dynamic Models
  - Cost Estimations
  - Performance Models
  - Pack Management
  - Abuse & Safety Models
- **Element 2: Develop Cell Models**
  - CAD Design (prismatic cylindrical)
  - Thermal Models
  - Electrode Design
  - Life Models
  - Abuse Models
  - Structural & Mechanical Models
- **Element 1: Develop Component Level Models**
  - Cathode Material Modeling
  - Anode Material Modeling
  - Electrolyte Modeling
  - Electrochemical Couples Modeling
  - Abuse Chemistry Modeling
  - Separator Modeling

Industry and University Collaborations through RFP

Material-Level Models Developed under BATT and ABR Programs

<u>Assignments for Coordination</u>

- Overall activity: NREL
- Element 1: LBNL
- Element 2: NREL
- Element 3: NREL
- Element 4: ORNL

Initiated Collaboration with Industry

Accomplishments

- Introduced the CAEBAT program at battery conferences and meetings with the United States Advanced Battery Consortium Tech Team
- Prepared a Statement of Work for RFP from industry (car makers, battery developers, battery integrators, universities, and software companies).
  - The purpose was to seek cross-cutting teams to "develop suites of software tools that enable EDV battery community to simulate and design battery packs."
- NREL issued the CAEBAT RFP on July 30, 2010; many proposals received by September 24, 2010.
- Total DOE/NREL funding is set to be $7.5M over three years with required 50% cost-sharing from participants a project totaling $15 M.
- Source Evaluation Team (SET) consisting of experts from NREL, DOE, and other organizations discussed the proposals during the first two weeks of October 2010.
- By the end of October, the SET reviewed, scored and ranked the proposals; recommended the top three teams for further consideration.

Pending Collaborations with Industry

Accomplishments

- Three industry-led teams were selected for further negotiation with potential awards

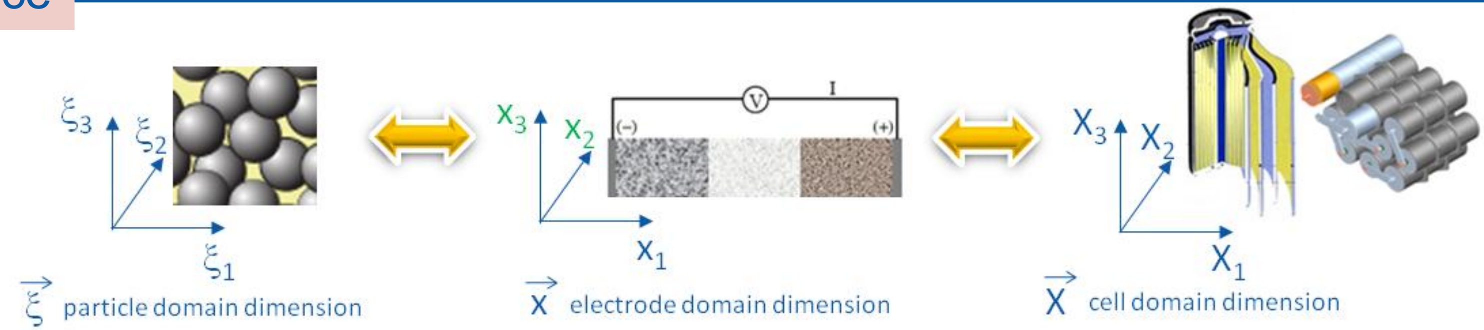
- Staff from NREL Contracts and Business Services, with input from three NREL technical monitors, initiated negotiations with the teams to arrive at the subcontracts based on Terms and Conditions dictated by the RFP and the DOE Prime Contract.

- As of the date of preparation of this presentation (3/21/2011), we have resolved all issues except for a few intellectual property (IP) concerns – NREL and the industry teams are determined to resolve the IP issues shortly.

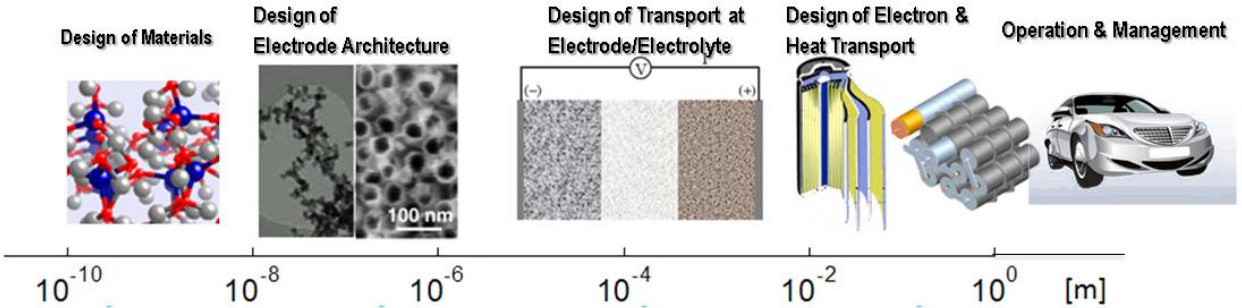
NREL Battery Modeling Under CAEBAT

NREL's Multi-Scale Multi-Dimensional Model

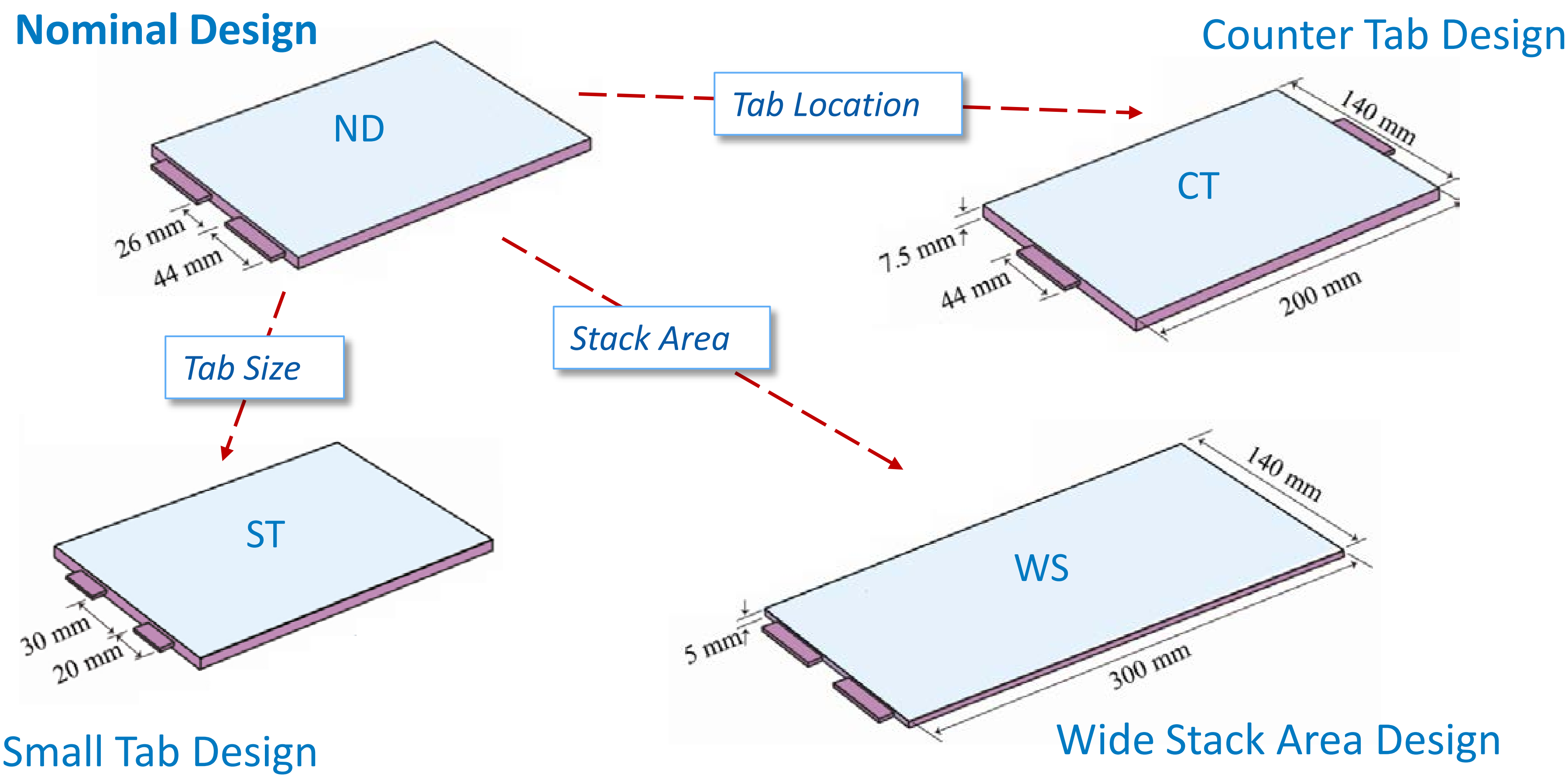
Relevance



- Introduces multiple computational domains for corresponding length scale physics
- Decouples geometries between submodel domains
- Couples physics in two ways using 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



We Selected These Cell Designs for Demonstrating MSMD Model Utility

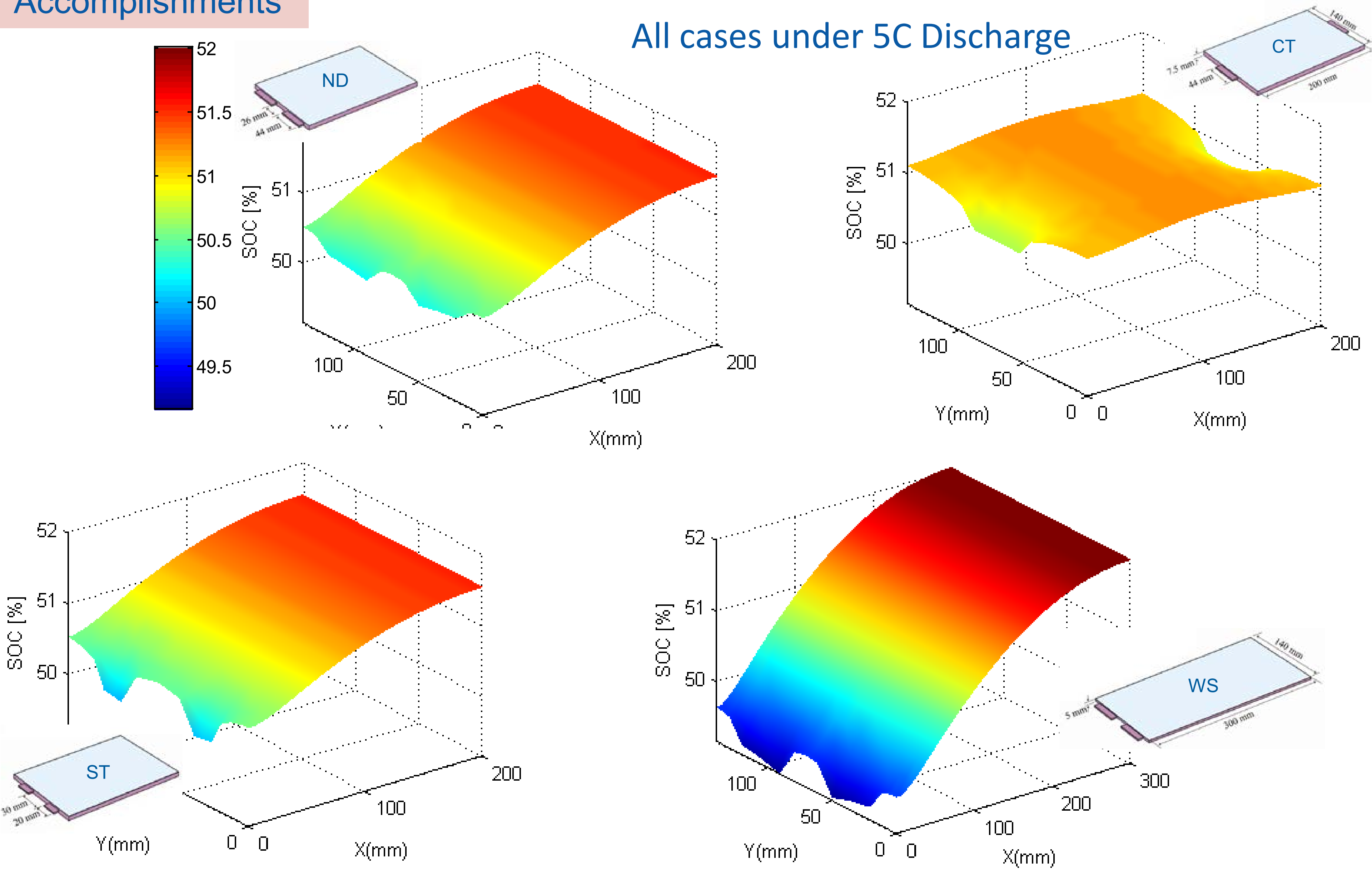


Case	Description	L_x [mm]	L_y [mm]	L_z [mm]	Tab width [mm]	Tab configuration
ND	Nominal design	200	140	7.5	44	Adjacent tabs
CT	Counter tab design	200	140	7.5	44	**Counter tabs**
ST	Small tab design	200	140	7.5	**20**	Adjacent tabs
WS	Wide stack-area design	**300**	140	5.0	44	Adjacent tabs

MSMD Model Shows Impact of Geometry and Tab Locations on Internal SOC Imbalance (Cell with wide stack area design is worst)

Accomplishments

All cases under 5C Discharge

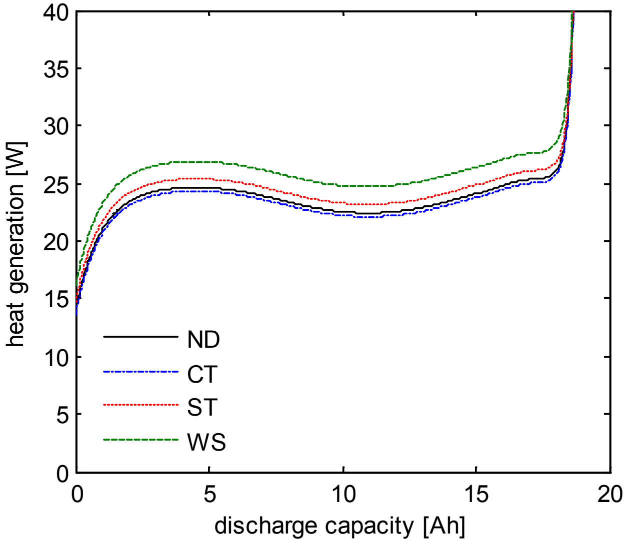


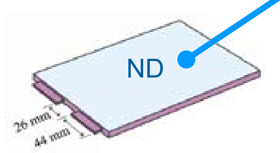
MSMD Model Shows Impact of Geometry and Tab Locations on Heat Generation and Temperature

Accomplishments

All cases under 5C Discharge

Total Heat Generation



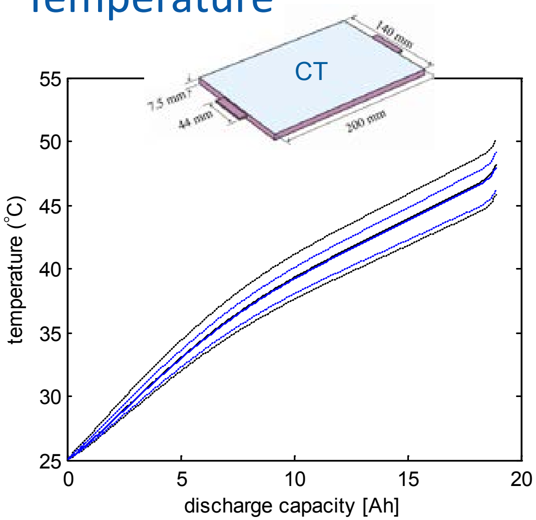


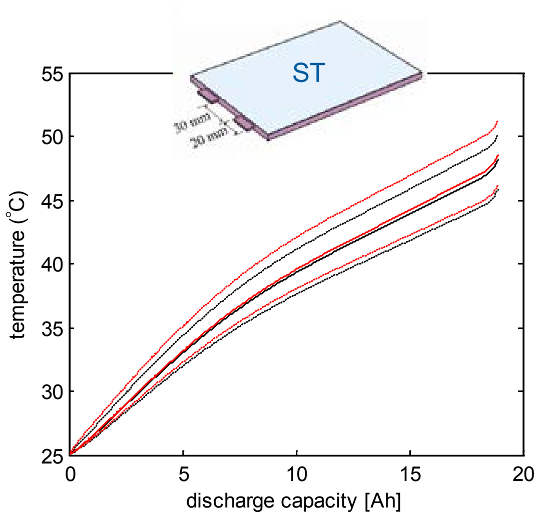
Single side cooling on top surface

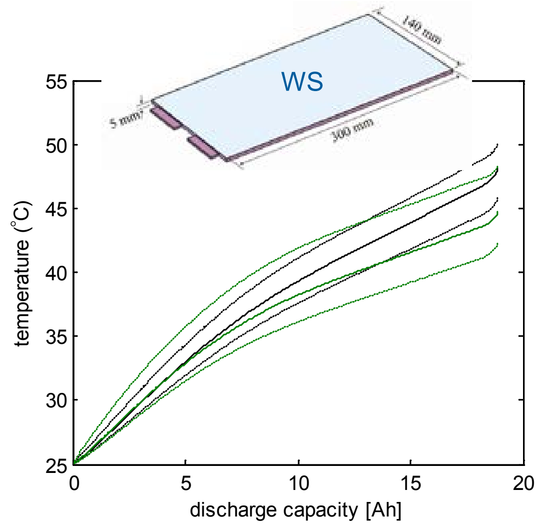
- ✓ With h = 25 W/m^{2}K
- ✓ At T_{amb}= 25°C

- Similar average temperatures: ND, CT, ST
- Smaller ΔT at CT
- Larger ΔT at ST
- Heat generation is highest with WS, but the average T at the End of Discharge (EOD) is lowest

Temperature







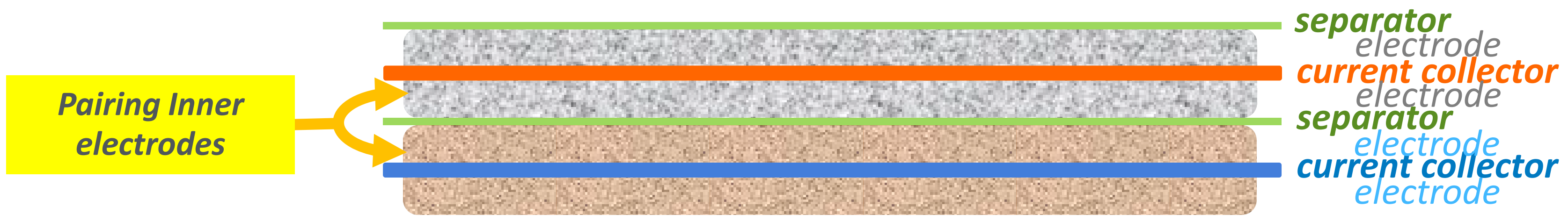
Developed Battery Model for Spirally Wound Cells

Accomplishments

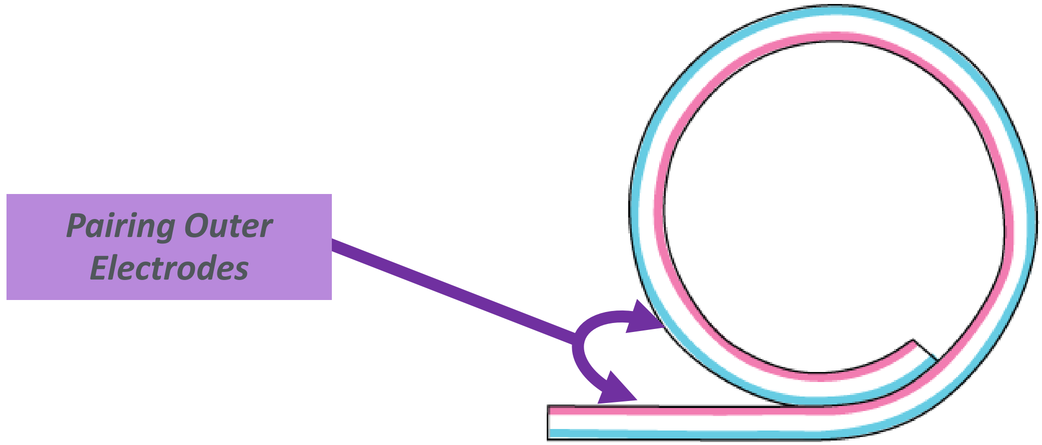
Spirally Wound Cell :

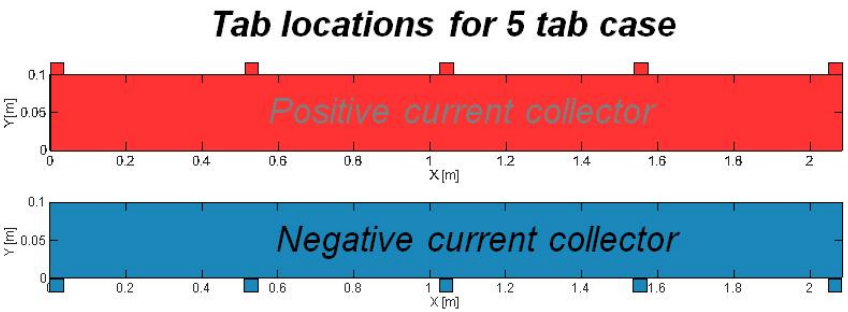
- *One pair of wide current collector foils*
- *Two pairs of wide electrode layers*
- *Complex electrical configuration*

***Stacking process:* Forming a pair between inner electrodes**



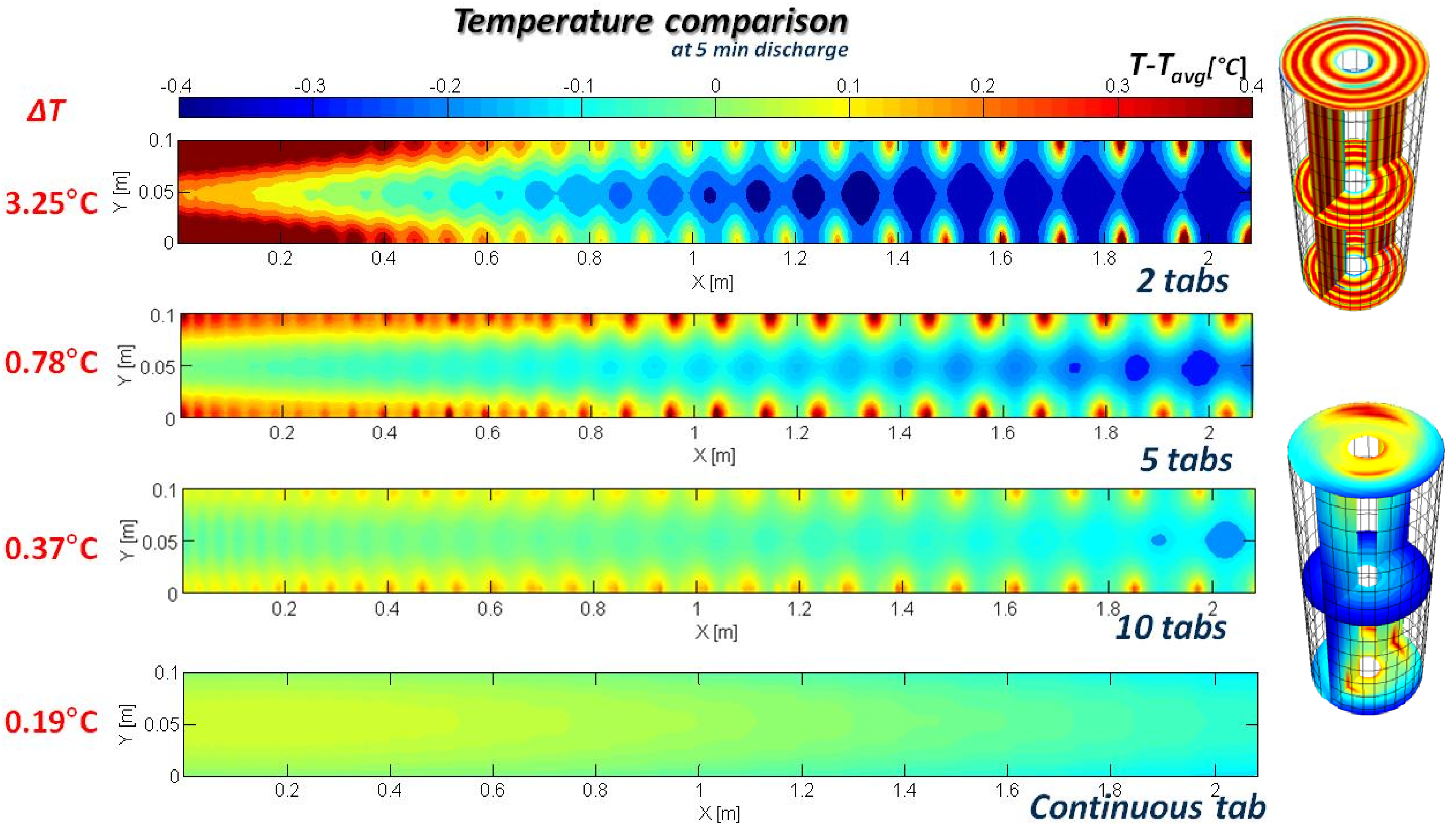
***Winding process:* Forming a second pair between outer electrodes**





The MSMD Model Showed the Larger the Number of Tabs the better the Thermal Performance

Accomplishments



Collaborations and Partnerships

- Collaborating with other national labs to add to the portfolio of capability for CAEBAT
  - ORNL (open architecture software)
  - LBNL (material and electrode models)
  - ANL (material, degradation and cost models)
  - SNL (material safety database and models)
  - INL (electrolyte and degradation models)
  - LLNL (safety modeling)
- Pending cost-shared subcontracts with three industry teams (in negotiations) to develop battery CAE design tools
- Colorado School of Mines – *integrated general chemistry solver for charge transfer and side reactions in Li-ion*

Publications and Presentations

Multi-Domain Modeling of Lithium-Ion Batteries Encompassing Multi-Physics in Varied Length Scales, Gi-Heon Kim, Kandler Smith, Kyu-Jin Lee, Shriram Santhanagopalan, and Ahmad Pesaran; submitted to *Journal of The Electrochemical Society*, March 2011.

Integrated Lithium-Ion Battery Model Encompassing Multi-Physics in Varied Scales, Gi-Heon Kim, Kandler Smith, Kyu-Jin Lee, Shriram Santhanagopalan, Ahmad Pesaran; presented at the 11th International Advanced Automotive Battery Conference, Pasadena, CA, January 24–28, 2011.

Accelerating Design of Batteries Using Computer-Aided Engineering Tools, Ahmad Pesaran, Gi-Heon Kim, Kandler Smith; presented at 25th Electric Vehicle Symposium, Shenzhen, China, November 5–9, 2010.

Prediction of Multi-physics Behaviors of Large Lithium-Ion Batteries During Internal and External Short Circuit, Gi-Heon Kim, Kyu-Jin Lee, Lawrence Chaney, Kandler Smith, Eric Darcy, Ahmad Pesaran; presented at Battery Safety 2010 in conjunction with 6th Lithium Mobile Power, Boston, MA, November 3, 2010.

3D Thermal and Electrochemical Model for Spirally Wound Large Format Lithium-ion Batteries, Kyu-Jin Lee, Gi-Heon Kim, Kandler Smith, presented at the 218th ECS Meeting, Las Vegas, NV, October 14, 2010.

Computer-Aided Engineering of Automotive Batteries, Ahmad Pesaran, Gi-Heon Kim, and Kandler Smith; presented at the AABC 2010 meeting, Orlando, FL, May 18–21, 2010.

Future Work: Battery CAE

- Finalize negotiations with the three industry teams to execute subcontracts per RFP terms
- Plan kick-off meetings with each CAEBAT-RFP project team to start work
- Finalize the CAEBAT project plan
- Interact with ORNL on the open architecture software
- Finalize roles of other national labs
- Integrate various models in one single platform for industry use
- Perform bottom-up model validation study
- Enhance physics of various models
- Incorporate enhanced solver capabilities and solution schemes
- Hold a conference on Computer-Aided Engineering and Modeling for Automotive Batteries

Summary: Computer-Aided Engineering for Batteries

- Computer-aided engineering (CAE) tools have been widely used by many industries to design products in a shorter amount of time and with lower cost.
- In April 2010, DOE initiated a new program activity (called CAEBAT) to incorporate existing and new battery models into software modeling suites/tools to shorten design cycle and optimize batteries (cells and packs) for improved thermal uniformity, safety, long life, low cost
- NREL was assigned to coordinate the program with other national labs.
- NREL issued a RFP ($7.5M for 3 years, plus cost share) and screened three industry teams for further negotiations – pending IP issues
- NREL has been enhancing and further developing its battery models to support CAEBAT program participants.

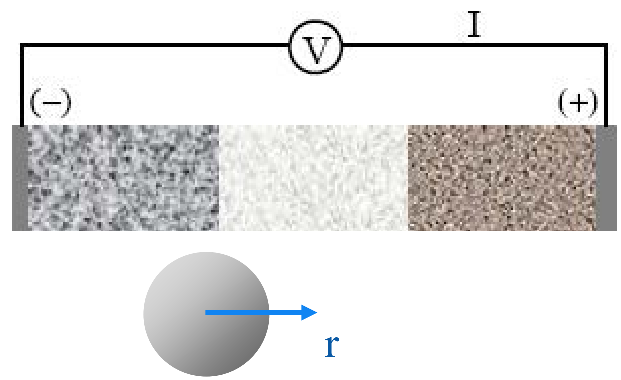
Technical Back-Up Slides

MSMD: Extending Beyond Porous Electrode Model

Charge Transfer Kinetics at Reaction Sites

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

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



Species Conservation

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

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

Charge Conservation

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

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

- Pioneered by Newman's group (*Doyle, Fuller, and Newman 1993*) – Dualfoil (cchem.berkeley.edu/jsngrp/fortran_files/Intro_Dualfoil5.pdf)
- Captures *lithium diffusion dynamics* and *charge transfer kinetics – porous media*
- Predicts *current/voltage response* of a battery
- Provides design guide for thermodynamics, kinetics, and transport across electrodes

> ➢ Difficult to resolve *heat* and *electron current* transport in large cell systems

Energy Conservation

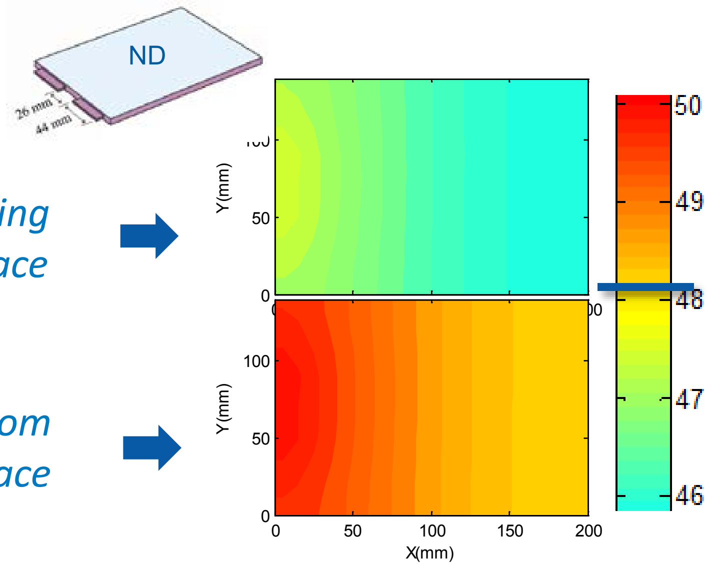
$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + q'''$$

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

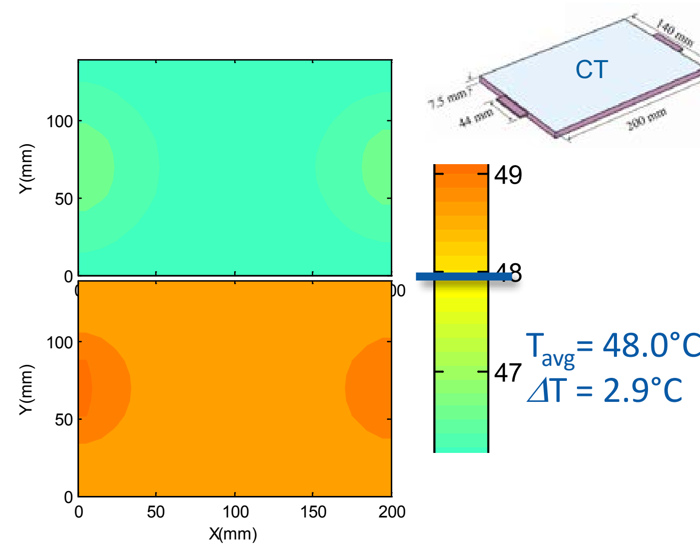
Temperature Imbalance at End of Discharge

Cooling Surface ➡

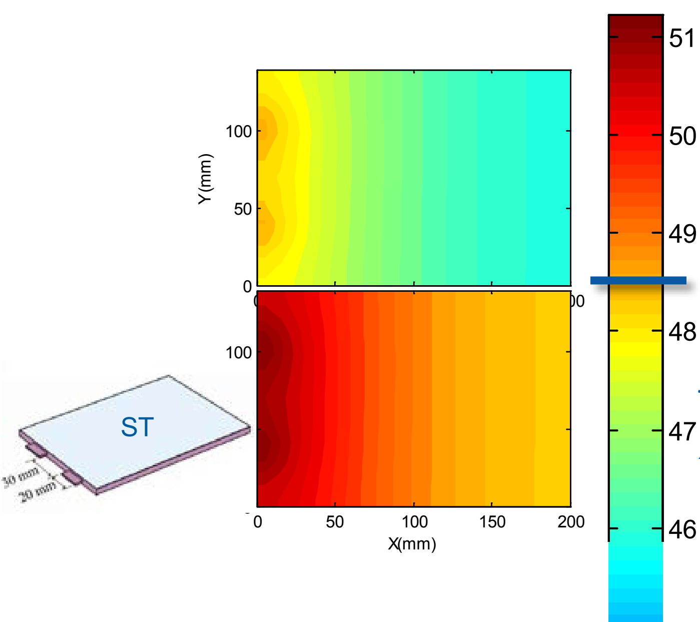
Bottom Surface ➡



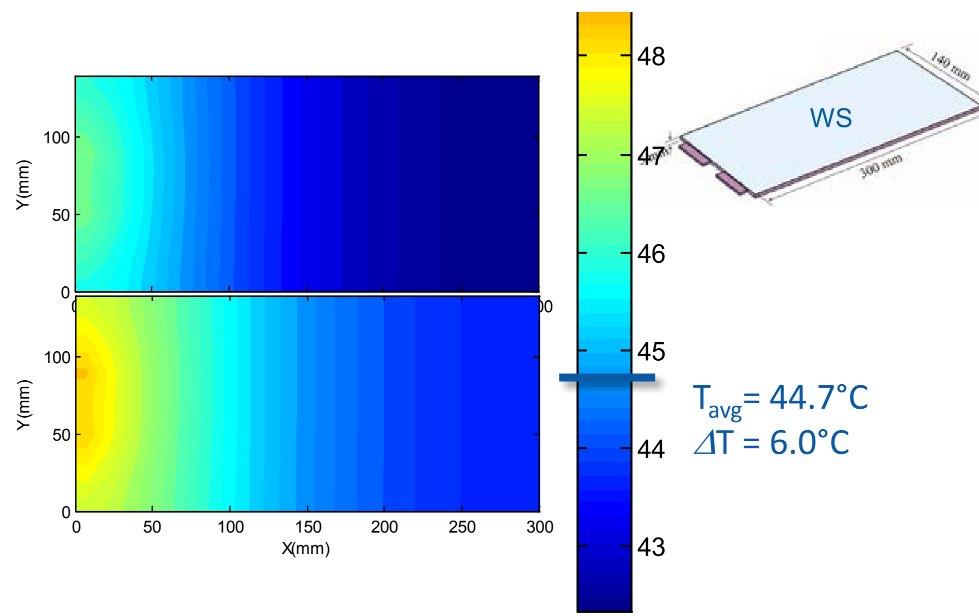
T_{avg}= 48.1°C
ΔT = 4.3°C



T_{avg}= 48.0°C
ΔT = 2.9°C



T_{avg}= 48.5°C
ΔT = 5.3°C



T_{avg}= 44.7°C
ΔT = 6.0°C

Number of Tabs Impact Performance