# Energy Storage R&D
# Thermal Management Studies and Modeling

**Ahmad A. Pesaran, Ph. D.**
**National Renewable Energy Laboratory**
**Golden, Colorado**

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This presentation does not contain any proprietary or confidential information.

# NREL Energy Storage Program

Our projects support the three major elements of the DOE's integrated Energy Storage Program to develop advanced energy storage systems for vehicle applications.

- Battery Development, Testing, Analysis
  1. Thermal characterization and analysis
  2. Energy storage simulation and analysis
- Applied Battery Research
  3. Li-Ion Thermal abuse reaction modeling

Will be discussed here in this presentation.

- Exploratory Battery Research
  4. High energy oxide anodes

Will be discussed by Anne Dillon on Wednesday afternoon.

# Outline

**To discuss in each section when applicable**

- Purpose of Work
- Barriers
- Approach
- Performance Measures
- Accomplishments
- Technology Transfer
- Publications
- Future Work/Plans
- Summary

- Thermal Characterization and Analysis
  - Measuring thermal properties
  - Thermal evaluation
  - Thermal analysis and modeling
  - Fabricating a new advanced calorimeter
- Energy Storage Simulation and Analysis
  - PHEV battery requirement analysis
  - HEV energy window analysis
  - PHEV battery tradeoff study
- Li-Ion Thermal Abuse Reaction Modeling
  - Cell modeling – simulating internal short
  - Cell-to-cell propagation in module
- IEA/HEV Implementing Agreement Support

# Purpose of Work

- **Purpose** (per Task 6 of the DOE's Vehicle Technologies R&D Plan)
  - Measure thermal properties of batteries/ultracapacitors.
  - Model the thermal performance of batteries and use computer-aided design tools to develop configurations with improved thermal performance.
  - Support USABC and FreedomCAR developers with thermal testing and modeling
- **Rationale**
  - Thermal control is critical to achieve the desired performance, life, and safety of energy storage system in vehicle application.
  - Thermal management system should keep cells with acceptable uniform distribution and within the desired range.

# Barriers

- The Vehicle Technologies Program has identified that major technical barriers to implementing energy storage (Li-Ion batteries) in advanced vehicles are
  - Life
  - Cost
  - Low-temperature Performance
  - Safety
- Temperature in actual use has significant impact on life, cost, performance, and safety of energy storage systems.
- Thermal management systems that do not add too much cost, impact volume, mass, and system complexity are needed.
- NREL is supporting developers to address the issues of thermal management by
  - Measuring thermal properties
  - Insight on thermal designs
  - Electro-thermal modeling and multi-physics analysis

# Approach

- Work with developers to obtain battery and ultracapacitor prototypes (cells, modules, packs) for thermal characterization and modeling.
- Use NREL unique calorimeter to provide information for thermal management system design
  - Measure heat generation of prototypes under different and realistic power/drive profiles
  - Measure heat capacity of prototypes
- Use infrared thermal imaging to identify hot spots and provide insight on thermal designs.
- Evaluate thermal performance of modules by thermal testing under realistic drive cycles and conditions.
- Use modeling tools such as electro-thermal and multi-physics analysis to identify designs that leads to better internal current and temperature distributions in cells and modules
- Fabricate a new calorimeter for testing large, liquid-cooled modules and packs.

# Thermal Characterization Approach

*Cells, Modules and Packs*

Tools:
- Calorimeter
- Thermal Imaging
- Electrical Cyclers
- Environmental Chambers
- Dynamometer
- Vehicle Simulation tools

Test Profiles:
- Normal operation
- Aggressive operation
- Driving cycles
  - US06
  - UDDS
  - HWY
- Discharge/charge rates
  - CC
  - FreedomCAR profiles

Measurements:
- Heat Capacity
- Heat Generation
- Efficiency
- Thermal Performance
  - Spatial temperature distribution
  - Cell-to-cell temp. imbalance
  - Cooling system effectiveness

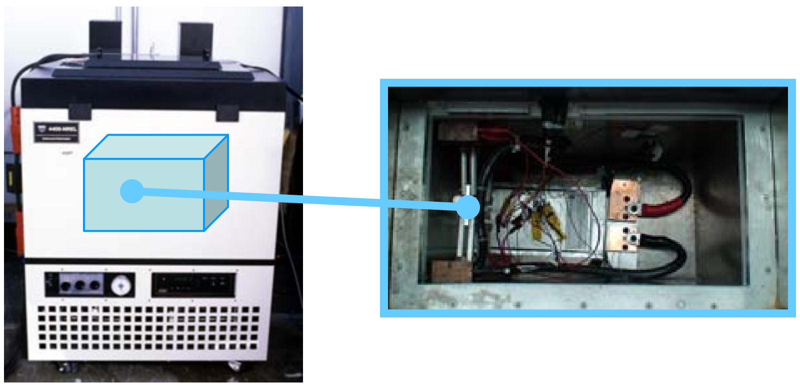
# Example Technical Accomplishments and Results

- Performance measures were collection thermal data on various batteries delivered by FreedomCAR developers
- Following are examples of testing, evaluation, and analysis in support of NREL FreedomCAR/USABC battery developers and other organizations
- Permissions were obtained to provide the infor[illegible]tion [illegible] developers
- Res[illegible]ep[illegible]E, USABC, and developers

# Thermal Characterization: CPI/LG Chem HEV Cells

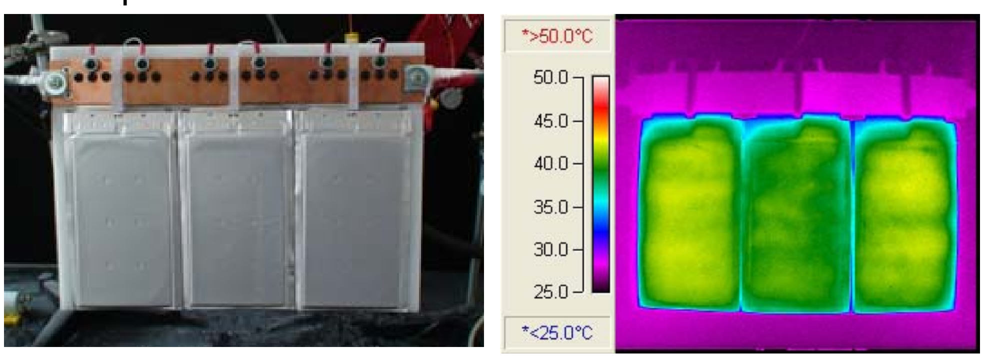
## Calorimetry

- Heat capacity & heat generation
- Temperatures: -30 to +45˚C
- Profiles: Driving cycles, full/partial discharge

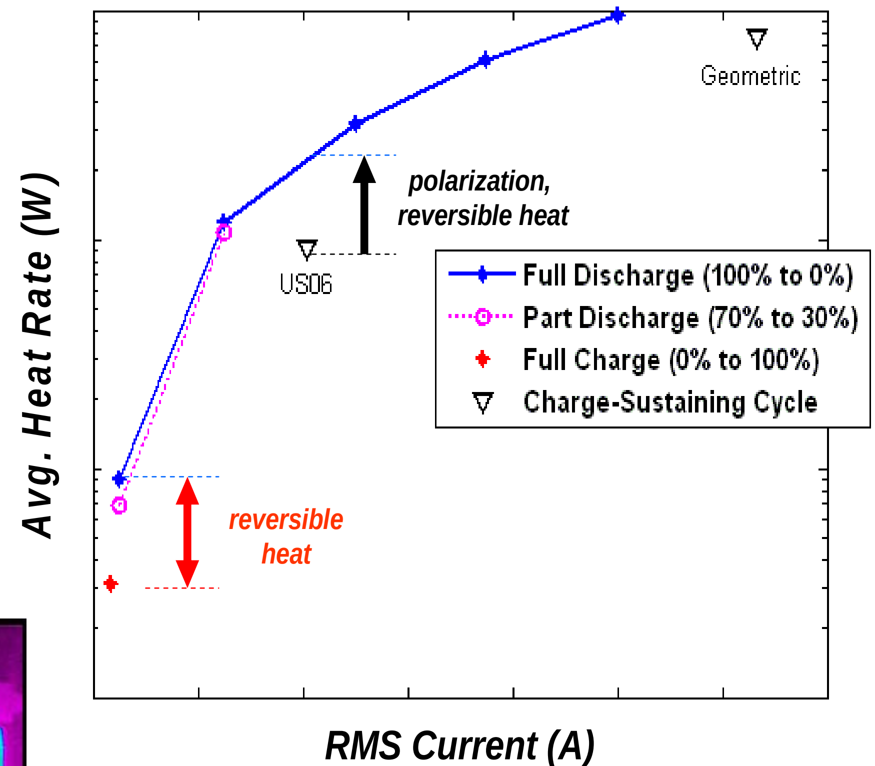


## Thermal Imaging at 20C Rate

- Temperature: Ambient




### *Example Heat Generation Data*

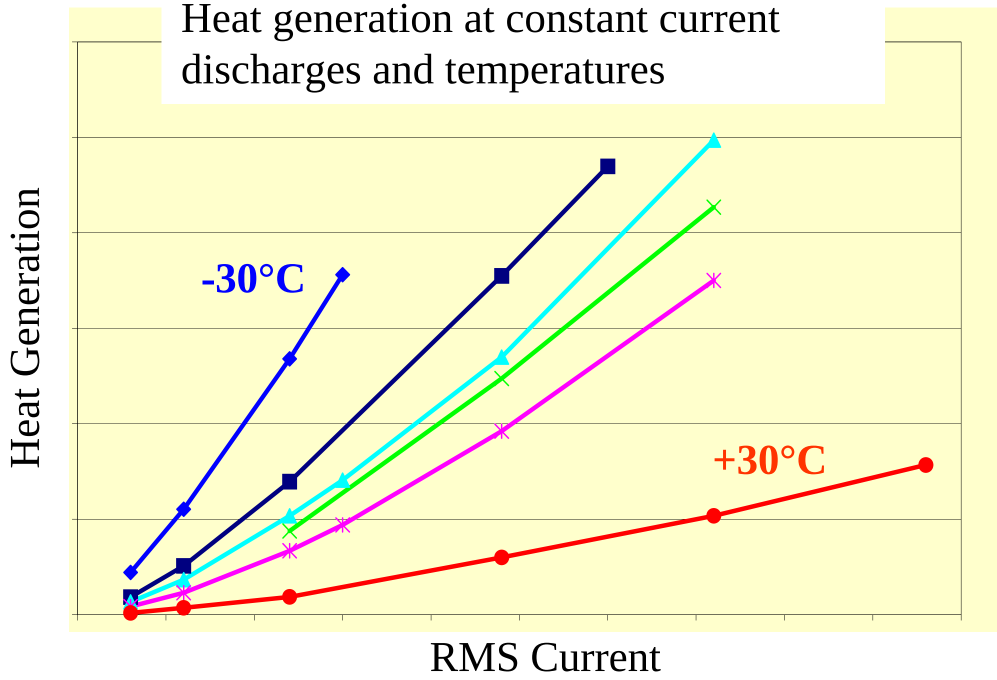



Efficiency (at 30°C and C/1) = 97.6%
Efficiency (at 30°C and US06) = 95.7%

# Thermal Characterization: Johnson Controls- Saft HEV Cells

## Calorimetry

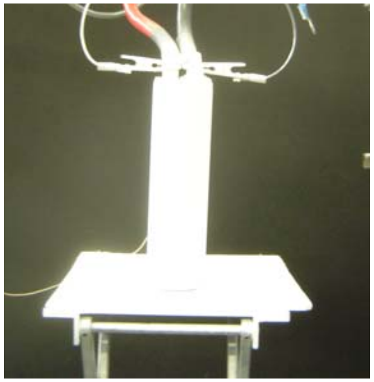
- Heat capacity & heat generation
- Temperatures: -30 to +30˚C
- Profiles: USABC 25 & 50 Whr cycles, CC discharge

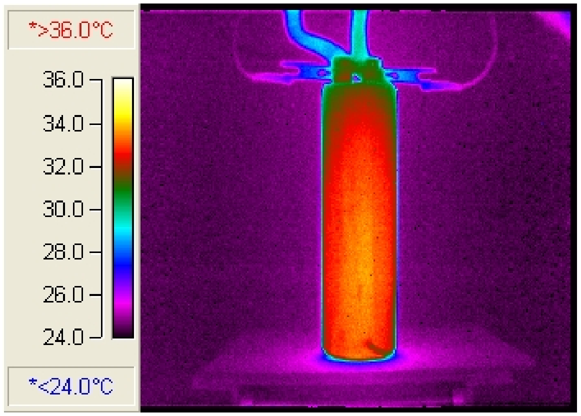



Efficiency (at 30°C and 5C) = 98%
Efficiency (at 30°C and 50 Wh Cycle) = 97%

## Thermal Imaging at 12C Rate

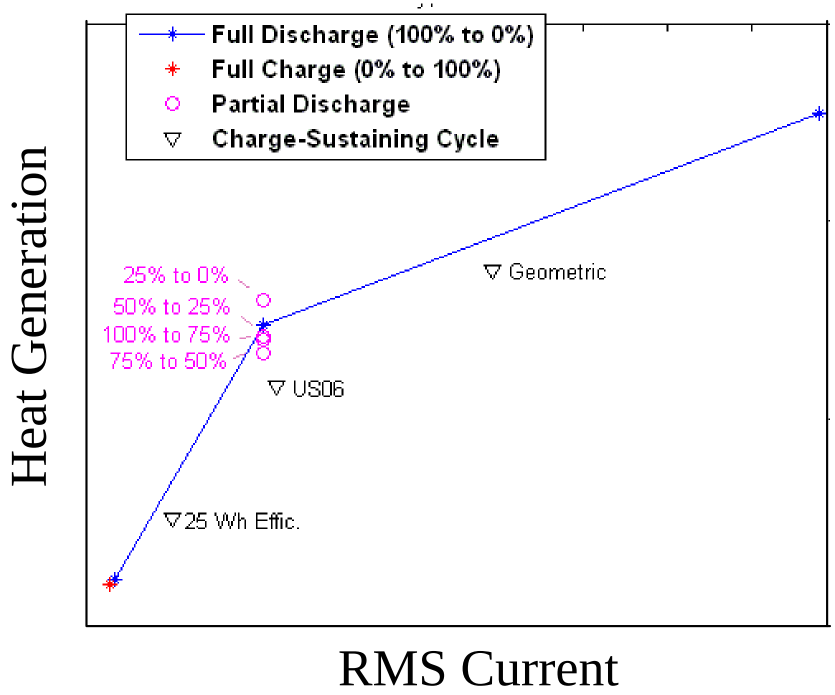
- Temperatures: Ambient
- Profiles: 100% SOC to 0% SOC

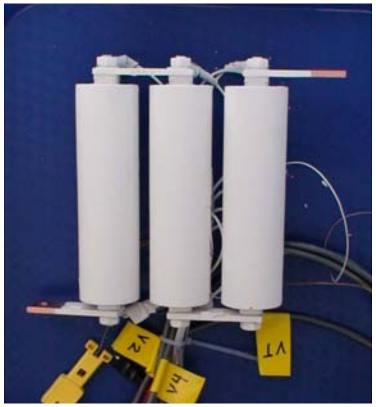


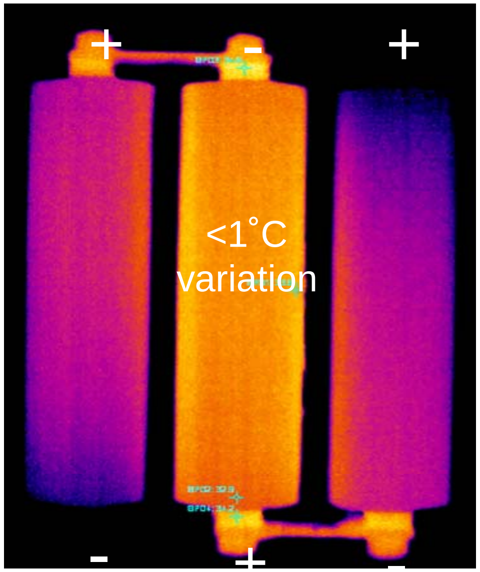


# Thermal Characterization: A123 Systems HEV Cells

- NREL and A123 Systems has signed a CRADA
  - Measuring battery heat generation
  - Thermal imaging of cells
  - Improving thermal design using modeling tools

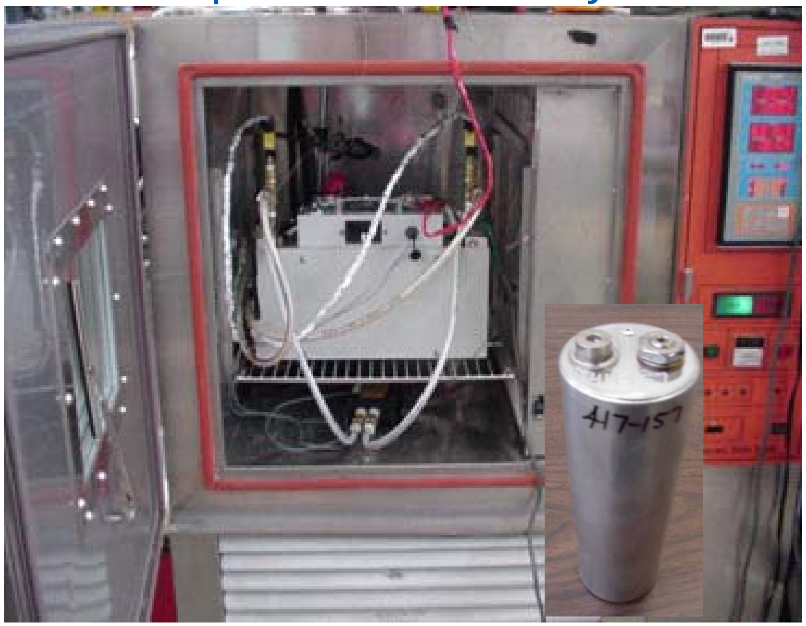


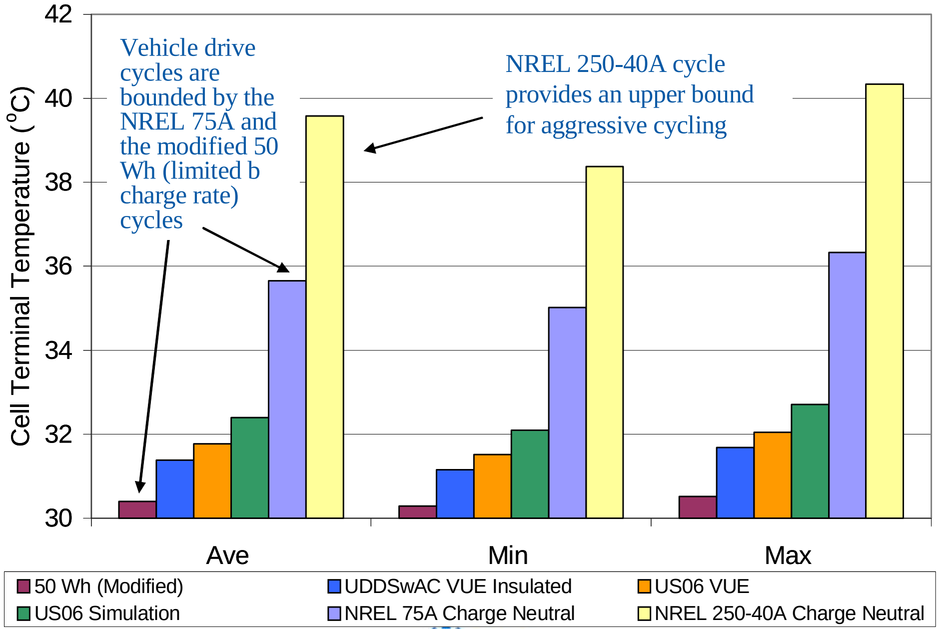





# Thermal Evaluation: Saft 42-V Liquid-Cooled Module

- Tested in environmental chamber with temperature controlled coolant
- Measured inlet, outlet and various cell temperatures at different power/drive cycles and ambient/liquid conditions
- Excellent thermal performance
  - $\Delta T_{terminal,ave}$ < 5°C for typical 42-V mild hybrid
  - $\Delta T_{terminal,ave}$ < 10°C for the most aggressive cell current limit tests
  - Temperature uniformity better than 2°C

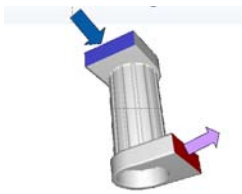


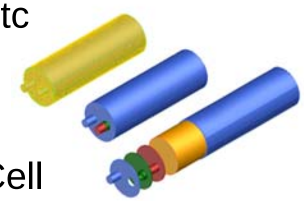



# Battery Thermal Modeling at NREL

## Cell Characteristics

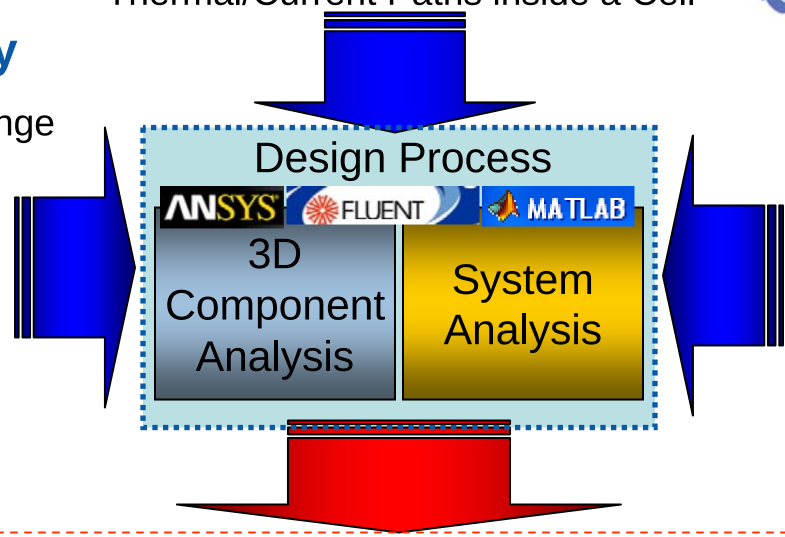
- Shape: Prismatic/Cylinder/Oval etc
- Materials
- Size/Dimensions/Capacity
- Thermal/Current Paths inside a Cell





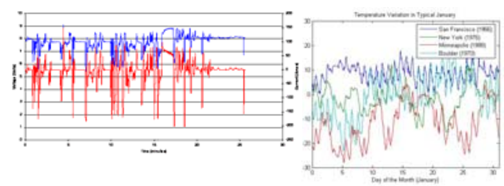
## Module Cooling Strategy

- Passive control with phase change
- Coolant type: Air/Liquid
- Direct Contact/Jacket Cooling
- Serial/Parallel Cooling
- Terminal/Side Cooling
- Module Shape/Dimensions
- Coolant Path inside a Module
- Coolant Flow Rate



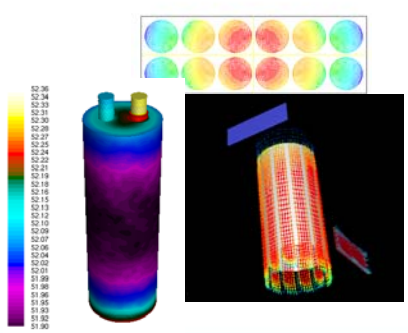

## Operating Conditions

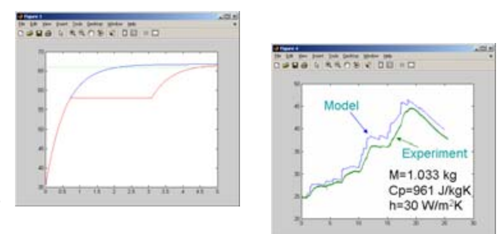
- Vehicle Driving Cycles
- Control Strategy
- Ambient Temperature
- etc



## Battery Thermal Responses

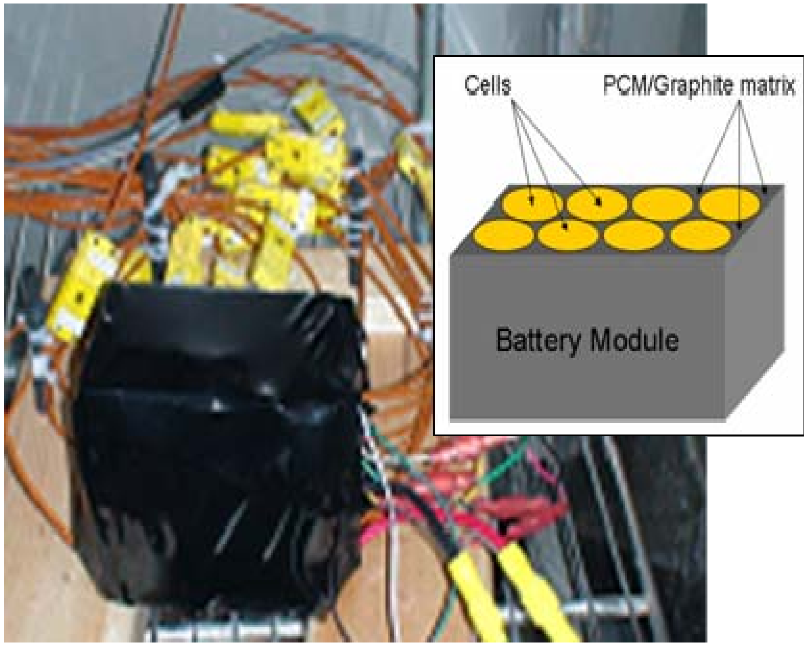
- Temperature History Cells/Module/Pack
- Temperature Distribution in a Cell
- Cell-to-Cell Temperature Imbalance in a Module
- Battery Performance Prediction
- etc



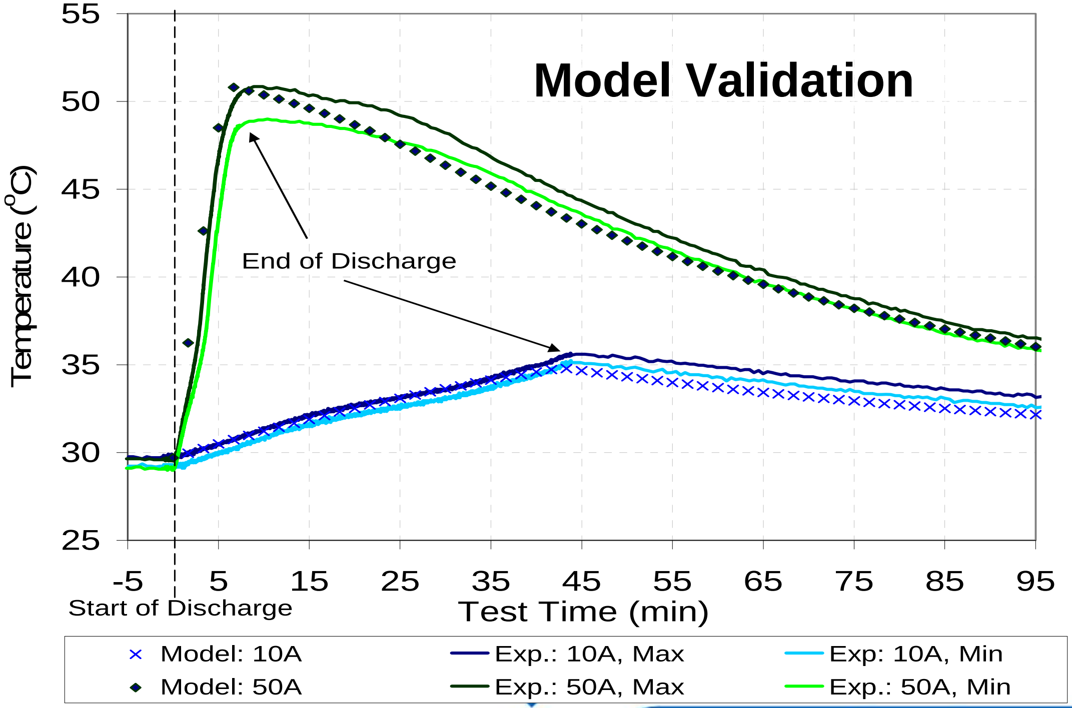


# Phase-Change Material (PCM) for Battery Thermal Management in HEVs & PHEVs

- Developed a system-level and a component-level model for evaluating PCM for thermal management
- Tested a prototype module provided by AllCell® Technologies
  - Module contained an array of 18650 Li-Ion cells surrounded by a graphite matrix impregnated with the "wax" (PCM)
- Validated and used models to compare management techniques

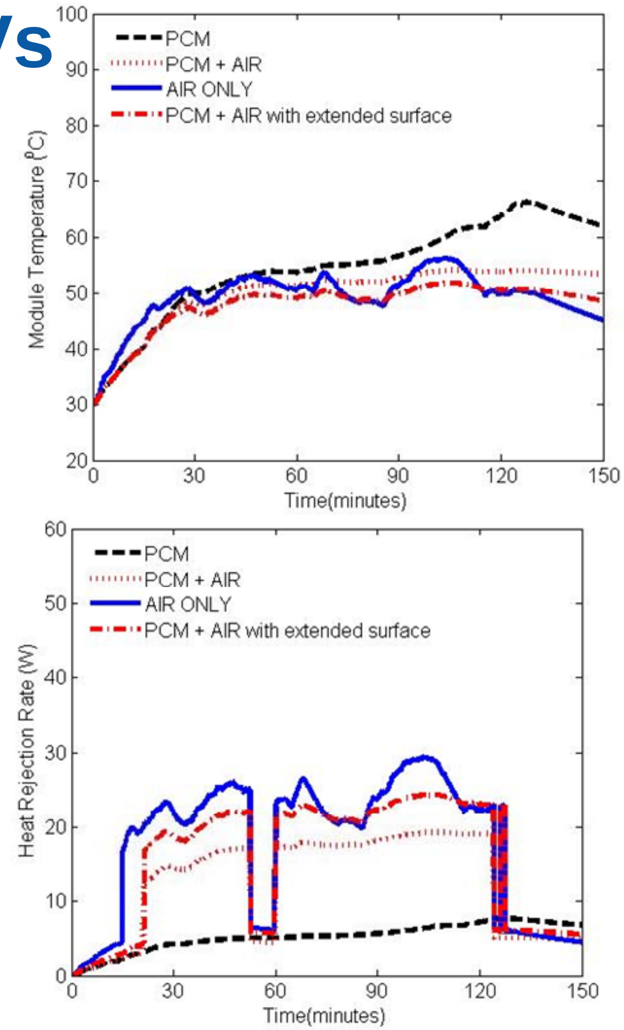



Prototype Module



# Study of PCM for Battery Thermal Management in HEVs & PHEVs

- **Results**
  - The PCM/graphite matrix effectively limits cell peak temperatures during short intense battery use
  - PCM by itself is not a cooling method and a cooling system must still be designed to handle the highest continuous demand
  - Reduced concern over peak intermittent thermal loads provides design flexibility (e.g., use of a smaller cooling system)
  - Multidimensional modeling indicated that the highly conductive matrix could improve temperature uniformity and limit thermal runaway

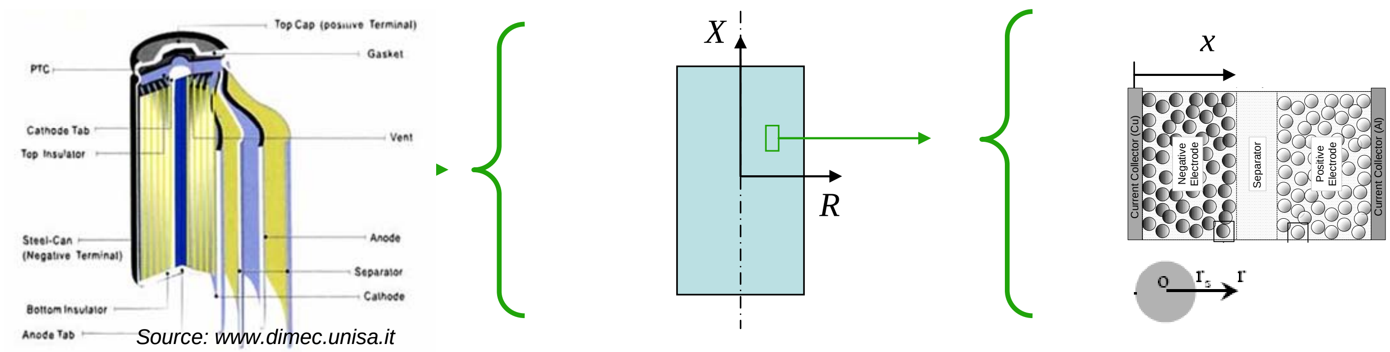



**Comparing Cooling Techniques**

# Developing a 3D Lithium-Ion Battery Performance Model

- For PHEV applications, large cells preferred to small cells:
  - fewer electrical connections, less balancing circuitry, *however…*
  - internal temperature gradients degrade life and performance.

**Detailed Structure** ≈ **Axisymmetric Thermal Model** + **Electrochemical Submodel**




*G. Kim, K. Smith, "Multi-Dimensional Electrochemical-Thermal Coupled Model of Large Format Cylindrical Lithium Ion Cells," Proceedings of 212th Electrochem. Soc. Mtg. Washington D.C., Oct. 7-12, 2007.*

*Model quantifies temperature imbalance, explores thermal-chemical-structural interactions under normal and abusive conditions.*

# Initial Results from the 3D Lithium-Ion Battery Performance Model

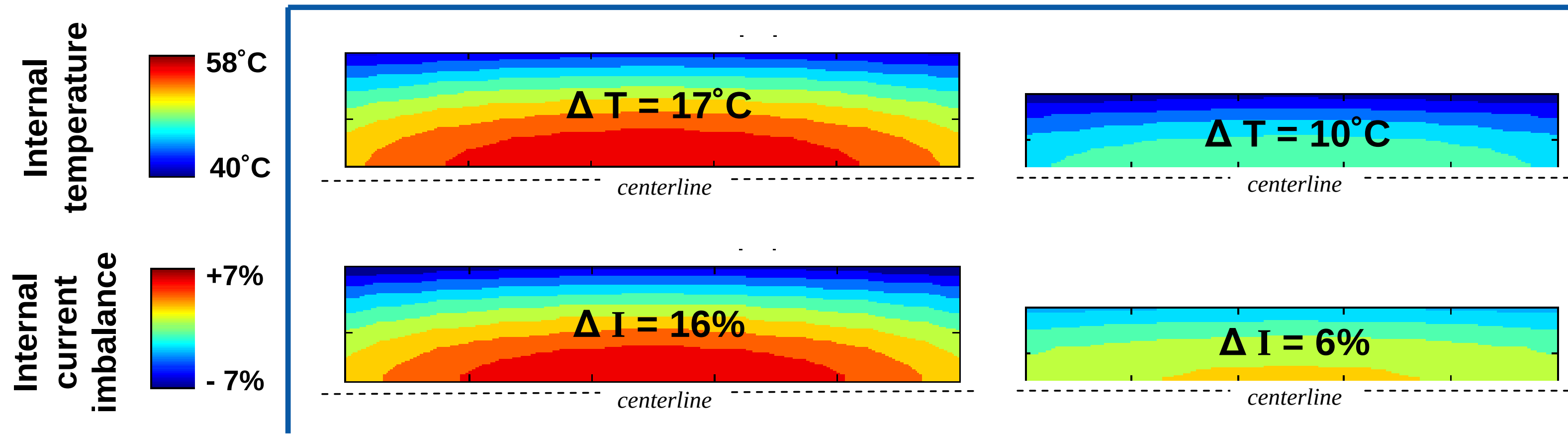
*Model quantifies internal temperature and current imbalance.*

*(Dependent on power profile, cooling method, cell size.)*

*200 A geometric cycle with liquid cooling.*

**40 Ah cell**
(baseline case)

**20 Ah cell**
(two cells in parallel equals 40 Ah)

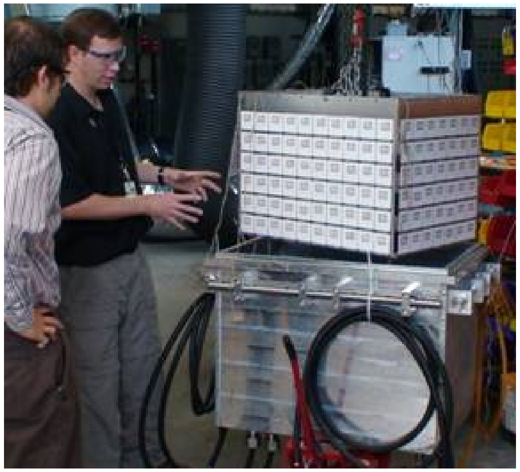



**FY08** →

- Include internal current paths
- Quantify heating under abuse conditions

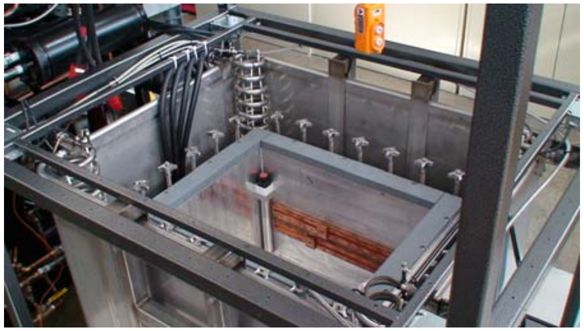
# Fabricating a Unique Calorimeter for Large, Liquid-Cooled HEV and PHEV Modules

- Designed based on lesson learned from existing calorimeter
- To evaluate thermal performance of batteries under real driving profiles
  - Operating T: - 40°C to +100°C
  - Bath T sensitivity: 0.005°C
  - Heat sensitivity: 10-20 mw
  - Heat Rate: 100 mW to 1000 W
  - Accuracy of ± 3%.
- More than 3000 parts from 200 suppliers
- Single-ended conduction calorimeter
  - Test chamber
    - Cavity for holding batteries
    - 206 Flux gauges to measure heat
  - Isotherm bath **submerging** test chamber
  - External shell
- Heating and cooling systems for isothermal bath and liquid-cooled loop



Flux Gauges of Test Chamber

Test Chamber



Test Chamber in Isothermal Bath Container

# Unique Large Calorimeter for Evaluating Liquid-Cooled Prototypes

| Specifications | Existing Calorimeter | Large Calorimeter |
|---|---|---|
| Maximum Voltage (Volts) | 500 | 600 |
| Sustained Maximum Current (Amps) | 250 | 600 |
| Excursion Currents (Amps) | 300 | 1000 |
| Battery Weight (kg) | 23 | 200 |
| Volume (liters) | 14.7 | 96 |
| Maximum Dimensions (cm) | 35 x 21 x 20 | 60 X 40 X 40 |
| Operating Temperature (°C) | -30 to 60 | -40 to 100 |
| Accuracy at minimum Heat (%) | 2% | 3% |
| Maximum Constant Heat Generation (Watts) | 150 | 1000 |
| Minimum Detectable Heat Effect (Joules) | 15 | 150 |
| Baseline Stability (mW) | 10 | 10-20 |

- Fabrication to be completed in March 2008
- Routine data collection starts in May 2008
- Could be used for other automotive components such as APE, motors, etc.

Existing calorimeter between an ABC-150 Cycler & a computer

New large calorimeter with heating and cooling system

# Future Work

- Continue working with HEV and PHEV battery developers on thermal characterization and analysis of batteries
  - EnerDel
  - A123 Systems
  - CPI/LG Chem
  - Johnson Controls Saft
  - Others
- Support battery developers with thermal management of batteries
- Develop and refine the electro-thermal model with other multi-physics analysis tools.

# Publications and Presentations

- G.-H. Kim and A. Pesaran. “Battery Thermal Management Design Modeling.” World Electric Vehicle Association (WEVA) Journal, Vol. 1, pp. 126-133, 2007.
- M. Keyser, J. Lustbader, K. Smith, G.-H. Kim, and J. Gonder, “*Thermal Characterization, Evaluation, and Analysis of Lithium-Ion Cells and Modules,*” *M*ilestone Report, NREL, Golden, Colorado, August 2007.
- G.-H. Kim, J. Gonder, J. Lustbader and A. Pesaran “Evaluation of HEV Battery Thermal Management with Phase-Change Materials,” paper to be presented at the 23rd Electric Vehicle Symposium, Anaheim, CA, December 2007.
- G.-H. Kim, K. Smith, “Multi-Dimensional Electrochemical-Thermal Coupled Model of Large Format Cylindrical Lithium Ion Cells,” Proceedings of 212th Electrochemical Society Meeting, Washington D.C., Oct. 7-12, 2007.
- A. Pesaran, et. al, “FY 2007 Energy Storage Program Report,” Annual Report, NREL/TP-540-42716, National Renewable Energy Laboratory, November 2007.
- Multiple presentations to FreedomCAR battery developers and USABC with “Battery Protected Information.”

# Purpose of Work

- **Purpose** (per Task 6 of the DOE's Vehicle Technologies R&D Plan)
  - Work with battery developers and USABC to improve and validate energy storage models for system simulations, for use in optimization studies and target analyses for different platforms and vehicle types.
  - Support USABC and FreedomCAR Energy Storage Tech Team to identify targets for PHEV batteries
- **Rationale**
  - Energy storage simulation and analysis is important for identifying requirements and tradeoff among performance, life, and cost.

# Approach

- Collaborate with USABC and FreedomCAR Teach Team members to identify assumptions and exchange information
- Develop energy storage models (Excel or Matlab) based on data
- Perform vehicle simulations using PSAT or other analysis tools
- Three activities performed in the last 15 months
  - PHEV battery requirement analysis
  - HEV energy window simulation
  - PHEV battery tradeoff analysis

# Development of PHEV Battery Requirements

- Worked with PHEV Battery Workgroup
  - Objective
    - Collaboratively develop and identify requirements for batteries for PHEVs based on analysis and vehicle simulation results
  - Purpose
    - Provides targets to for battery developers when developing PHEV batteries

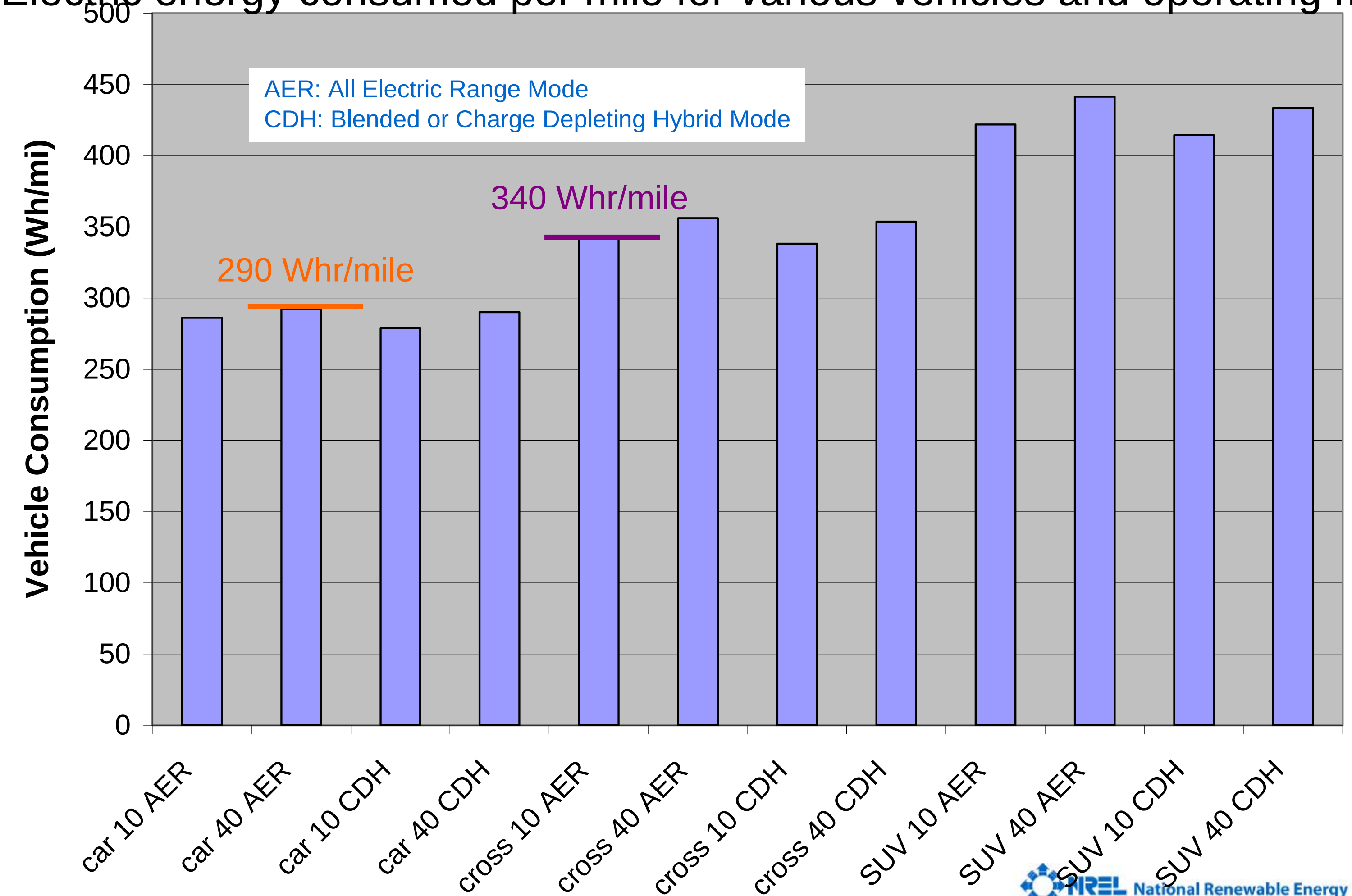
# PHEV Battery Requirement
## Analysis for Power and Energy

- Process included defining
  - vehicle platforms (mass, aerodynamic, and rolling resistance)
  - vehicle performance targets (acceleration, top speed, grade)
  - the desired equivalent electric range
  - the operating strategy (all-electric and blended)
  - the usable SOC window.
- The analysis and simulations provided
  - electric vehicle consumption (Wh/mile)
  - peak power requirements for a particular drive cycle
  - peak power requirements during charge-sustaining operation.

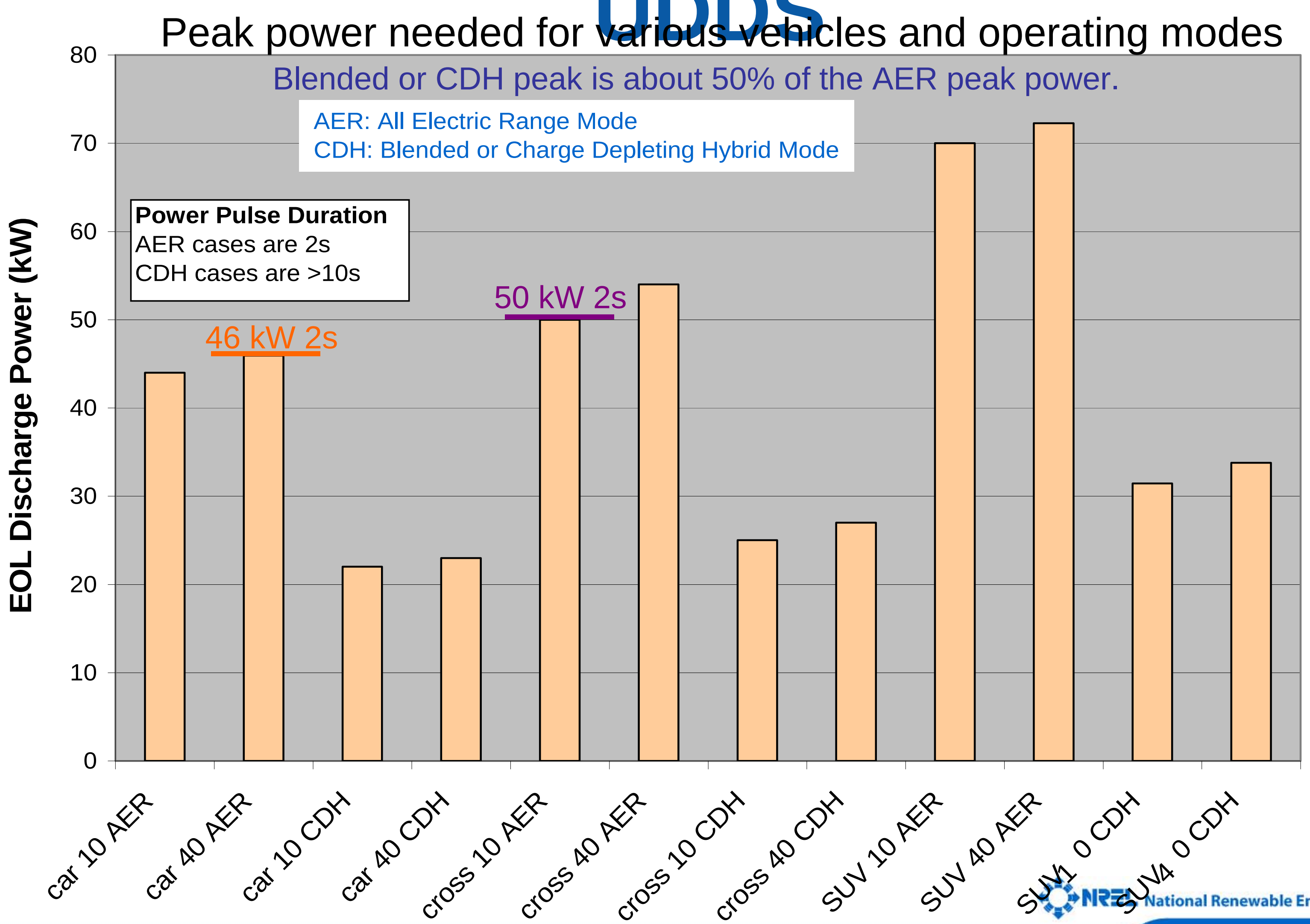
# PHEV Battery Requirement

## Analysis Results for Energy - UDDS

Electric energy consumed per mile for various vehicles and operating modes



# PHEV Battery Requirement Analysis Results for Power - UDDS



# PHEV Battery Requirement

## Bases for Selection of Battery Requirements

- The battery requirements were recommended based on two sets of electric range and time-frame
  - A 10-mile all-electric-range (over UDDS) for a crossover vehicle in the mid-term (2012)
    - Supporting potential early market experience

    **High Power to Energy Ratio (P/E) Battery**
  - A 40-mile all-electric-range (over UDDS) for a midsize car in the long-term (2015-2016)
    - Supporting President's Initiative

    **High Energy to Power Ratio (E/P) Battery**

# Final PHEV Battery Targets

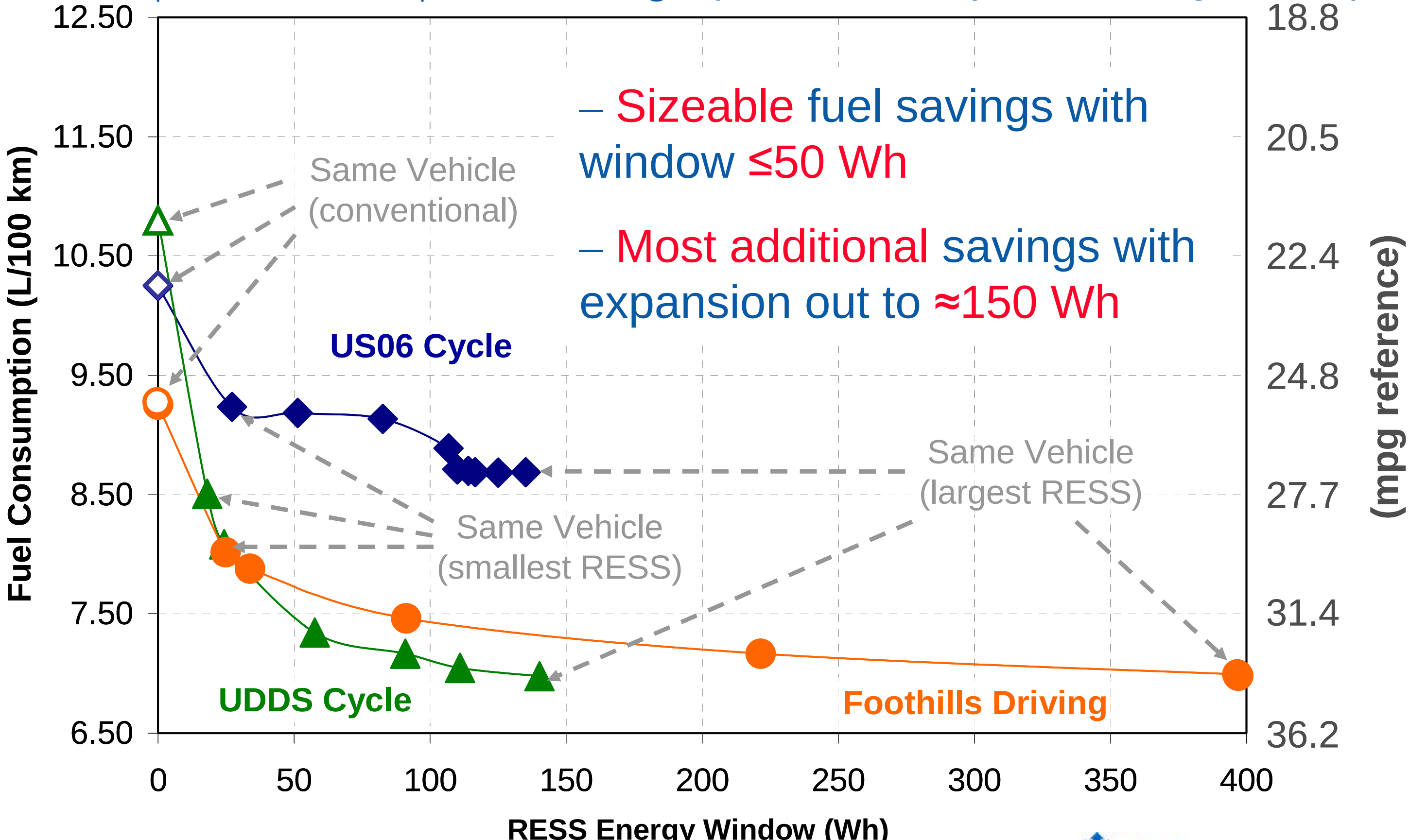
Requirements of End of Life Energy Storage Systems for PHEVs

| Characteristics at EOL (End of Life) | | High Power/Energy Ratio Battery | High Energy/Power Ratio Battery |
|---|---|---|---|
| Reference Equivalent Electric Range | miles | **10** | **40** |
| Peak Pulse Discharge Power - 2 Sec / 10 Sec | kW | **50 / 45** | **46 / 38** |
| Peak Regen Pulse Power (10 sec) | kW | **30** | **25** |
| Available Energy for CD (Charge Depleting) Mode, 10 kW Rate | kWh | **3.4** | **11.6** |
| Available Energy for CS (Charge Sustaining) Mode | kWh | **0.5** | **0.3** |
| Minimum Round-trip Energy Efficiency (USABC HEV Cycle) | % | **90** | **90** |
| Cold cranking power at -30°C, 2 sec - 3 Pulses | kW | **7** | **7** |
| CD Life / Discharge Throughput | Cycles/MWh | **5,000 / 17** | **5,000 / 58** |
| CS HEV Cycle Life, 50 Wh Profile | Cycles | **300,000** | **300,000** |
| Calendar Life, 35°C | year | **15** | **15** |
| Maximum System Weight | kg | **60** | **120** |
| Maximum System Volume | Liter | **40** | **80** |
| Maximum Operating Voltage | Vdc | **400** | **400** |
| Minimum Operating Voltage | Vdc | **>0.55 x Vmax** | **>0.55 x Vmax** |
| Maximum Self-discharge | Wh/day | **50** | **50** |
| System Recharge Rate at 30°C | kW | **1.4 (120V/15A)** | **1.4 (120V/15A)** |
| Unassisted Operating & Charging Temperature Range | °C | **-30 to +52** | **-30 to +52** |
| Survival Temperature Range | °C | **-46 to +66** | **-46 to +66** |
| Maximum System Production Price @ 100k units/yr | $ | **$1,700** | **$3,400** |

http://www.uscar.org/commands/files_download.php?files_id=118

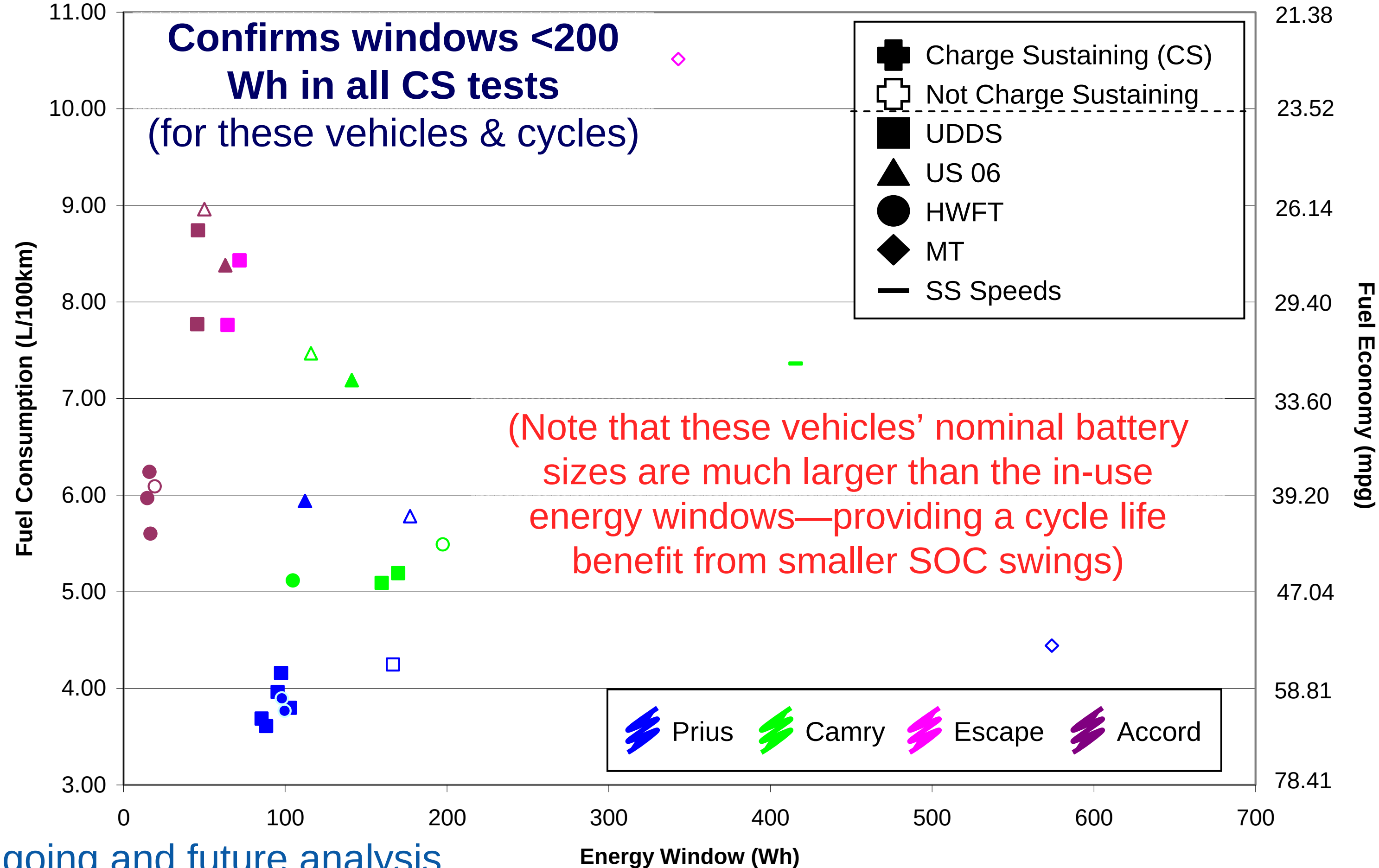
# Impact of Energy Window Size on the Fuel Economy of Power-Assist HEVs

- – Simulate HEVs with a range of RESS* capacities over multiple drive cycles
- – Observe window (max - min energy state) and fuel savings for each cycle
- – Confirm insensitivity of results to control parameter and DOH** variation
- For all cases, ↑ window → ↑ fuel savings (with eventually diminishing returns)




*RESS = Rechargeable Energy Storage System; **DOH = Degree of Hybridization

# Analysis of Energy Window in Commercial Hybrids



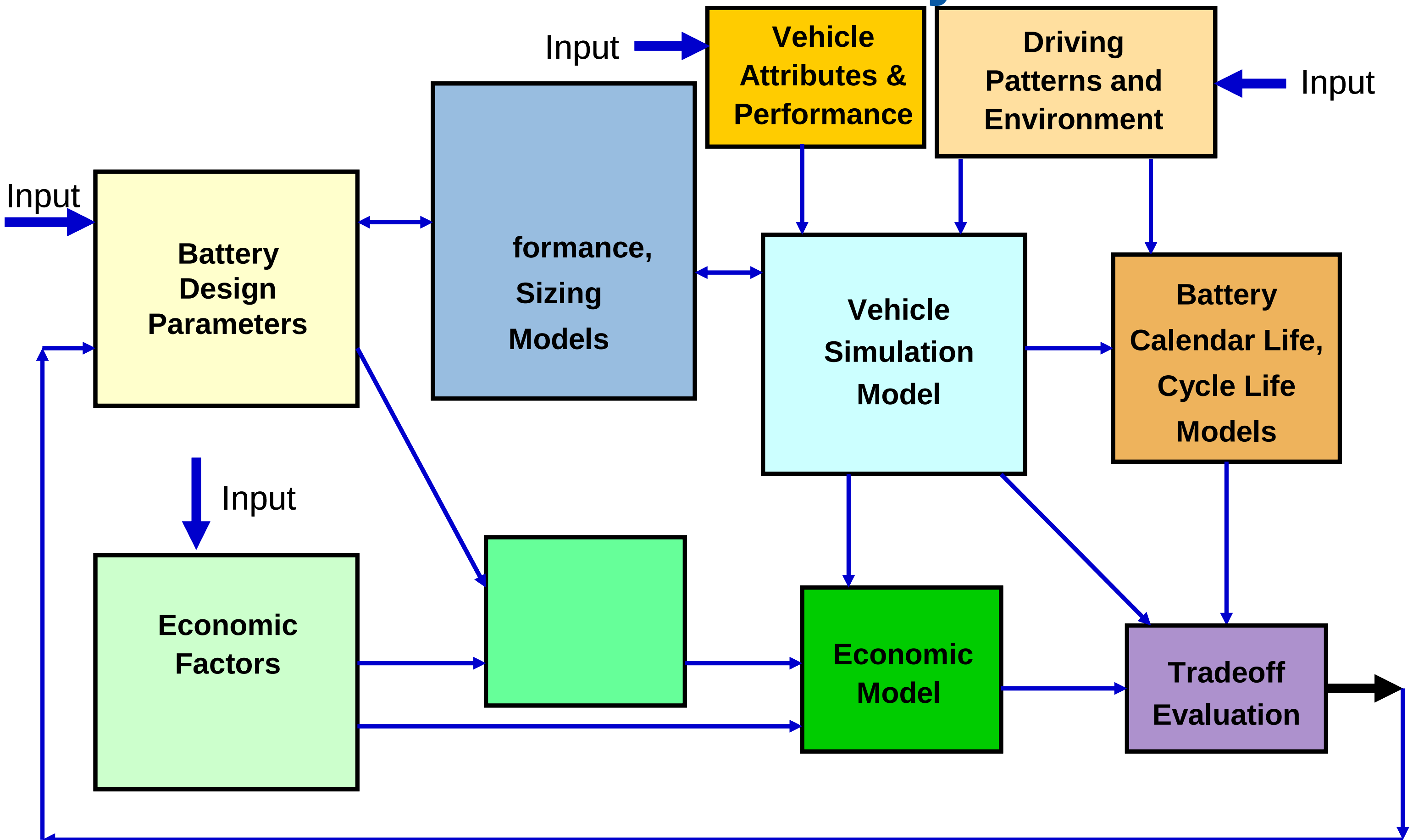

- Ongoing and future analysis
  - Required battery over-sizing to achieve desired cycle life reduces smaller window $$ benefit (often greater cycling in small windows; & $/kW dominates)
  - Consider ultracapacitors for small in-use energy window designs ($/kW less of a cost driver and lower required size margin for achieving cycle life)

# PHEV Battery Tradeoff Study
## Objectives

- Develop fast-running fundamental battery modeling tools which may be implemented for all varieties of Li-ion chemistries and power/energy designs.
- Validate the battery performance (1-D electrochemical) models against Saft VL41M PHEV battery data.
- Propose battery cost and life models.
- Link the battery performance, cost and life models to vehicle simulation tools.
- Outline a parametric study to identify an “optimal” PHEV battery design from USABC requirements.
- Outline a study to simulate the “optimal” vehicle/battery’s performance and life under a variety of scenarios.

# PHEV Battery Tradeoff Study

## Linking Battery Models to Vehicle Simulations for Tradeoff Analysis



# PHEV Battery Tradeoff Study

## Approach

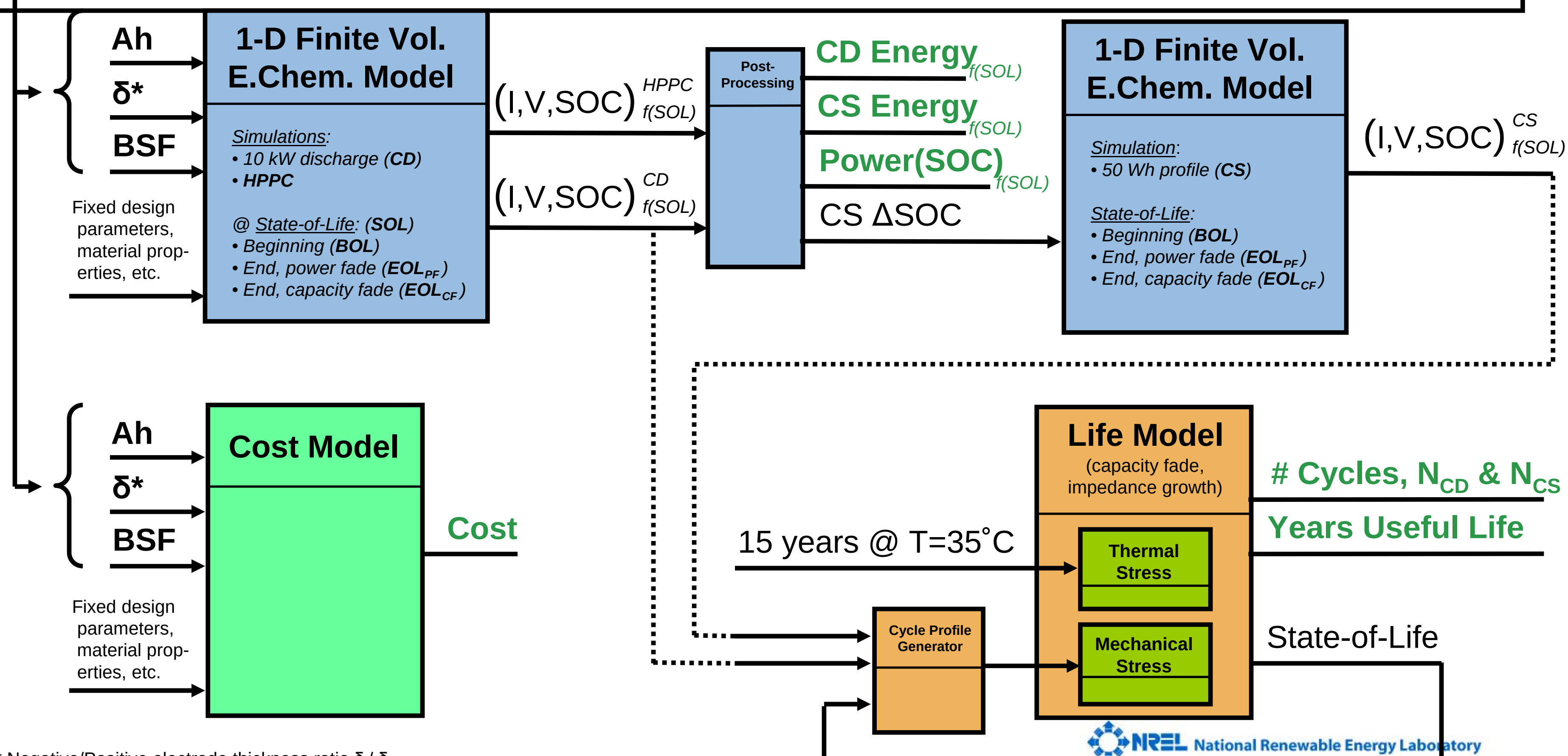
- By using physics-based models we hope to:
  - improve understanding of battery design/performance/life tradeoffs
  - develop capability to predict battery life under any usage scenario
  - reduce the number of iterations in the prototype battery design & testing process
  - reduce the experimental burden of battery technology life verification
- Use credible cost models developed by others
- Use vehicle simulation tools
- Run optimization routine to come up with designs that have best combination of performance, life and cost

# PHEV Battery Tradeoff Study

## Battery Optimization Study

***Parametric study** (capacity, electrode thickness, BSF) to explore tradeoffs in **performance, life and cost** of various PHEV battery designs relative to USABC requirements.*

(Individual elements of this flowchart are explained on subsequent slides.)

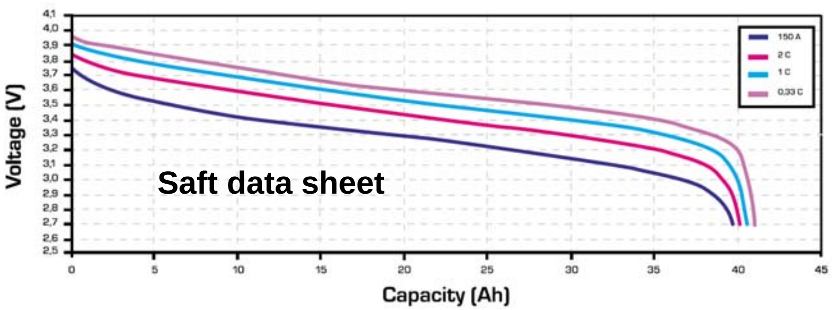


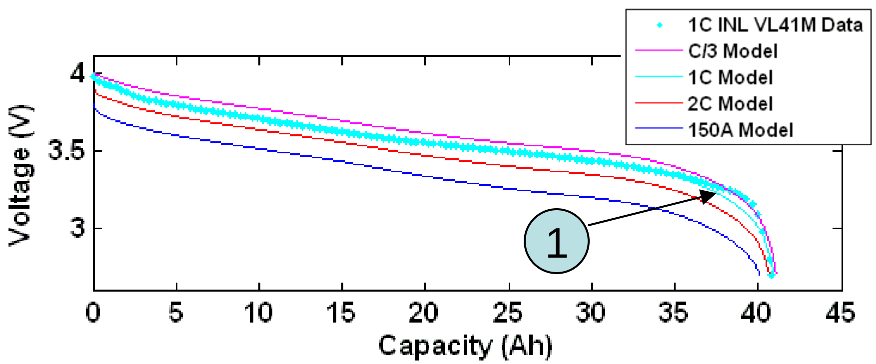

* Negative/Positive electrode thickness ratio $\delta_-/\delta_+$ assumed constant

# PHEV Battery Tradeoff Study

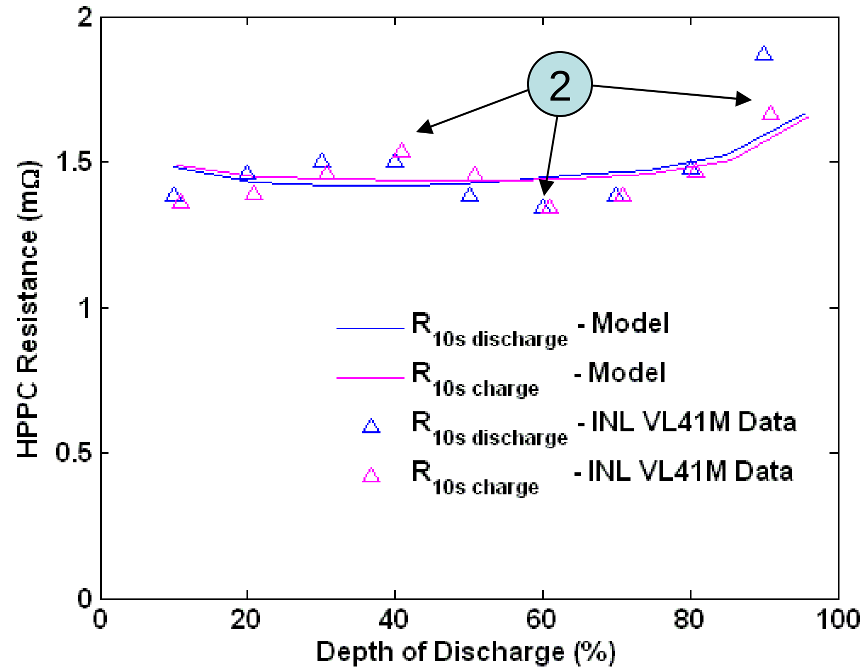
## Fast Running Electrochemical Model Solved with Variable State Method (Saft VL41M)

**Constant current discharge:**
- Saft data sheet (C/3, 1C, 2C, 150A)
- INL data (1C)




**HPPC:**
- INL data

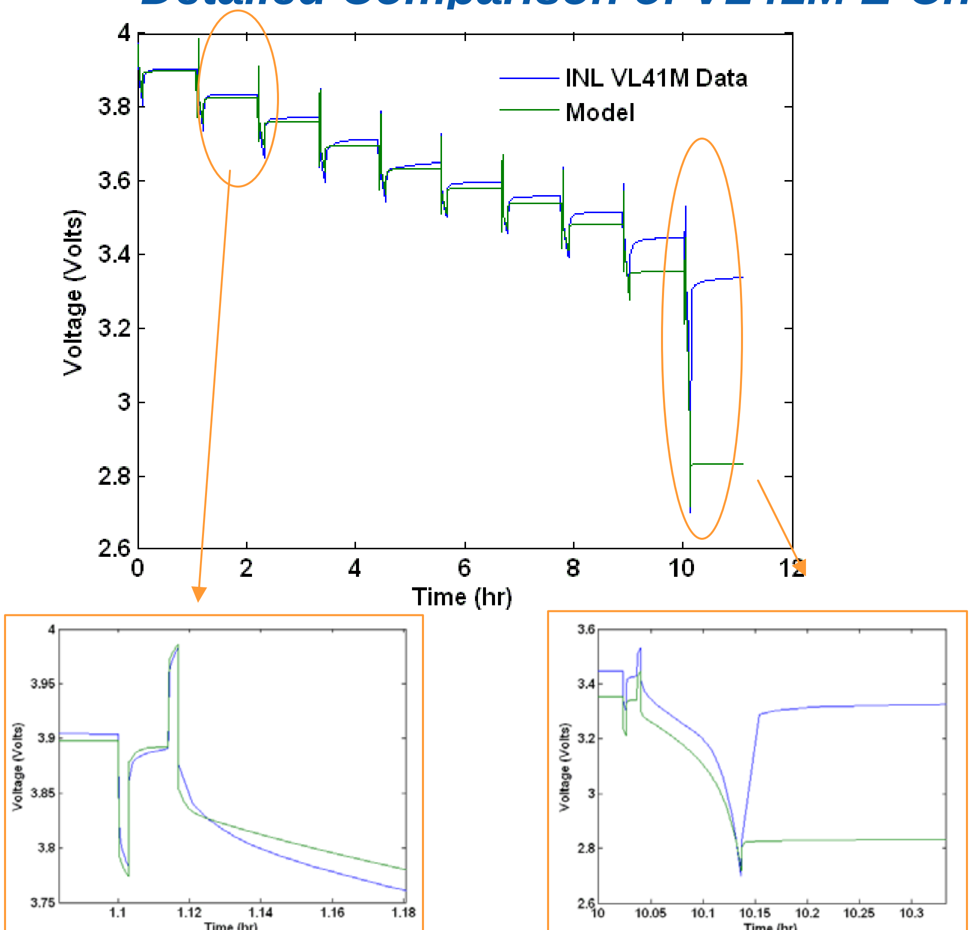



1. Small difference in voltage near end of discharge likely due to poor OCP curve fit.
*To create model, $OCP_-$ for MCMB (assumed anode material) was taken from literature and subtracted from VL41M data to fit $OCP_+$. In FY08, we will continue to improve the model via a manual iterative approach.*

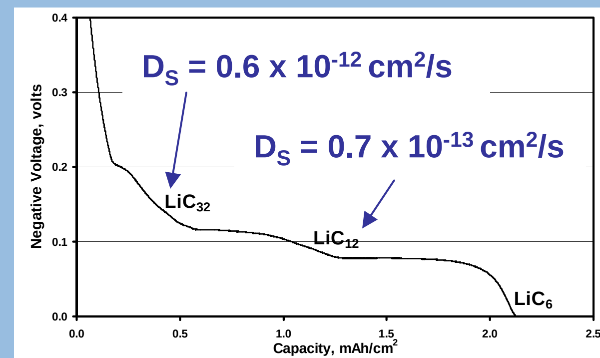
2. Model matches overall resistance, but fails to capture detailed DOD-dependency.
*Explained in more detail on next slide…*

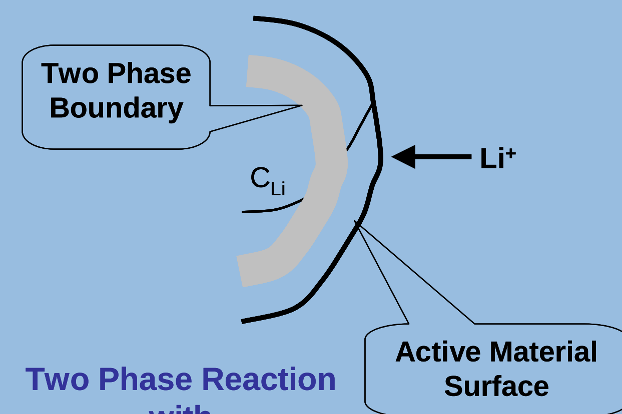
# PHEV Battery Tradeoff Study

## *Detailed Comparison of VL41M E-Chem SVM vs. INL HPPC Dataset*




*(from presentation by Dennis Dees/ANL at May, 2007 ATD Review meeting)*



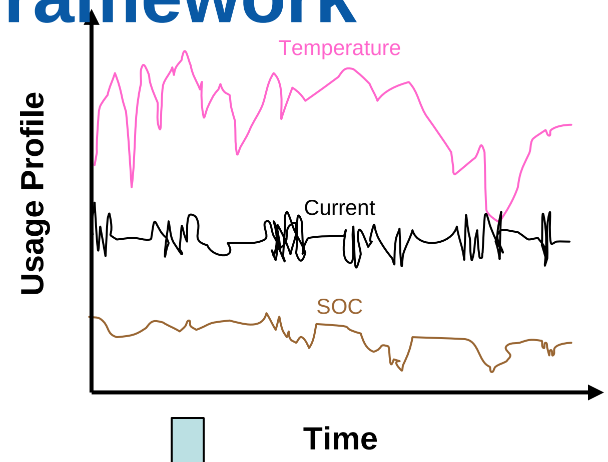

**Two Phase Reaction with Finite Transition Rate**

• Although the present model (with constant $D_{s-}$ and $D_{s+}$) is in generally good agreement with data, it does not properly predicts voltage relaxation. We expect to improve the model by incorporating Dees' two phase model (variable $D_{s-}$) shown at right.

# PHEV Battery Tradeoff Study
## Proposed Life Modeling Framework

***Objective:*** Quantify degradation for any given usage profile

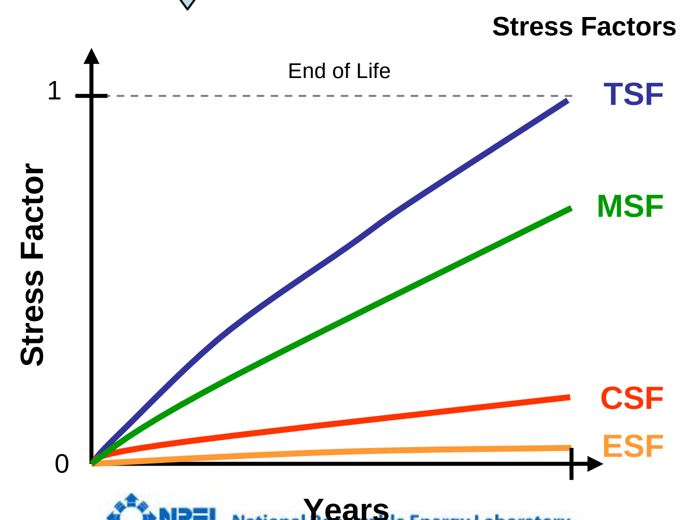
- Time at *T*
- Time at *SOC*
- # cycles at $\Delta DOD_i$
- rate dependency*




***Method:*** Stress factors
- 0 at beginning of life
- 1 when FreedomCAR power or energy goals no longer are met

Mechanical (cycling stress, expansion/contraction)
\+ Thermal (chemical reactions at T, SOC)
\+ Electrochemical* (side reactions in use and standby)

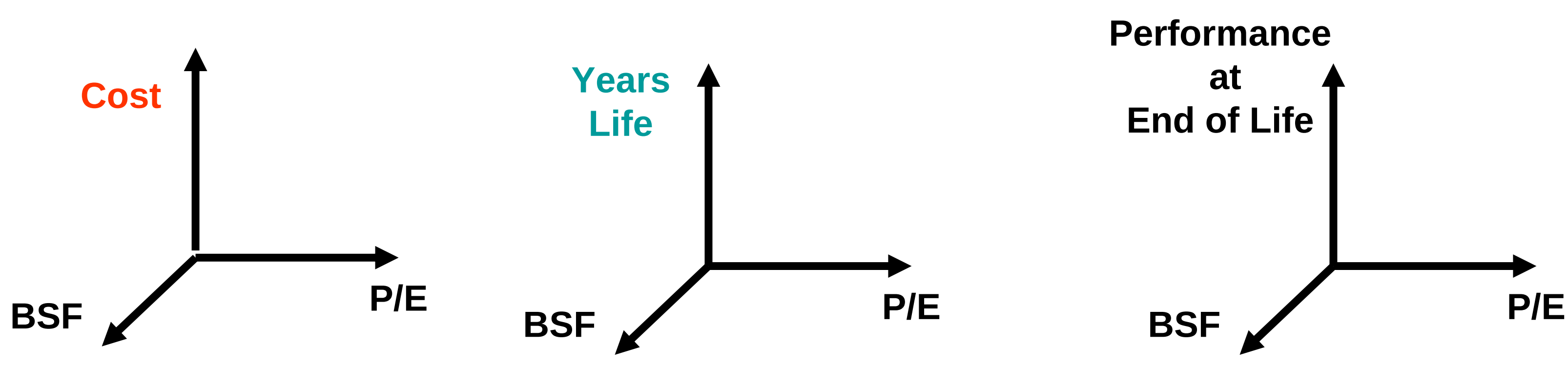
= Total Stress Factor
- 0 at beginning of life
- ~1 when FreedomCAR power or energy goals no longer met




* *Rate dependency & electrochemical stress will be left out of initial FY08 effort until sufficient experience with model and/or experimental data is accumulated.*

# PHEV Battery Tradeoff Study

## End result: Better understanding of battery design tradeoffs when designing to USABC requirements.




## But how will this battery perform in the real-world?

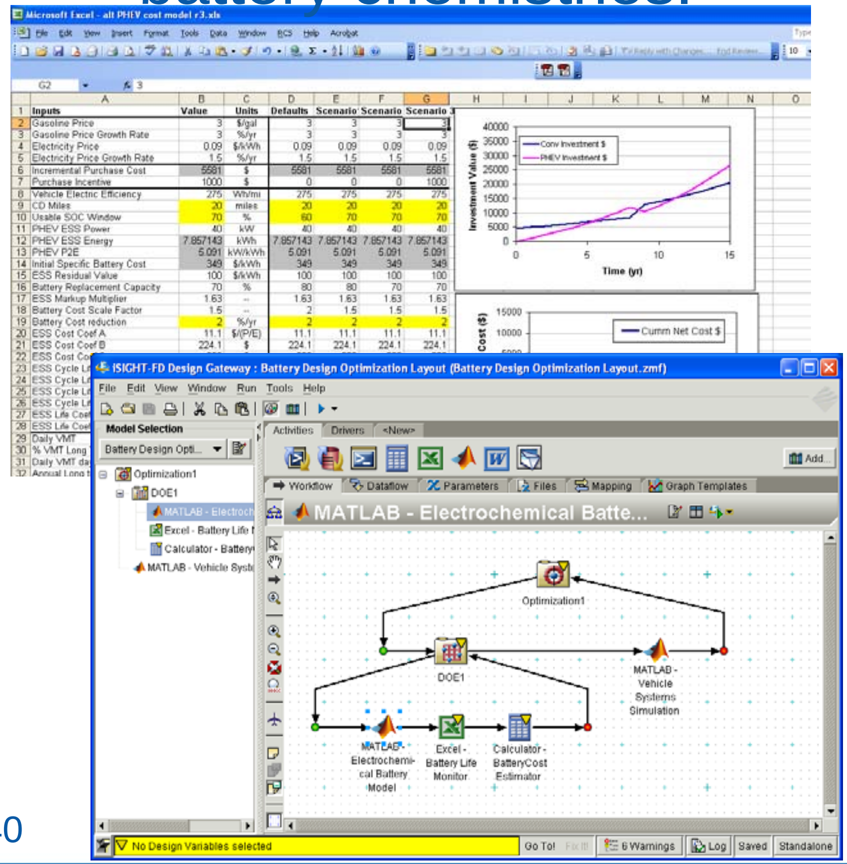
- **Driving characteristics**: *Aggressive vs. non-aggressive*
- **Climate**: *Arizona vs. North Dakota*
- **Charging**: *Nighttime vs. Opportunity*

# PHEV Battery Tradeoff Study

## Future Work

- Perform optimization studies for various Li-ion battery chemistries.






- Analyze performance/ life/cost tradeoffs of alternative PHEV battery usage scenarios (vehicle to grid, renewable electricity, battery replacement,…)
- Incorporate battery performance/life/cost models into global systems optimization procedure to better explore scenarios.

# Publications and Presentations

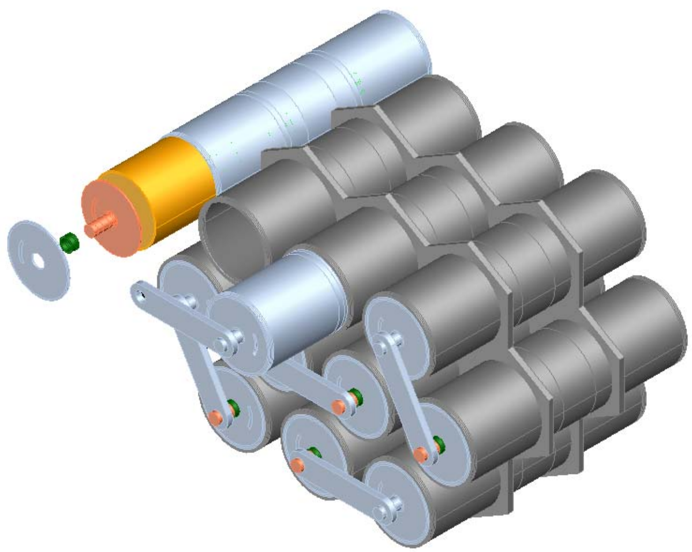
- T. Markel and A. Simpson, "Cost-Benefit Analysis of Plug-In Hybrid Electric Vehicles," *World Electric Vehicle Association (WEVA) Journal,* Vol. 1, pp. 053-063, 2007.
- A. Pesaran, "Battery Choices and Potential Requirements for Plug-In Hybrids," Presented at the Plug-in Hybrid Electric Truck Workshop Hybrid Truck Users Forum, Los Angeles, California, February 2007.
- A. Pesaran and T. Markel, "Battery Requirements and Cost-Benefit Analysis for Plug-In Hybrid Vehicles," Proceedings of the *24th International Battery Seminar and Exhibit*, Fort Lauderdale, Florida, March 2007.
- T. Markel and A. Pesaran, "PHEV Energy Storage and Drive Cycle Impacts," Presented at *Advanced Automotive Battery Conference*, Long Beach, California, May 2007.
- A. Pesaran and J. Gonder, "Factors & Conditions for Widespread Use of Ultracapacitors in Automotive Applications," Proceeding of *Advanced Capacitor Summit*, San Diego, California, July 2007.
- A. Pesaran, T. Markel, H. Tataria, and D. Howell, "Battery Requirements for Plug-In Hybrid Electric Vehicles – Analysis and Rationale" 23rd Electric Vehicle Symposium. Dec. 2007.

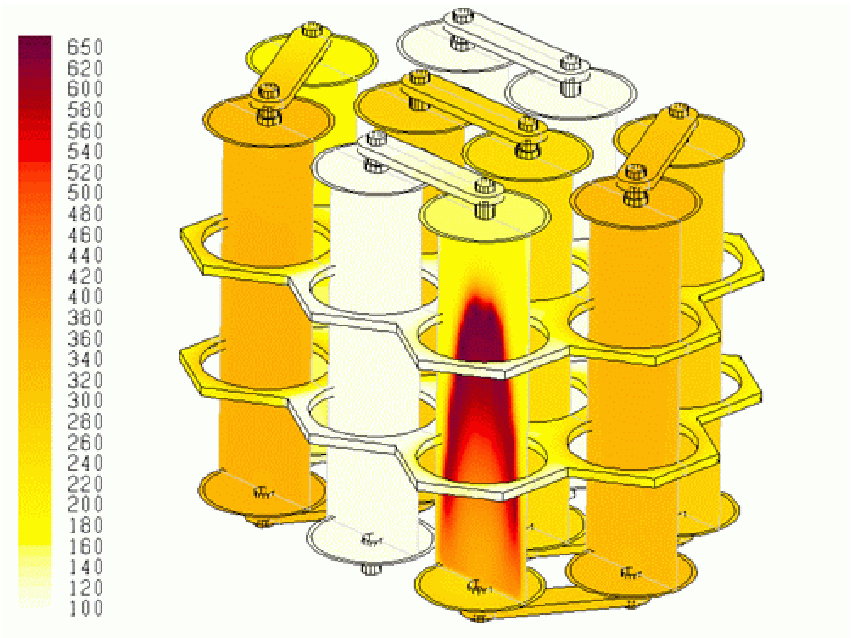
# Applied Battery Research

## 3. Li-Ion Thermal Abuse Reaction Modeling

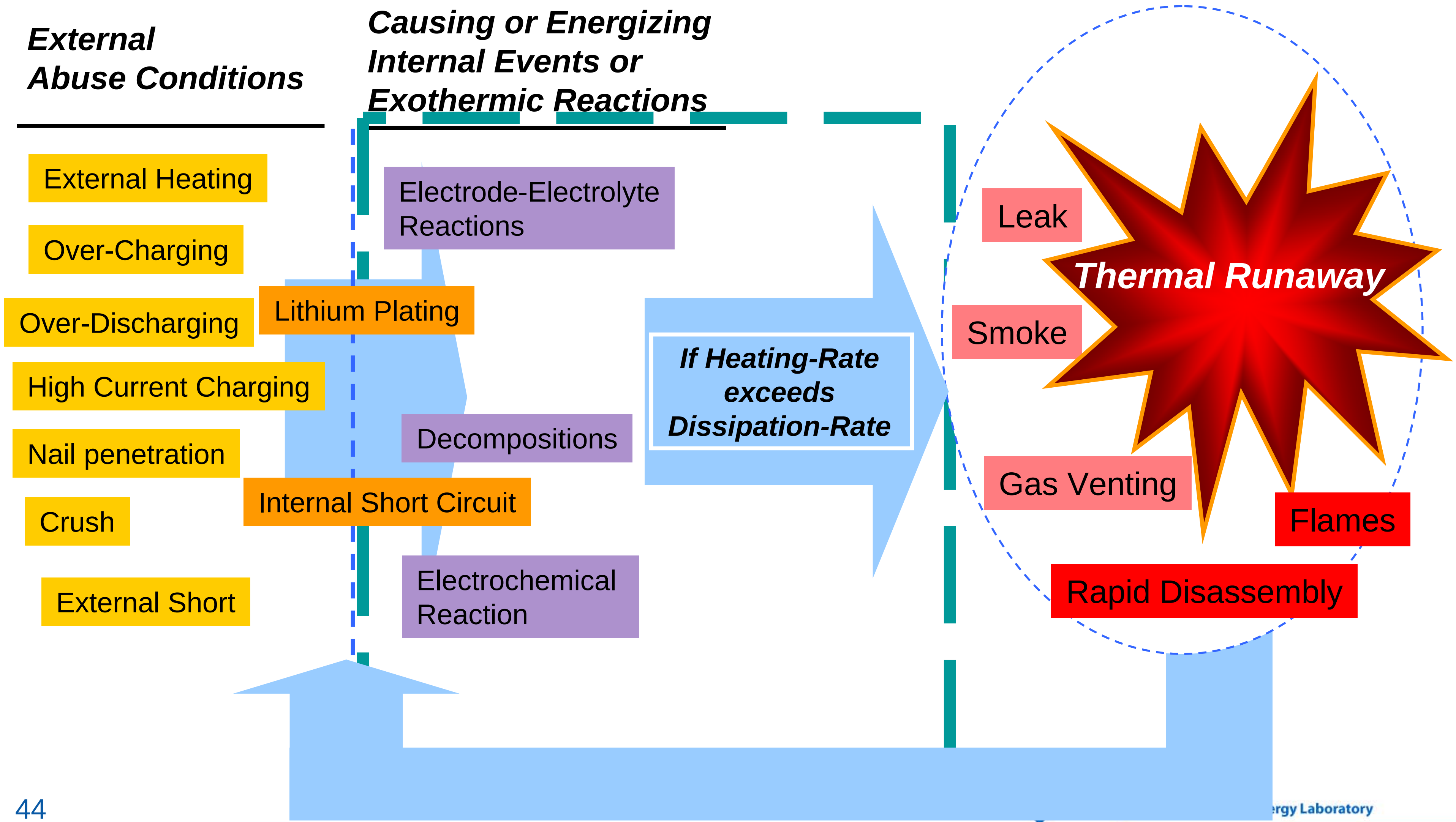
- One of major barriers that the DOE Vehicle Technologies Program is addressing is safety of Li-Ion batteries.
- Safe and abuse tolerant Li-Ion batteries systems need to be developed for vehicle applications.
- NREL is supporting the development of abuse tolerant batteries by developing design models.

# Methodology for Understanding Impacts of Battery Design Parameters on Thermal Runaway in Lithium-Ion Cells/Modules





# Thermal Runaway



# Objectives of this Study

*Thermal abuse behaviors of Li-Ion batteries are greatly affected by the local conditions of heat and materials*

- To develop 3D Li-Ion battery thermal abuse "reaction" models for cell and module analysis.
- To understand the mechanisms and interactions between heat transfer and chemical reactions during thermal runaway for Li-Ion cells and modules.
- To develop a tool and methodology to support the design of abuse-tolerant Li-Ion battery systems.

# Approach

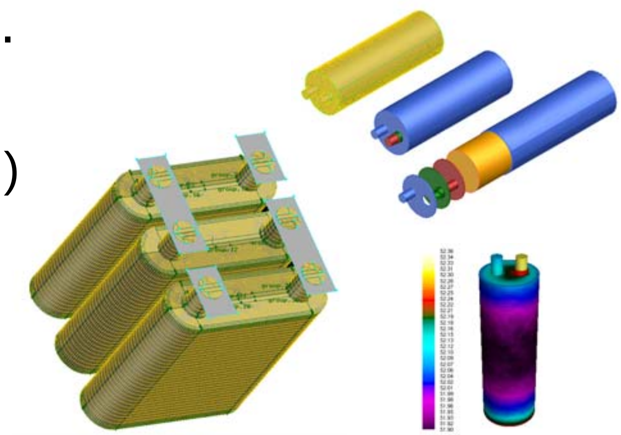
- Formulate *Exothermic Reactions* at elevated temperatures

> *Reproduce thermal abuse modeling of Li Ion cells provided by Hatchard et al. (J. Electrochem. Soc. 148, 2001)*
> *Consulted with Bob Spotnitz for reaction formulation*

→ Component reactions were fitted to Arrhenius type reactions.
→ Kinetic parameters were determined with ARC(/DSC) data.

- Extend to *Multi-dimensional Models* capturing *actual thermal paths* and geometries of cells and modules.

→ A commercial finite volume method (FVM) solver, FLUENT, was used.



# Cell Level Thermal Runaway Analysis

- **Internal Short Simulation**
  - ✓ Impact of short location in a cell
  - ✓ Impact of thermal property of cell materials

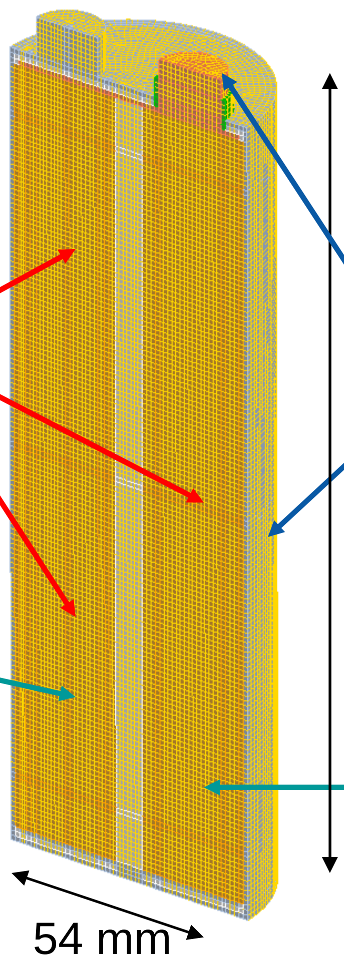
# Model Description

½ Model with Symmetry Plane

- MESH
  - ✓ Computational Grid: 200K
  - ✓ Grid Size: ~1mm by 1mm by 1mm
  - ✓ max: 2.01 $mm^3$ ,min: 0.31 $mm^3$

***Hot-Spot***

- Localized energy (5% of stored electric energy) would be released in a short period of time inside a cell core.




***Thermal Boundary Conditions***

- Natural/forced convection
- Gray-body radiation

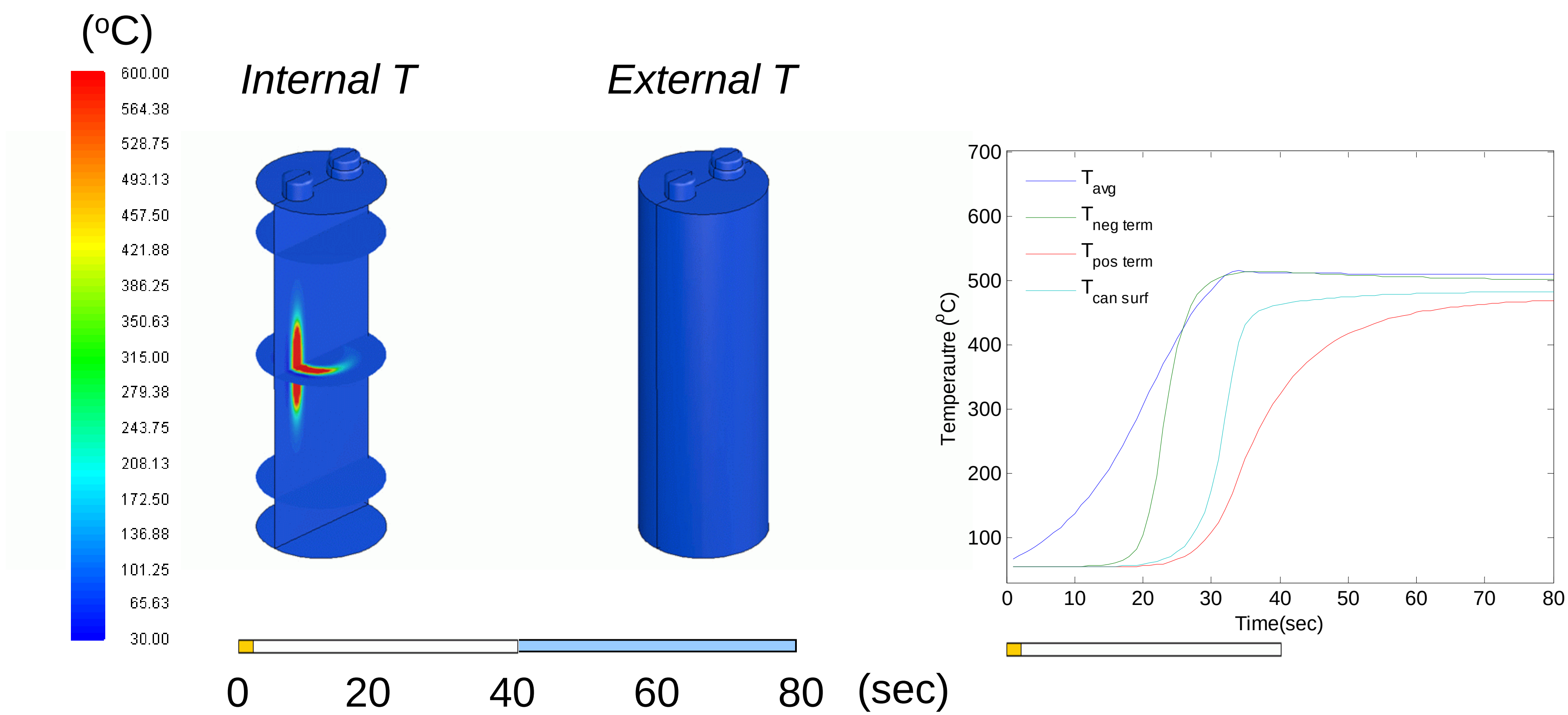
*Heat Sources*

- Exothermic reaction heat
- No resistive/Joules heating

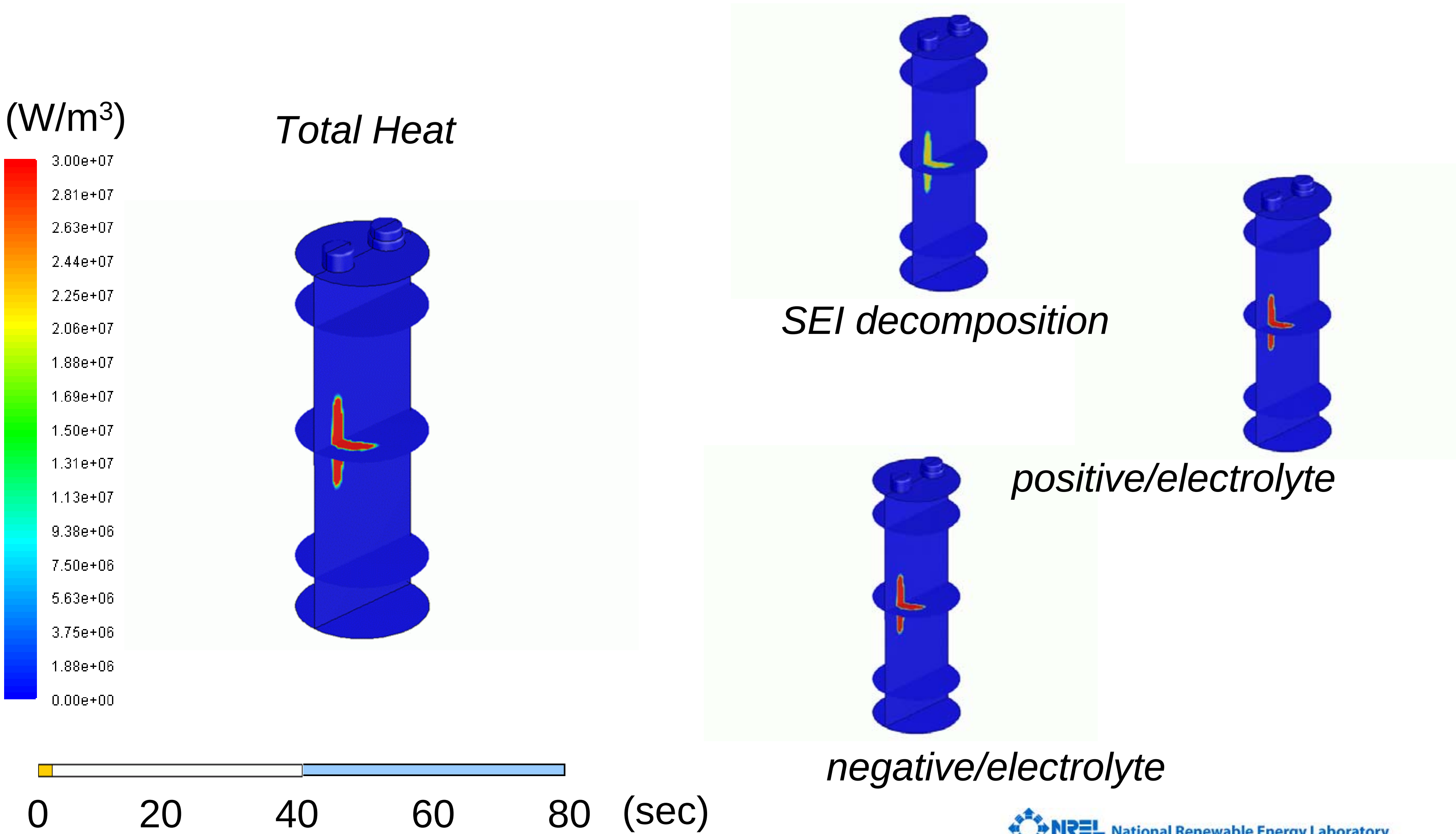
*Core Material*

- Cylindrically Orthotropic Properties

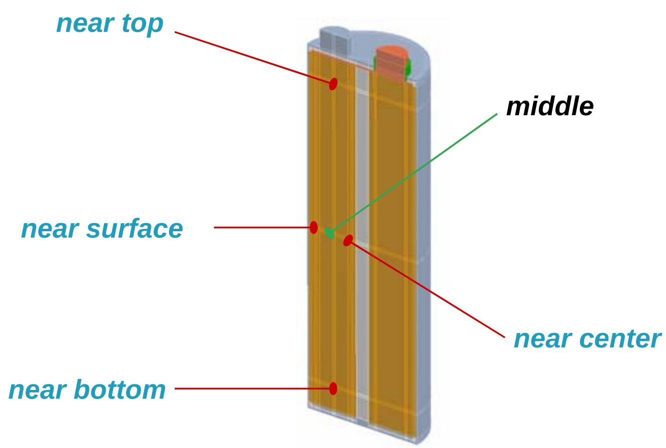
# Temperature Evolution



# Volumetric Heat Generation



# *Impact* of Short Location




Layer structure of electrodes
→ *preferred directions of reaction propagation*

Initial location of short &
Thermal paths and material distributions
→ *propagation pattern*
→ *heat release duration*

# *Impact* of Thermal Property

***Heat Capacity***

*5% less* ← $C_p$ → *5% more*

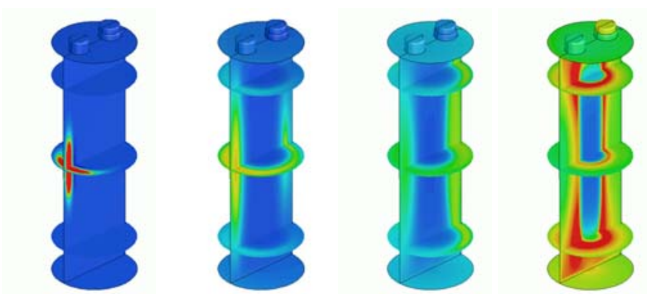
***Thermal Conductivity***

*50% less* ← $k$ → *50% more*

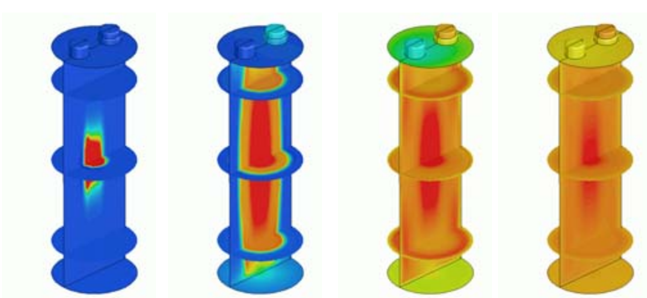
Electrode/current collector thicknesses &
Relative amount of component materials
→ *volumetric heat generation*
→ *thermal properties of electrode sandwich*

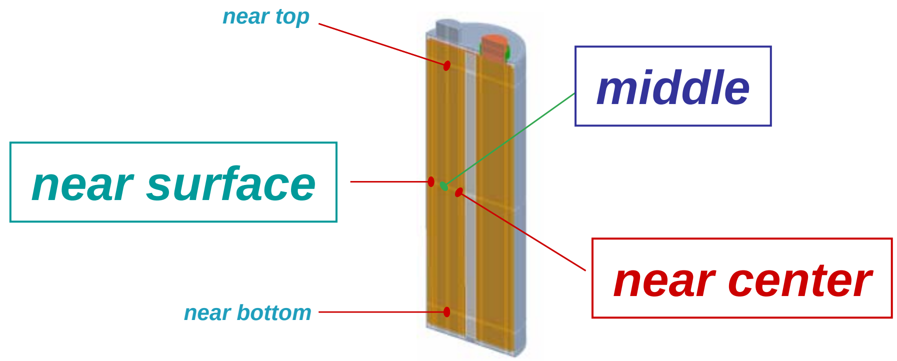
# Short near exterior surface .vs. Short near center of a cell

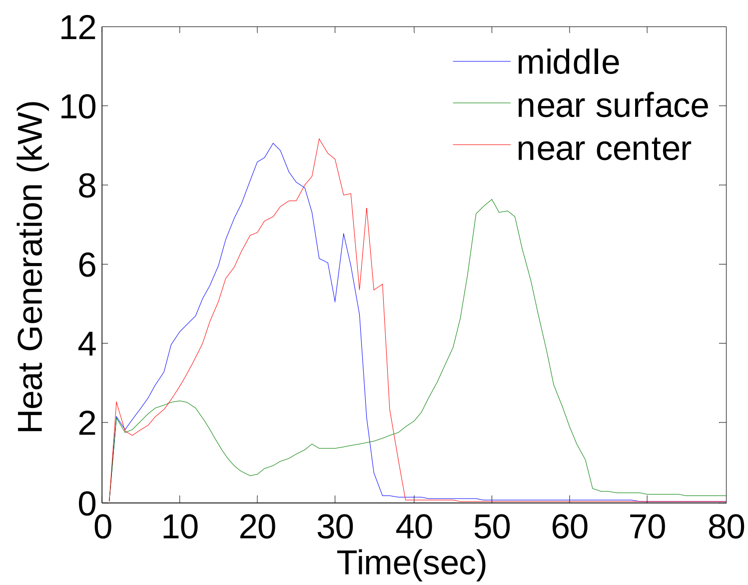
*temperatures*



2 20 38 54 sec

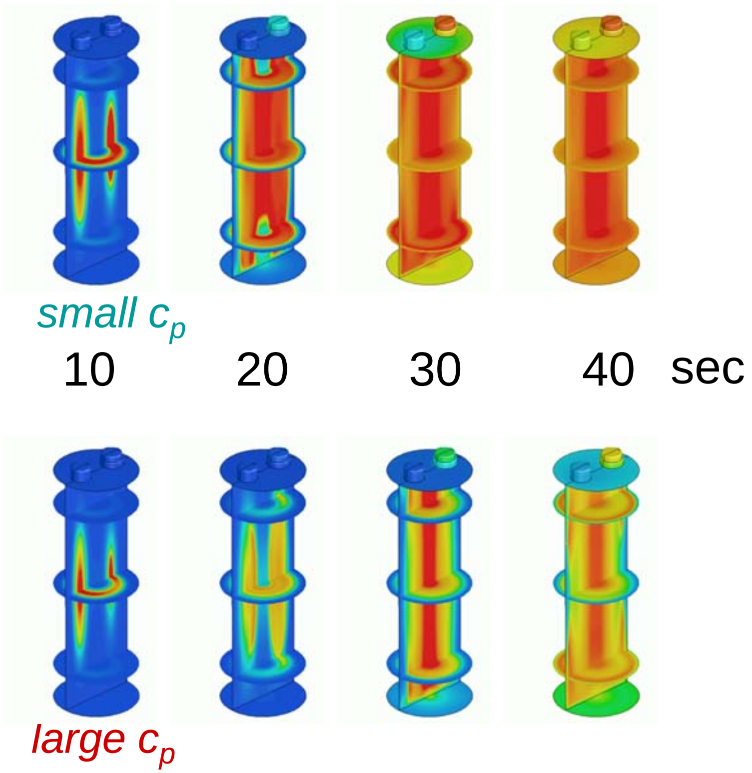




# $c_p$ impact

*temperatures*

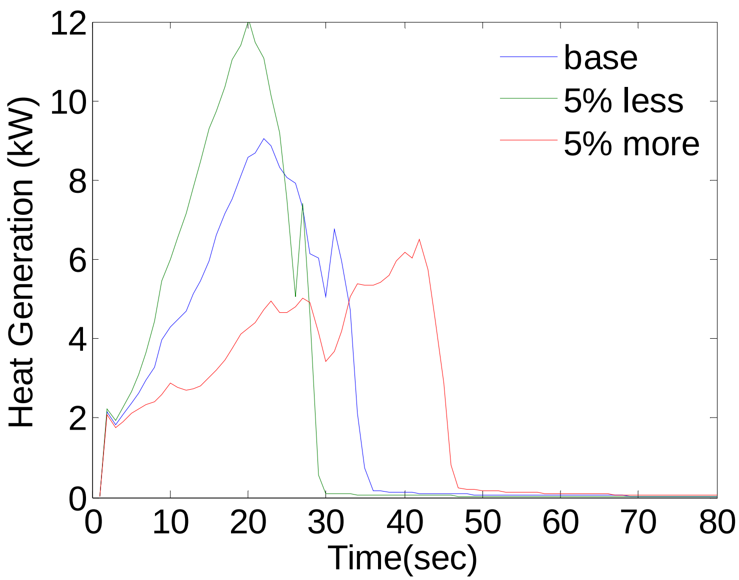



***Heat Capacity***

5% less ← $C_p$ → 5% more

***Thermal Conductivity***

*50% less* ← $k$ → *50% more*



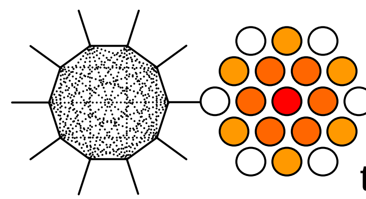
# Module Level Analysis of Cell-to-Cell Thermal Runaway Propagation

***How can a module be more resistive to cell-to-cell thermal runaway propagation?***

# We propose that ***Cell-to-Cell Propagation*** in a Module is …

*A result of **INTERACTION** between the distributed chemical sources and the thermal transport network through a module.*

dispersed sources



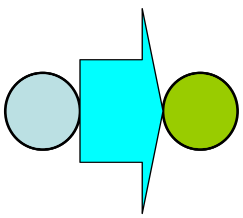
thermal network

***Approach** for the analysis of this system*

- Formulated *exothermic chemical reactions* of a cell at elevated temperatures.
- Quantified *heat transfer among the cells* in a module
  - → Radiation Heat Transfer
  - → Conduction Heat Transfer
  - → Convection Heat Transfer

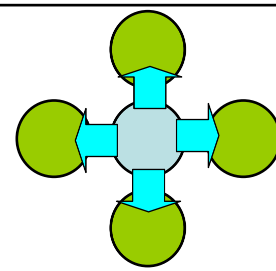
# Would Fast Heat Transfer be Good? or Slow Heat Transfer?

Concentrated Delivery



Fast: Bad
Slow: Good

Distributed Delivery



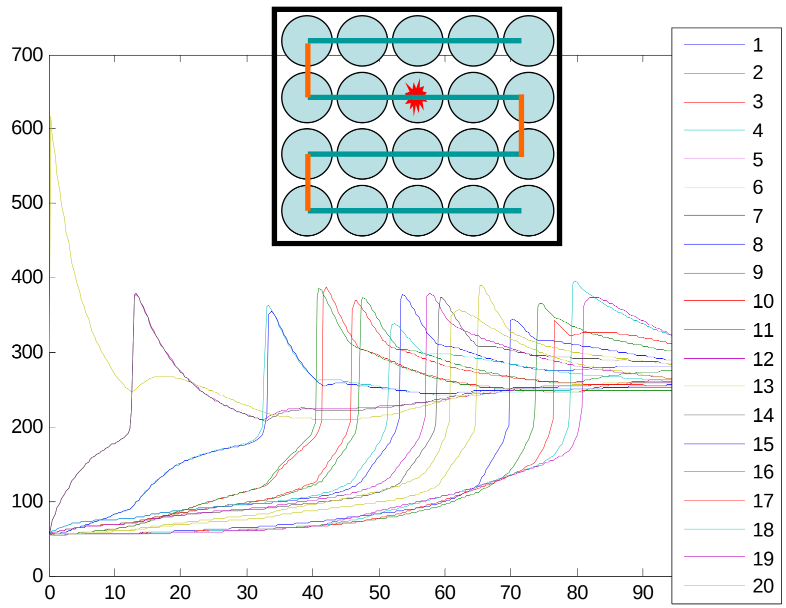
Fast: Good
Slow: Bad

*Example*: Thin series connector and Thick parallel connector are good for propagation-resistive design

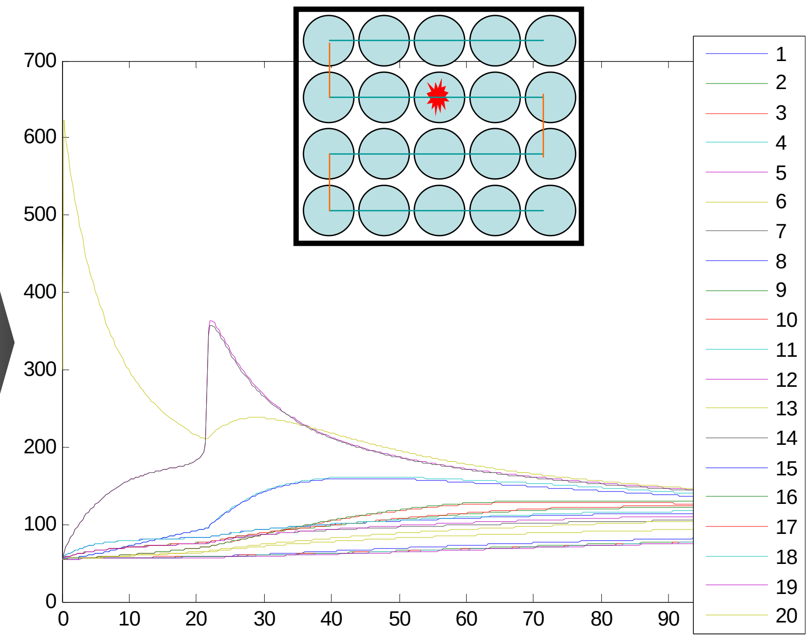
# *Impact* of Cell-Cell Connector Size

***Module Propagation Analysis Example***

Electric connector cross section was reduced by 33% from the base case.




***Base Case***



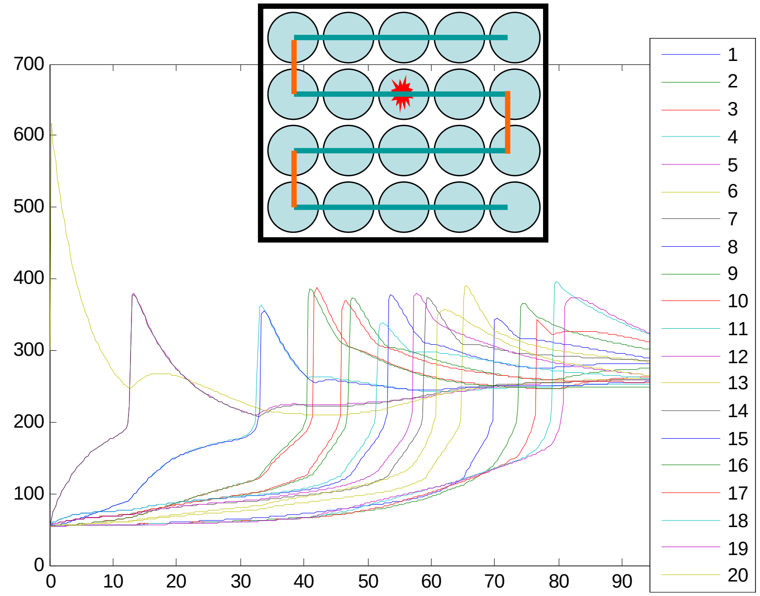

***Smaller cell-cell Connector***

It appears that fewer cells will go into thermal runaway with smaller cell-cell connector.

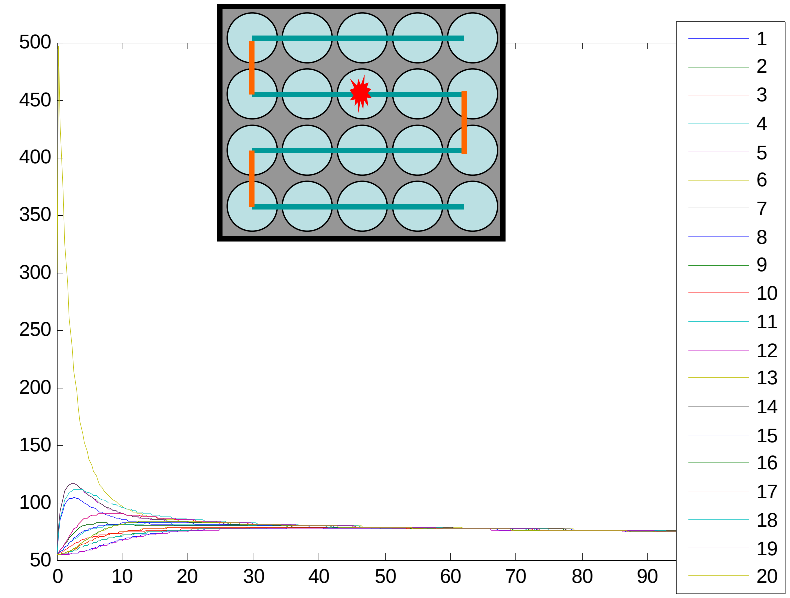
# ***Impact*** of a "Highly Conductive Heat Transfer Medium"

***Module Propagation Analysis Example***

Rather than air used in the Base Case, a highly conductive PCM/Graphite Matrix filled the space between the cells in the module.




***Base Case (air)***




***PCM/Graphite Matrix Imbedded****

It appears that a very conductive medium may reduce the chance for propagation.

NOTE: * PCM/Graphite Matrix is a highly porous graphite structure that is impregnated with phase change material (PCM) based on S. Al-Halaj, et. al information.

# Summary

- Li-Ion Reaction chemistry was implemented into a finite volume 3D cell model addressing various design elements.
  - ✓ Simulated oven test and internal short-circuit events
  - ✓ Examined impact of cell design parameters

- Propagation of abuse reaction through a module was simulated.
  - ✓ A complicated balance between heat transfer network and dispersed chemical sources.
  - ✓ This balance is affected by module design parameters such as cell size, configuration and size of cell-cell connectors, and cell-cell heat transfer medium.

- A feature designed for improving normal operation of battery system need to be evaluated in thermal aspects.

# Future Work

- Improve model through the comparison with experimental data from other Labs
- Continue on examining the impact of design variables
- Address limitation of the model
  - e.g.) venting impact and pressure impact
- Expand the model capability to address various chemistries and materials such as iron phosphate
- Investigate internal/external short by incorporating thermally coupled electrochemistry model into the three dimensional cell model
- Work with developers on specific cell and module designs

# Publication/Presentation

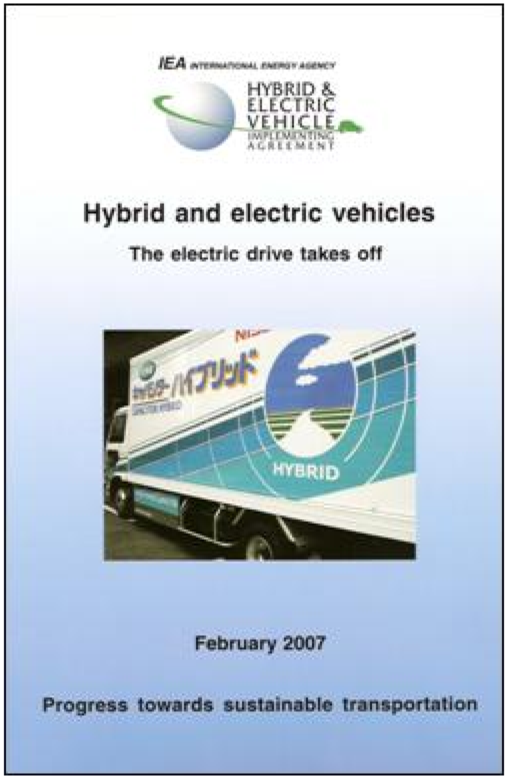
- G.-H. Kim, A. Pesaran, and R. Spotnitz, “A Three-Dimensional Thermal Abuse Model for Lithium-Ion Cells,” *Journal of Power Sources*, Vol. 170, pp.476-489, July 2007).
- G.-H. Kim and A. Pesaran. “Analysis of Heat Dissipation in Li-Ion Cells & Modules for Modeling of Thermal Runaway,” *The 3rd International Symposium on Large Lithium Ion Battery Technology and Application* (LLIBTA/AABC-2007), Long Beach, California, May 2007.
- G.-H. Kim, A. Pesaran, and K. Smith, “Li-Ion Thermal Abuse Modeling,” 76th meeting of the Lithium Battery Technical/Safety Group (LBTSG):, Cleveland, OH, September 2007
- G.-H. Kim, K. Smith, A. Pesaran and R. Spotnitz, “Analysis of Thermal Behavior of Li-Ion Batteries using Thermal Abuse Reaction Model,” *212th ECS Meeting*, Washington DC, October

# NREL also Supports the IEA/HEV Implementing Agreement

- The International Energy Agency (IEA) acts as energy policy advisor to 27 member countries in their effort to ensure reliable, affordable and clean energy for their citizens (www.iea.org)
- IEA/HEV Implementing Agreement (IA) is collaboration between 15 member companies to share information about governmental program, lessons learned, and latest technologies on hybrid vehicles (www.ieahev.org)
- The goal is to gain timely and reliable access to the latest activities and data exchanges among member nations and thus move to the front line of awareness on developing trends, markets, and component technologies and needs.
- DOE's Vehicle Technologies Office represents US in the IEA/HEV IA
- There are several Annexes in the HEV IA, which DOE supports.

# NREL Support of the IEA/HEV Implementing Agreement

- NREL supports the participation of US in the IEA/HEV IA and its Annexes
  - Overall HEV IA effort
  - Annex VII (Hybrid Vehicles)
  - Annex XII (Heavy-Duty Hybrid Vehicles)
  - Annex XIII (Fuel Cell Vehicles)
- NREL provides technical expertise and support to Annex XII and Annex XIII by participation at expert meetings and contribution to work plan
- IEA/HEV IA produces a comprehensive annual report summarizing the results of efforts and findings



# Technology Transfer

- The data generated, models developed, and techniques conceived are transferred to battery developers and others to support their implementation in their design and prototypes being developed toward a marketplace application
- We collaborate one-on-one with battery developers to enhance the thermal performance of batteries
- We disseminate information through conferences and journal articles to shed light on important design issues and available tools
- We participate at International Energy Agency to exchange public, non-propriety information

# Summary

- This presentation summarized NREL three major activities
  1. Thermal characterization and analysis
  2. Energy storage simulation and analysis
  3. Li-ion thermal abuse reaction modeling
- These actives support DOE goals, FreedomCAR targets, USABC Tech Team, and battery developers
- NREL transfers technology either through one-on-one collaborations or dissemination of information in international conferences and journals

http://www.nrel.gov/vehiclesandfuels/energystorage/publications.html

# Acknowledgements


- Programmatic Support from DOE's Vehicle Technologies Program
  - David Howell
  - Tien Duong
- Contributions by NREL Colleagues
  - Matt Keyser
  - Kandler Smith
  - Gi-Heon Kim
  - John Powell
  - Tony Markel
  - Jason Lustbader
  - Jeff Gonder
- Technical Guidance and Exchange with USABC and Energy Storage Tech Team
  - GM
  - Chrysler
  - Ford
  - Southern California Edison
- Input and Prototypes from Battery Developers
  - A123 Systems
  - Saft
  - Johnson Controls
  - CPI
  - LG Chem
  - AllCell Technologies