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Computer-Aided Engineering and Secondary Use of Automotive Batteries

The 10th Advanced Automotive Battery Conference
Orlando, Florida
May 19-21, 2010

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U.S. Department of Energy

NREL/PR-540-48145

Funded by Energy Storage R&D (David Howell), Vehicle Technologies Program, Office of Energy Efficiency and Renewable Energy, U.S. Department of Energy

Content

- Computer-Aided Engineering for Automotive Batteries
  - Accelerating design and development
  - State-of-the-art
  - Gaps and needs
  - Future plans

- Secondary Use of PHEV and EV Batteries
  - New interest
  - Potential second use applications
  - Gaps and needs
  - Future activities

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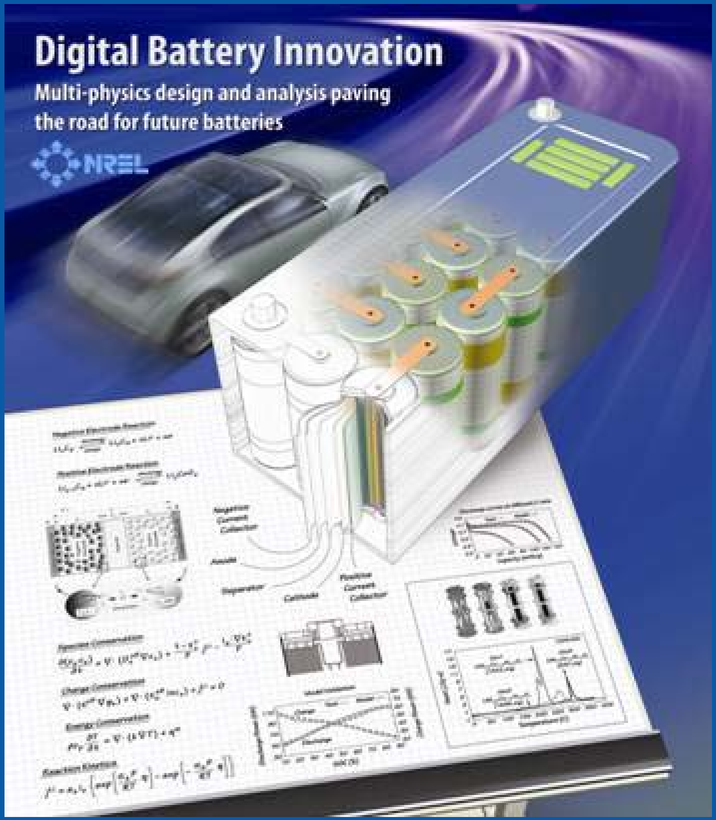

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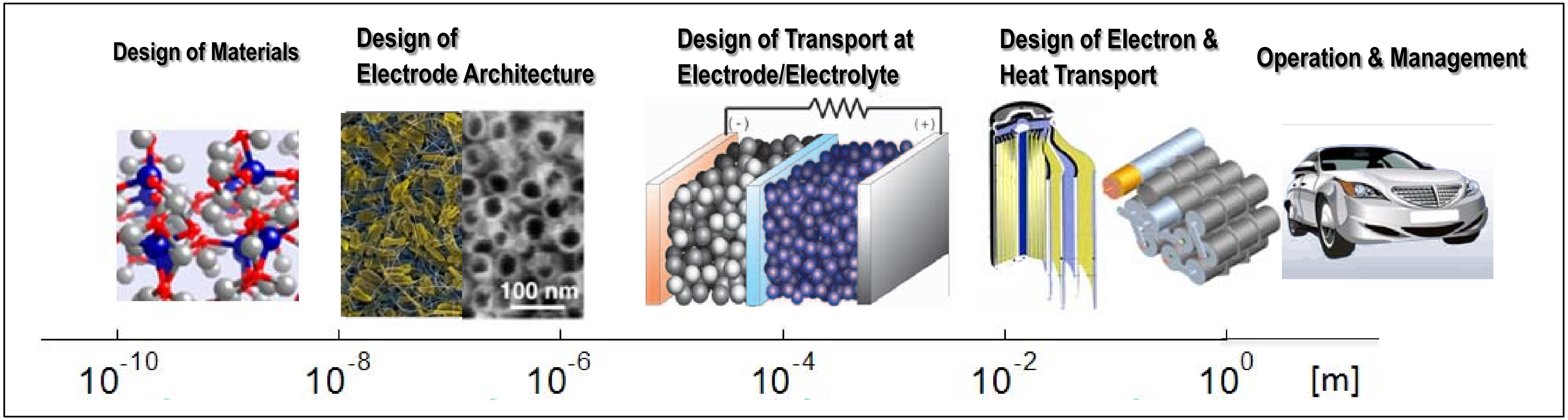
Introduction – Battery CAE

- Computer-aided engineering (CAE) is a proven pathway, especially in automotive industry, to
  - Improve performance by resolving relevant physics in complex systems
  - Shorten product development design cycle and thus reduce cost
  - Provide an efficient manner for evaluating parameters for robust designs
- Most battery CAE models could be enhanced
  - Academic models include relevant physics details, but neglect engineering complexities
  - Industry models include relevant macroscopic geometry and system conditions, but use too much simplification in fundamental physics
- DOE- and private-industry-funded projects have demonstrated the value of battery CAE
  - Most in-house custom model codes, however, require expert-users
- Battery CAE capabilities need to be transferred to industry
  - In time to impact the transition toward sustainable electric mobility
  - Reduce the process of design, build, test, break, redesign, rebuild, retest,…

Multi-Scale Physics in Li-Ion Battery

Various physics interact across wide range of length and time scales



Present industry needs

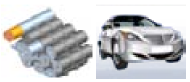
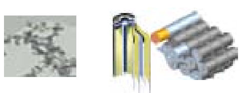
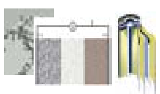
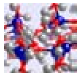
- ***Performance & Life Models:*** *Coupling electrode-level performance/life with cell/pack-level heat/current transport*
- ***Safety Models:*** *Coupling electrode-level chemical reactivity and cell/pack-level heat transport*
- *Need to include both science and engineering*

Active research areas

- ***First Principals Material Evaluation***
- ***Electrode Architecture Design***

NREL Battery Modeling Portfolio

(diverse, but not integrated)

Model	Length Scale pm --- nm --- µm --- mm ---- m	Geometry	Physics / Application
Vehicle/component (PSAT/ANL & Advisor/NREL)		Lumped	• Drivetrain power balance / Drive cycle • Battery usage & requirements • Control strategy design
Battery cost		Lumped	• Empirical • System cost (\$/*kW*, \$/*kWh*)
Battery life		Lumped	• Empirical • Life prediction ($t, N_{cyc}, T, \Delta DOD, SOC$)
Equivalent circuit (e.g. PNGV, FreedomCar)		Thermal/electrical network	• Electrical & thermal • Performance, design, safety evaluation
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
Molecular dynamics		3-D	• Atomic & molecular interactions • Material design

Battery CAE : What Should One Expect?

- **Multi-scale Physics Interaction**: Integrate different scale battery physics in computationally efficient manner
- **Flexibility**: Provide a modularized multi-physics platform – Enable user choice from multiple submodel options with various physical/computational complexity
- **Expandability**: Provide an expandable framework to "add new physics of interest" or to "drop physics of insignificance/indifference"
- **Validation and Verification:** The correct equations are solved and they are solved accurately

Length-Scale Mapping for Li-ion Battery Models

(Examples and not a complete list)

U of Michigan
Meso-Scale Model

ANSYS/CD-adapco
CAD, FEA, CFD Solvers

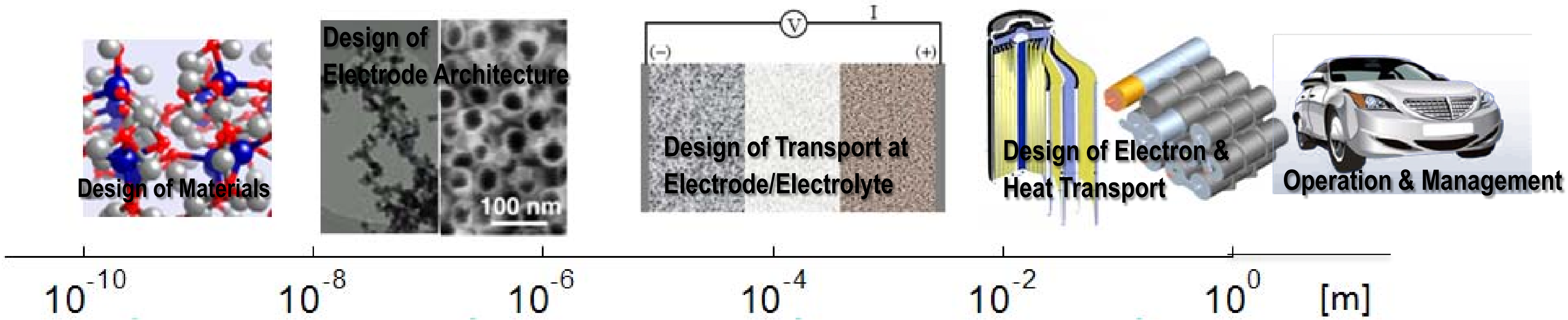
LBNL, MIT, ANL
First Principles ,

ANL, NREL, AVL
Vehicle Simulator

UC Berkeley
Dualfoil, 1D electrochem.

INL
Electrolyte models

NREL, USC, Battery Design
1D, 2D, 3D, multi-scale electrochem.

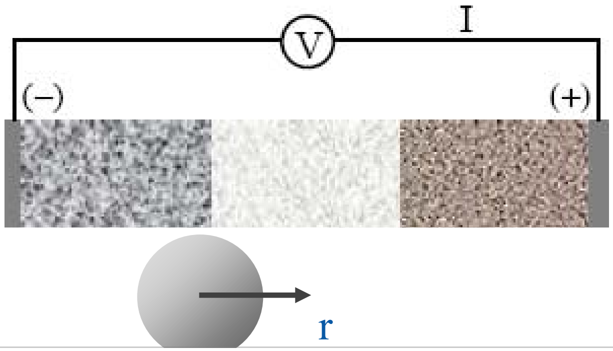


Example
Electrode-Scale Performance Model

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

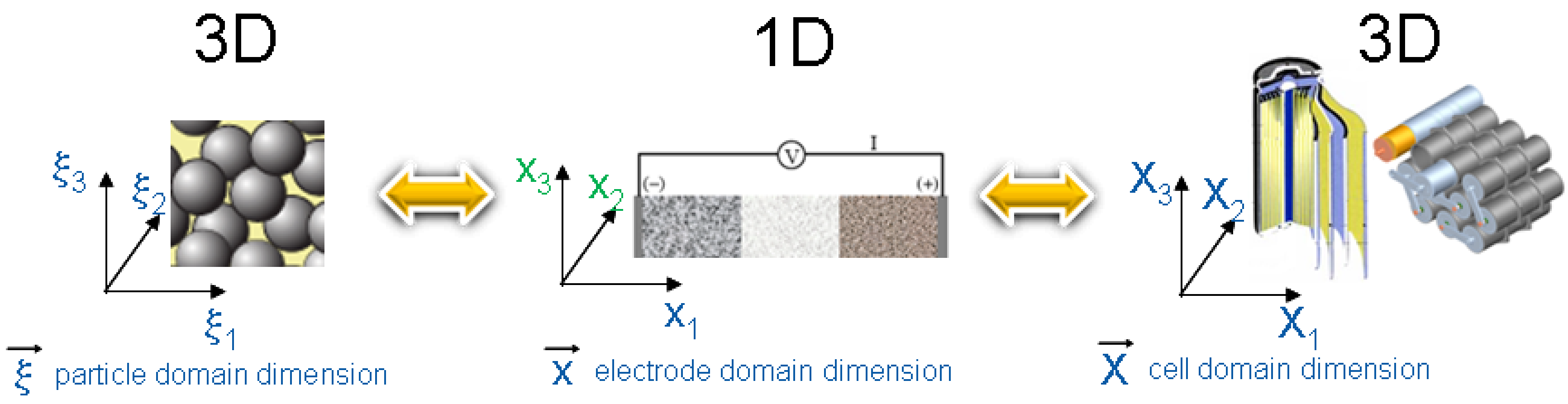
Energy Conservation

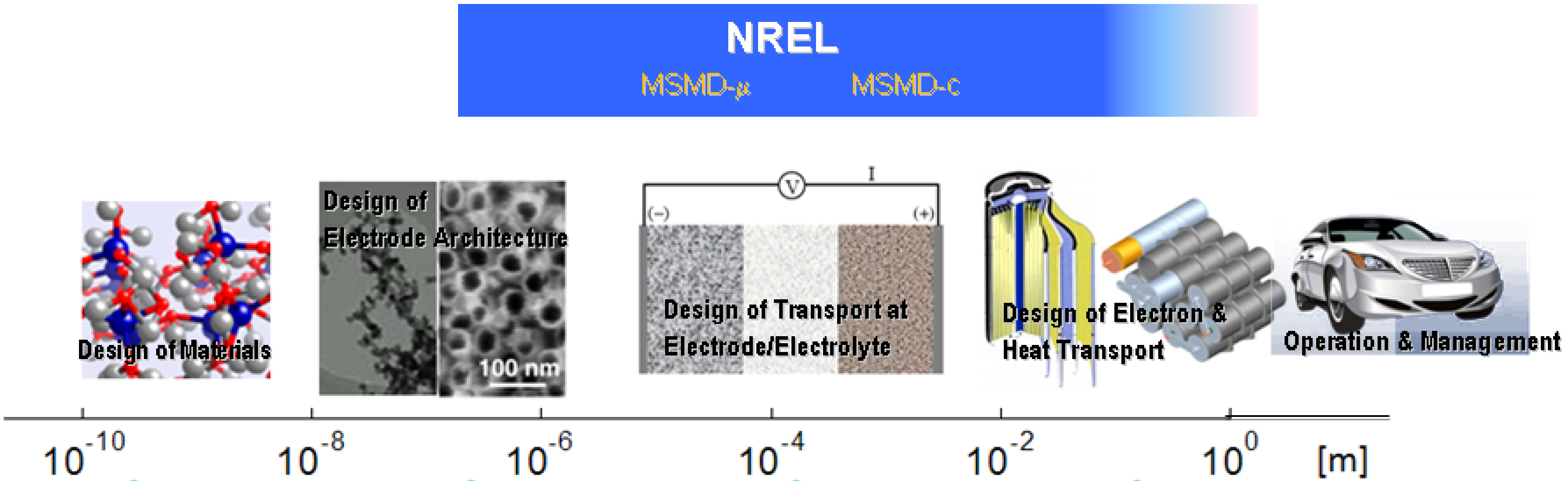
$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + q'''$$

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

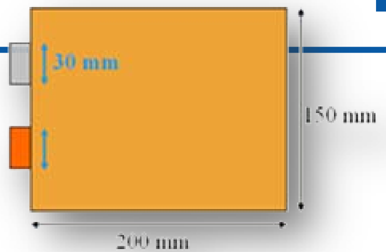
Extending Newman's model to Thermal-EChem 3D

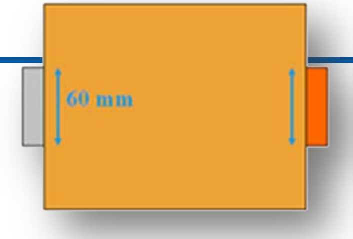
NREL's Multi-Scale Multi-Dimensional (Domain) Model Approach





Example Results of Battery Modeling Multi-Physics Interaction



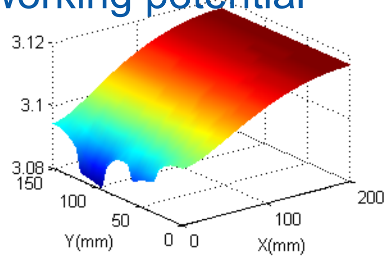


Comparison of two 40 Ah flat cell designs

2 min 5C discharge

- *Larger over-potential promotes faster discharge reaction*
- *Converging current causes higher potential drop along the collectors*

working potential



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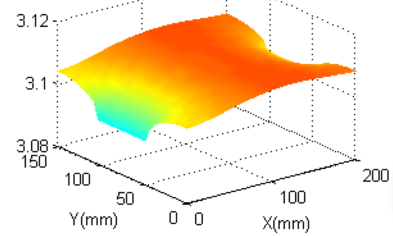
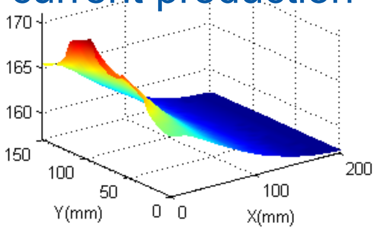


electrochemical current production



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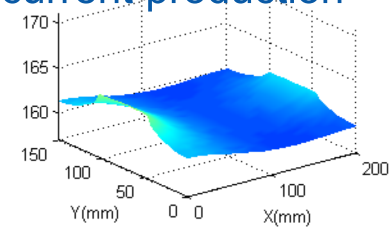

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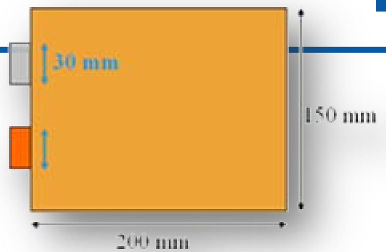
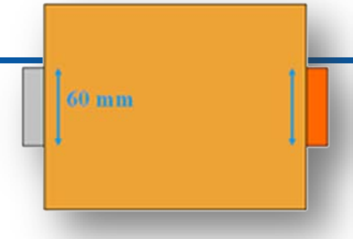
Multi-Physics Interaction





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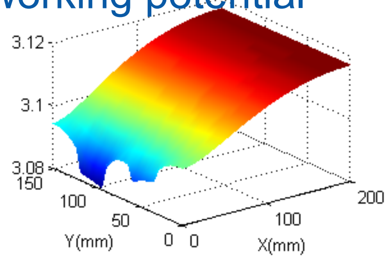
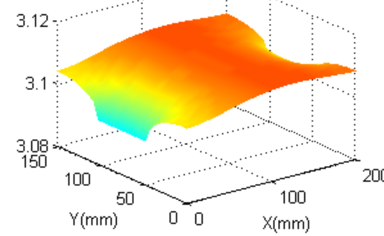
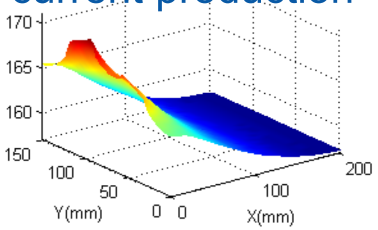


working potential



electrochemical current production



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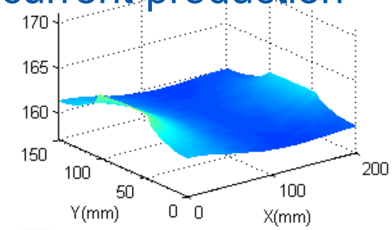
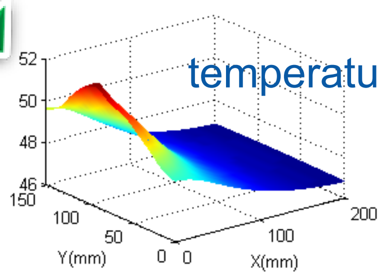
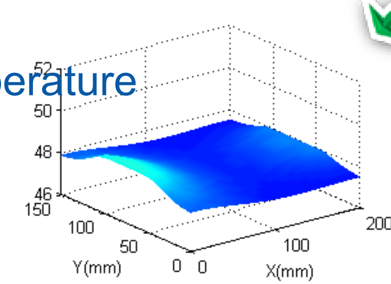


- *High temperature promotes faster electrochemical reaction*
- *Higher localized reaction causes more heat generation*

temperature



temperature



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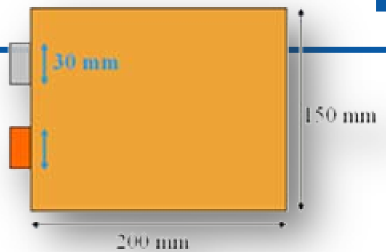

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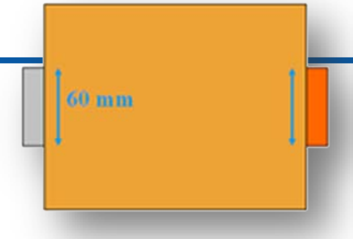

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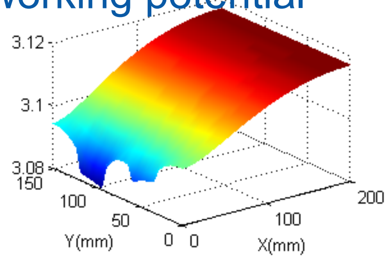
working potential



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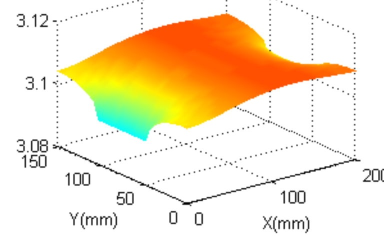

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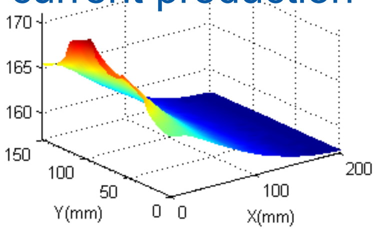

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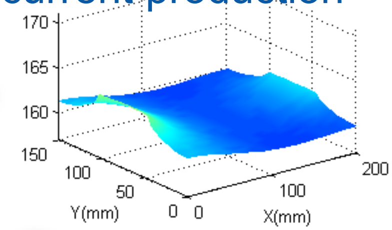

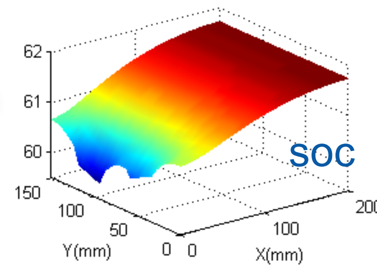

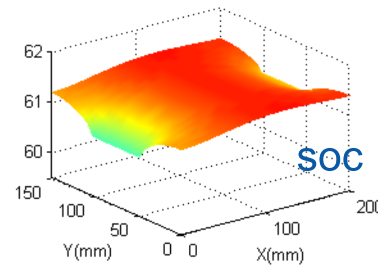

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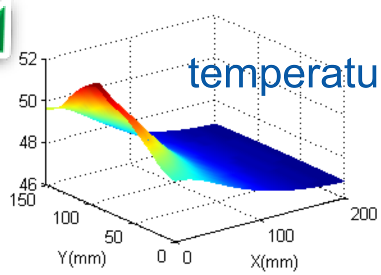
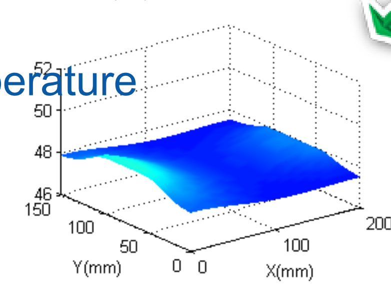


temperature



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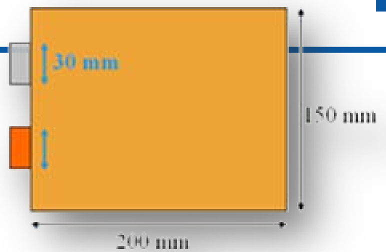

Comparison of two 40 Ah flat cell designs

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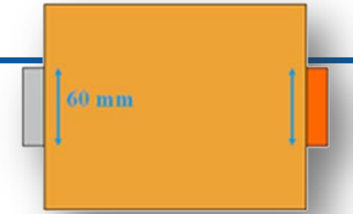

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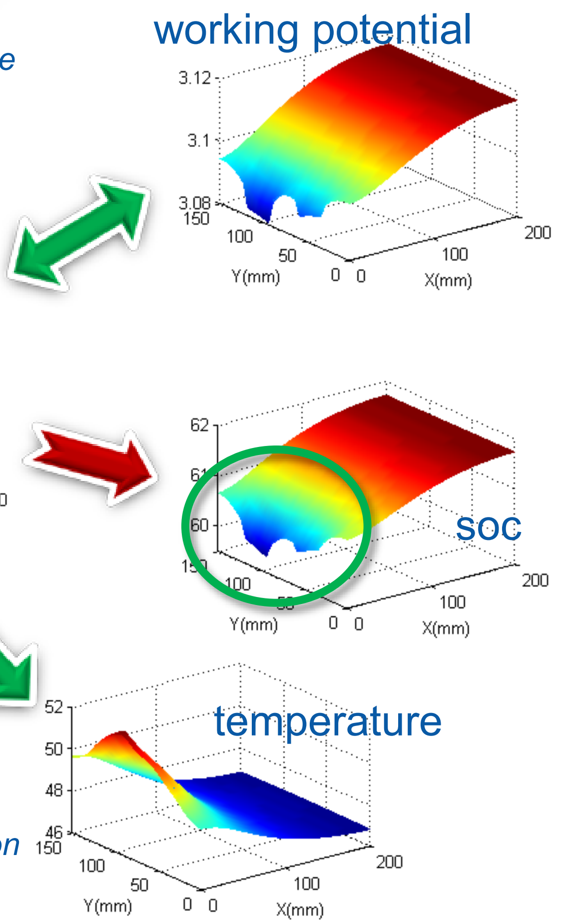

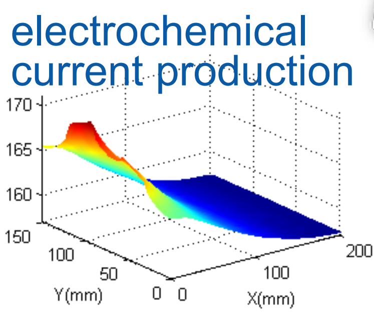

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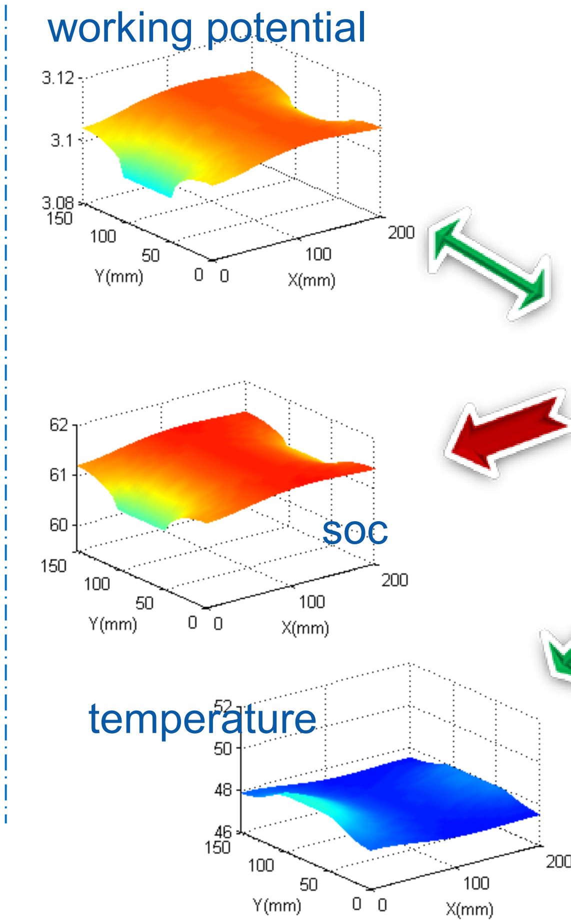
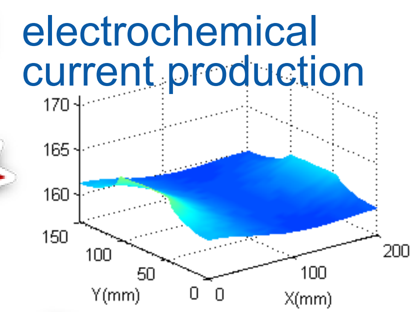
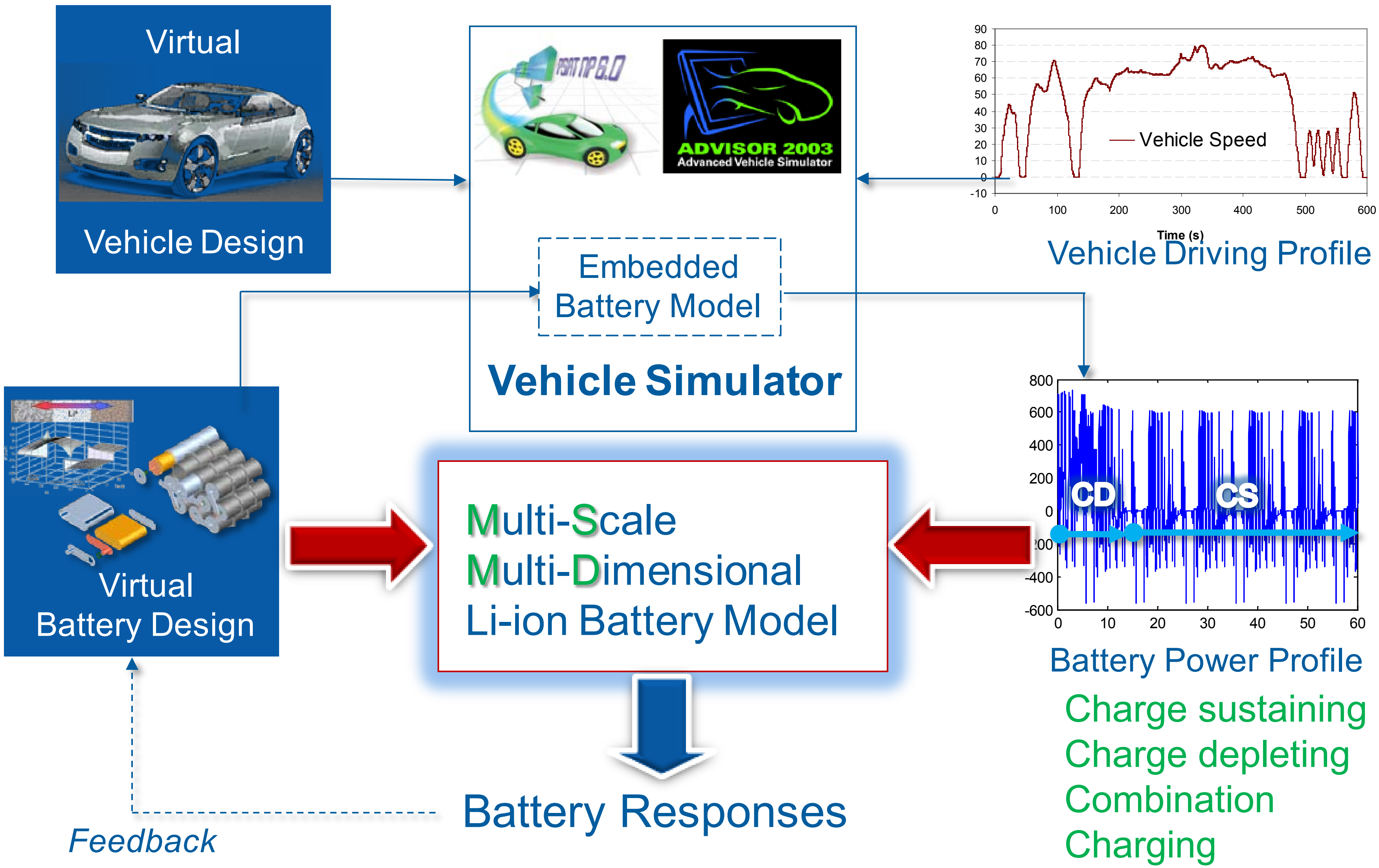


This cell is cycled more uniformly, can therefore use less active material ($) and has longer life.



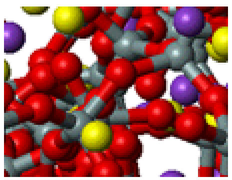
Virtual Design Evaluation
Integrated Battery – Vehicle Approach



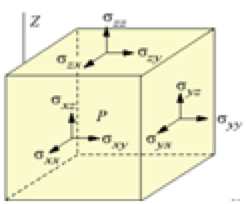
Need to Develop Modular Plug-and-Play Modeling Design Concepts

Material Level Models ⟷ **Electrode Level Models** ⟷ **Component Level Models** ⟷ **Vehicle Level Models**

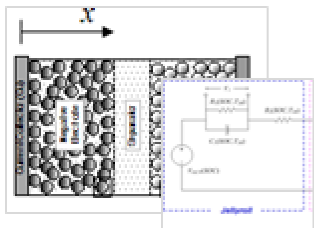
First Principles



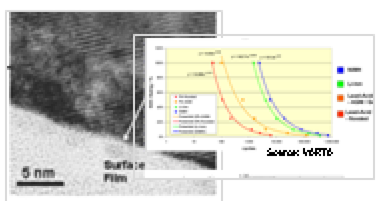
Material Stress



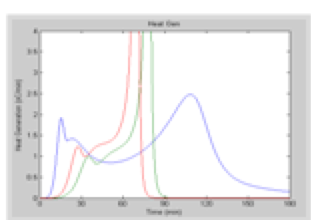
Performance



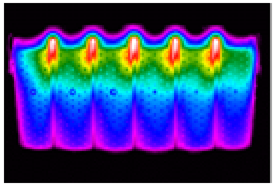
Electrochemical & Material Stress



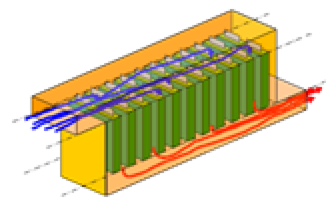
Abuse



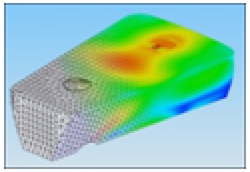
Current & Heat Transport



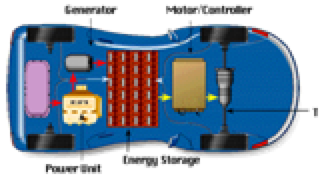
Fluid Dynamics



Stress & Vibration



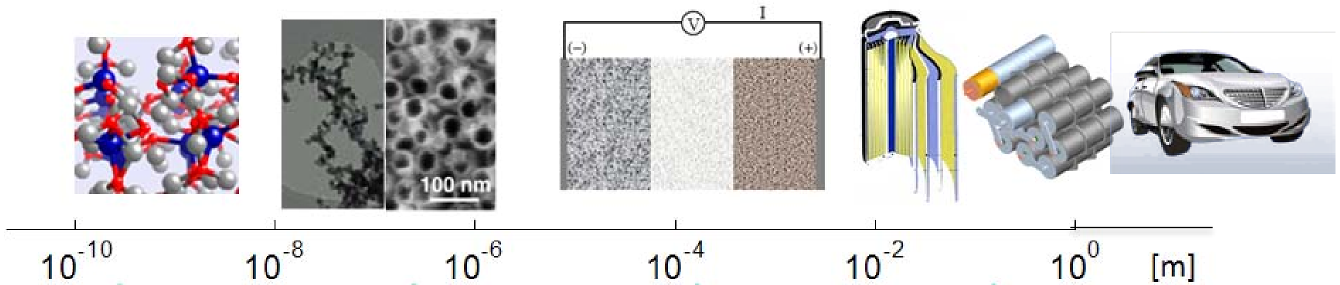
Power Demand



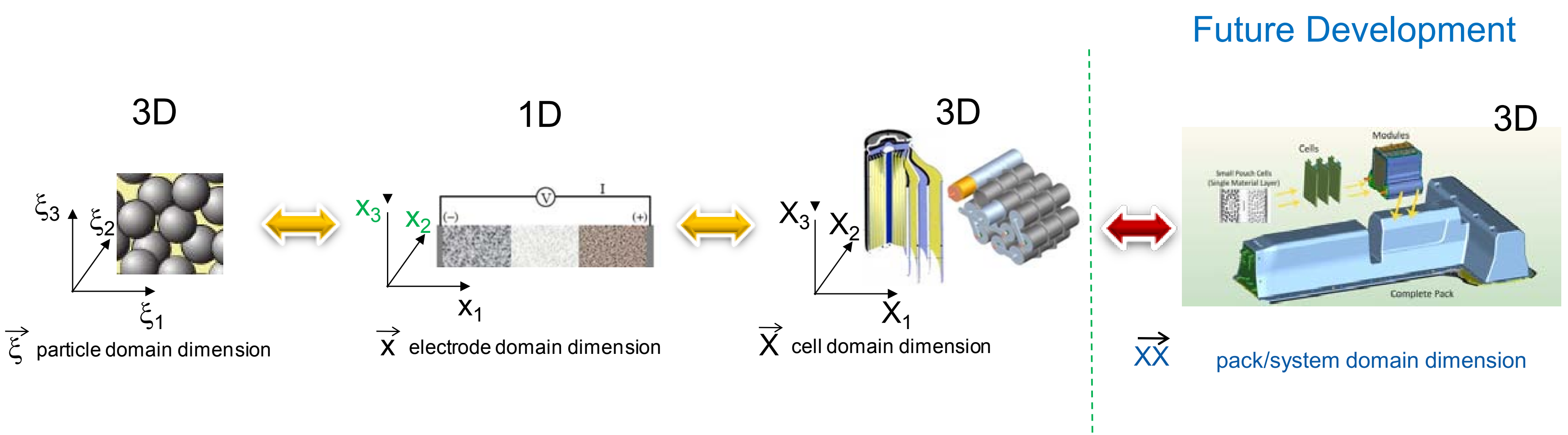
External Thermal Load

Future Plans – Battery CAE

- Integrating various models in one single platform for industry to use
- Bottom-up model validation and demonstration study
- Enhancing physics models



- Enhancing solver capability & solution schemes



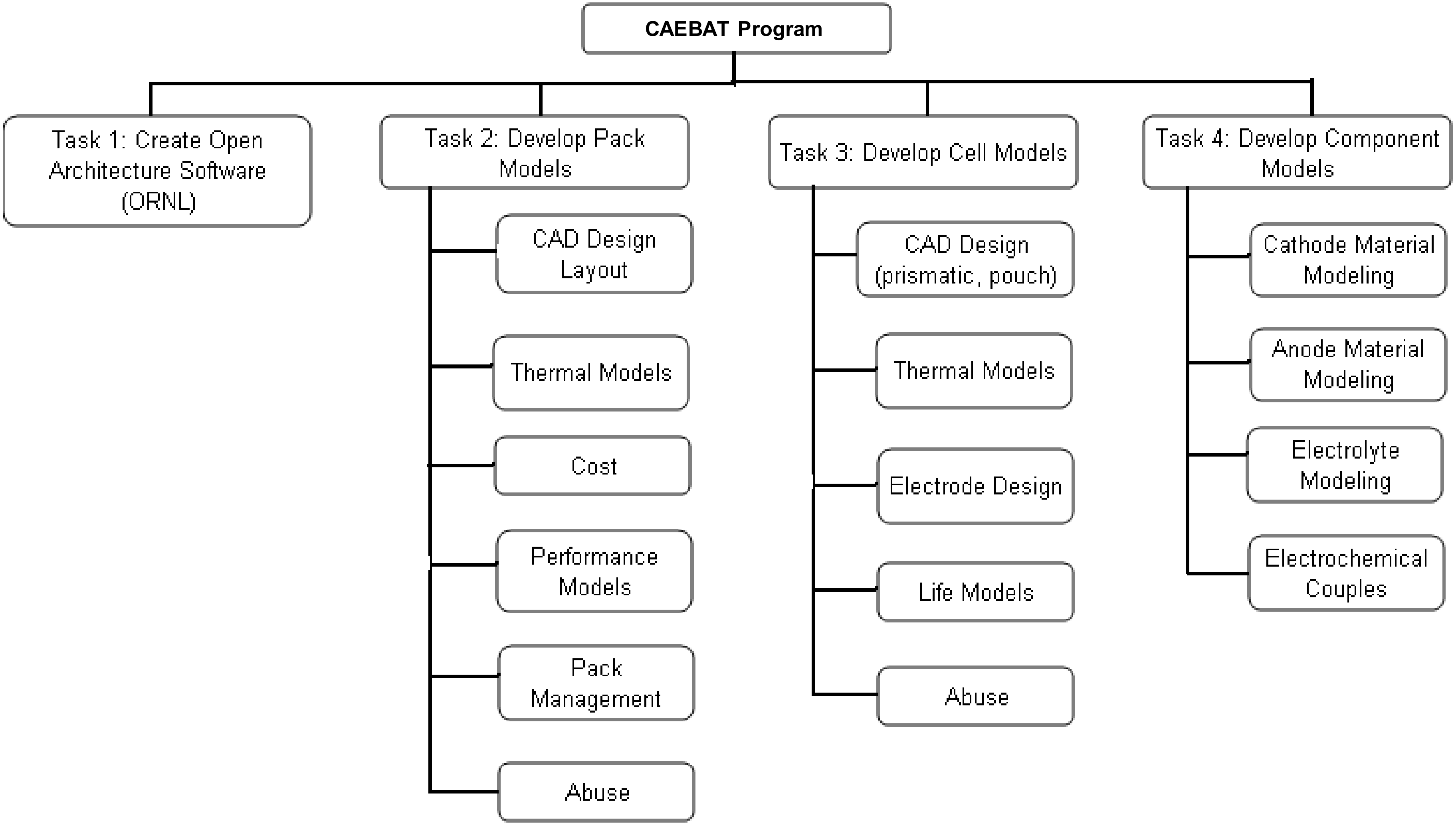
A New Activity – CAE for Batteries

- In the last several years, DOE's Vehicle Energy Storage Program has been funding battery modeling as part of its
  - Exploratory Battery Activity (BATT)
  - Applied Battery Research Activity (ABR)
  - Battery Development Activity
- DOE has been evaluating approaches to integrate these battery modeling activities and make them more accessible as design tools for industry
- In April 2010, DOE initiated implementing the Computer-Aided Engineering for Electric Drive Vehicle Batteries (CAEBAT) activity
  - Objective is to incorporate existing and new models into software battery modeling suites/tools
  - Goal is to shorten design cycle and optimize batteries (cells and packs) for improved thermal uniformity, safety, long life, low cost

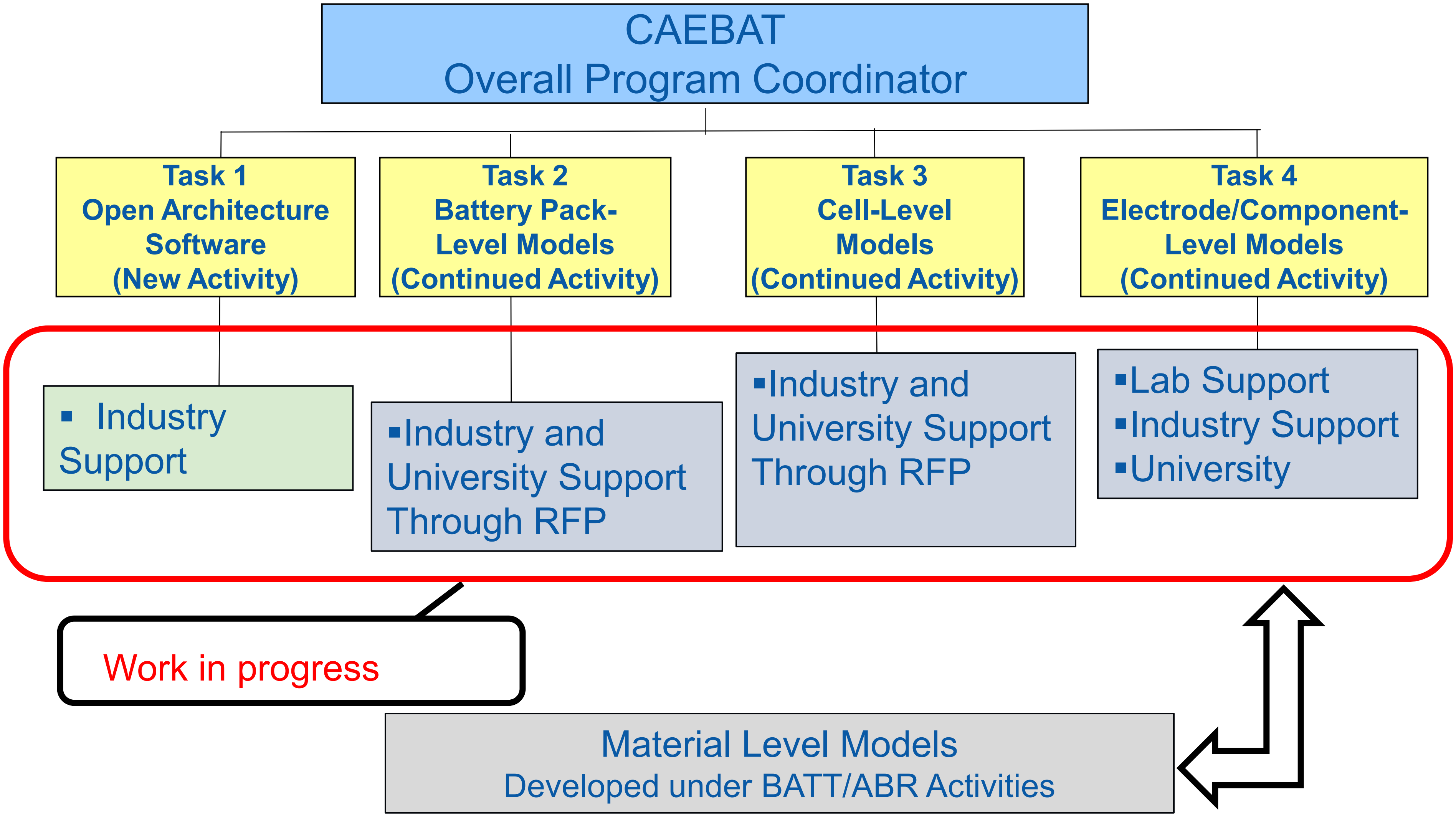
CAEBAT Operating Structure and Plans

- Operate similarly to BATT and ABR activities
- Include several National Laboratories
- One Lab coordinating the activities for DOE (NREL for CAEBAT)
- Include competitive collaborations with universities and industry (cell developers, pack integrators, vehicle makers, and software venders)
- Include structured tasks and subtasks dealing with materials/components, cells, packs, and open software architecture
- Seek collaboration with federal, state, and private organizations for leveraging resources
- Conduct annual planning, progress, and review meetings

Elements of CAEBAT Structure



CAEBAT Program



Planned Activities – CAEBAT Program

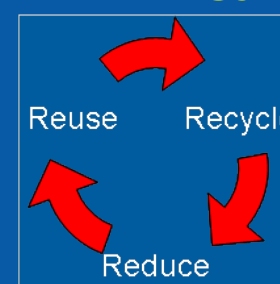
- Interact with other, National Labs, industry, and universities
- Develop detailed description of tasks and overall program plan
- Conduct model development and integration in National Labs and later by industry and universities
- Issue Request for Proposals (RFP) in July, receive proposals, review them, and select awardees by end of September
  - Multi-year, multi-partner projects
- More to come……………….

Secondary Use of PHEV and EV Batteries – Opportunities & Challenges

The 10th Advanced Automotive Battery Conference
Orlando, Florida
May 19-21, 2010

Jeremy Neubauer
Ahmad Pesaran
National Renewable Energy Laboratory

David Howell*
U.S. Department of Energy



Funded by Energy Storage R&D (David Howell),
Vehicle Technologies Program U.S. Department of Energy

Background – Battery Secondary Use

- It is a common belief that batteries in PHEVs and EVs expect to reach the end of their useful life when their capacity, energy, and/or power capabilities drop by 20% to 30%.
  - The reason is to have a vehicle that performs roughly the same at the beginning and end of the life of the battery.
- At the end-of-life, the "retired" PHEV or EV battery may still have reasonable energy capabilities for other applications such as stationary use.
- Secondary use of EVs (mostly NiMH) batteries was briefly studied in the past, but no implementation occurred
  - 1997 ANL study sponsored by USABC
  - 2002 Sentech study sponsored by SNL/DOE
  - "Electric Vehicle Battery 2nd Use Study" by Southern California Edison
- Due in part to the limited market of PHEV/EVs at the time, no second use programs have been implemented yet
  - Sensitivity to uncertain degradation rates in second use
  - High cost of battery refurbishment and integration
  - Low cost of alternative energy storage solutions
  - Lack of market mechanisms and presence of regulation
  - Perception of used batteries

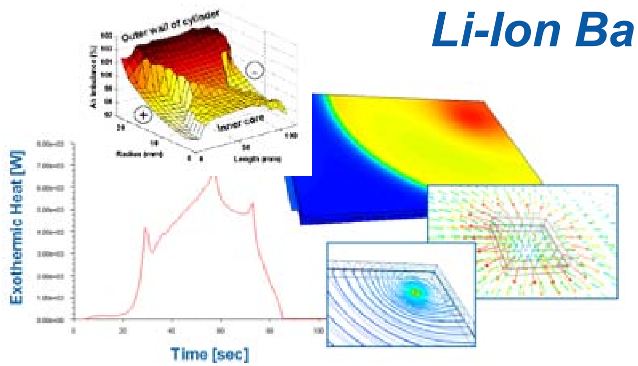
New Interest in Battery Secondary Use

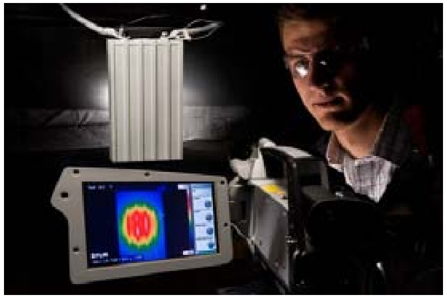
- New opportunities and dynamics for secondary use of "retired" electric drive vehicle batteries
  - Recent strong interest in PHEVs and EVs for reducing emissions, energy security, peak oil, and high price of oil.
  - Improved performance and life Li-Ion batteries, but still with high cost
  - Growing use of renewable solar and wind electricity; increased market penetration may benefit from energy storage
  - New trends in utility peak load reduction, energy efficiency, and load management
  - Smart grid, grid stabilization, low-energy buildings, and utility reliability has the need for energy storage such as batteries
  - Large investment in battery manufacturing for green economy
  - Reducing the initial cost of batteries by the value obtained in second use applications.

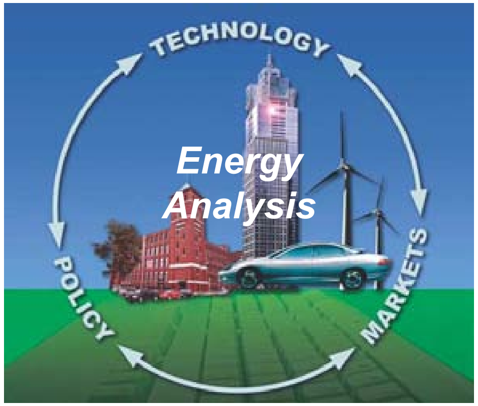
Current Second Use Activities

- **AEP & EPRI**… considering a Community Energy Storage (CES) appliance, which they've stated is *"the ideal secondary market we have been seeking for used PHEV batteries"*
- **UC Davis**… with funding from CEC has released an RFP titled "*Second Life Applications and Value of Traction Lithium Batteries"* to investigate profitable second use strategies and develop a Home Energy Storage Appliance (HESA)
  - The California Center for Sustainable Energy and its partners were selected for an Award
- **UC Berkeley/CEC**… investigated strategies to overcome the battery cost of plug-in vehicles by the value of integrating post-vehicle battery to grid
- **Rochester Institute of Technology**… funded by NYSERDA to investigate the second use of lithium ion batteries
- **Nissan**… has partnered with Sumitomo to initiate a business plan centered on recovering and reselling used automotive batteries
- **Enerdel** … is working with Itochu to develop energy storage systems for apartment buildings to *"help develop a secondary market"* for used batteries
- **Better Place**… is *"evaluating … second life applications for used batteries"* in partnership with Renault-Nissan
- **NREL**… funded by DOE to investigate the potential and value of PHEV/EV battery in second use and obtain data on performance of used batteries

NREL: Uniquely Positioned to Investigate Second Use





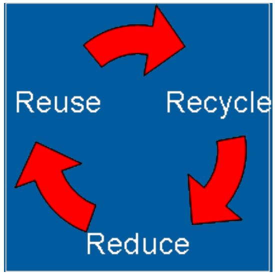


NREL Battery Secondary Use Project

Objective

- Evaluate the merits and value of end of vehicle life batteries for use in other applications – address challenges

Potential Benefits



- Reducing the (first) cost of batteries for PHEV and EV applications
- Reducing the cost and environmental impacts of recycling and disposal of batteries before their “true” end of life.
- Providing advanced inexpensive batteries for nonvehicle applications such as renewable electricity and home use

Approach

Phase 1: Assess Merit → **Phase 2:** Verify Performance → **Phase 3:** Facilitate Implementation

Phase 1: Assess the Merit
Some Second Use Applications

- Grid-Based Stationary
  - Energy Time Shifting
  - Renewables Firming
  - Service Reliability / Quality
  - Home Energy Appliance

- Off-Grid Stationary
  - Backup Power
  - Remote Installations

- Mobile
  - Commercial Idle Off
  - Utility & Rec. Vehicles
  - Public Transportation

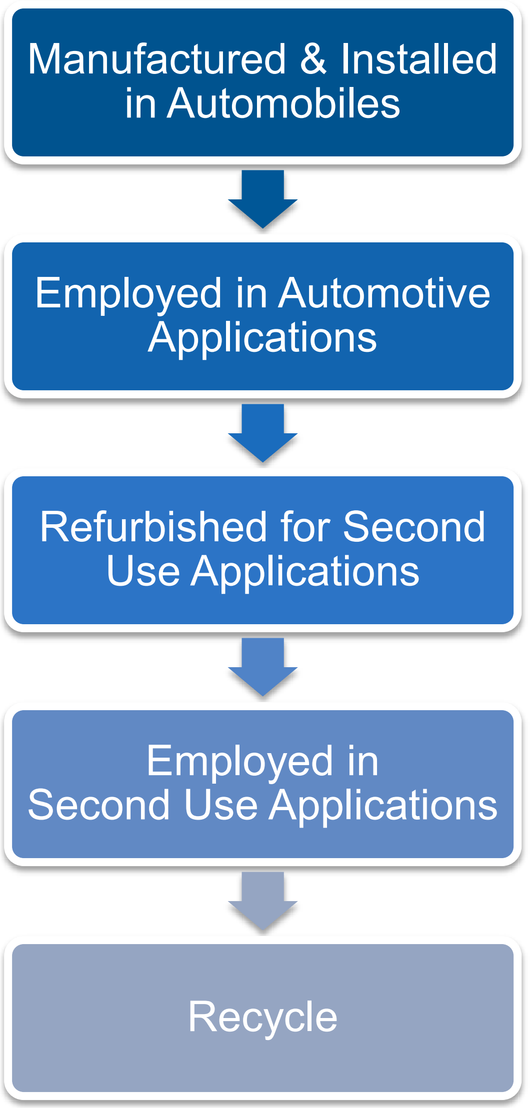
Phase 1: Assess the Merit

Application Identification

- All applications are considered, but high-value / high-impact ones are most desirable
- Accurate use profiles and economic data are needed
- Application value and impact will be estimated before progressing to a detailed investigation
- For each application, consider…
  - How does a battery retired from automotive service perform when subjected to the second use profile?
  - What are the projected revenues and costs?
  - What are the safety concerns and liabilities?
  - How do the performance, life, and cost of a second use battery compare with those of competing technologies?
  - What are the regulatory issues or other barriers specific to this application?
  - Is the scale of this application well suited to the expected availability of retired PHEV/EV batteries?

Phase 1: Optimizing Use Strategies

- For a given second use application, there can be many different ways to implement it
- Changing these variables can have a significant impact on total lifetime value and general feasibility
- In this segment, the use strategy of the battery is optimized via the developed tools and practical considerations



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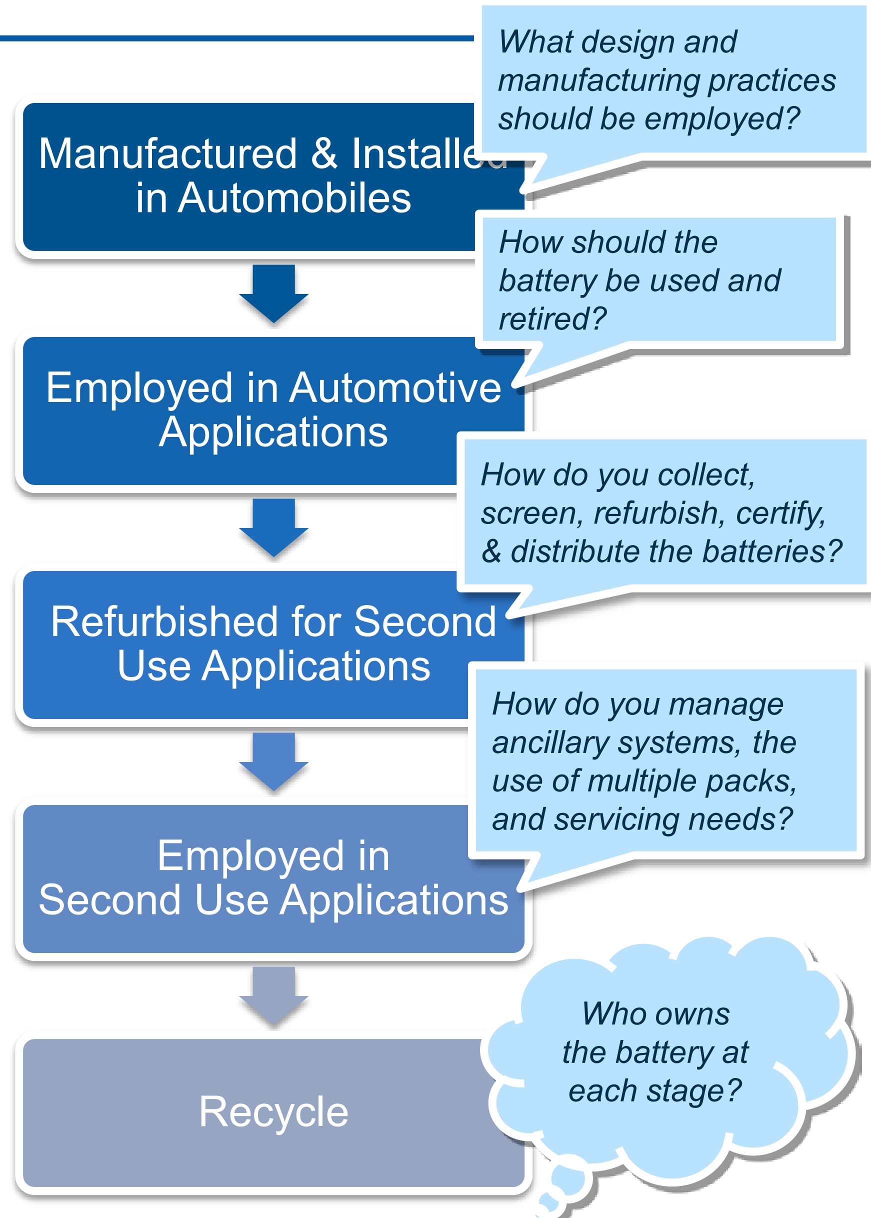
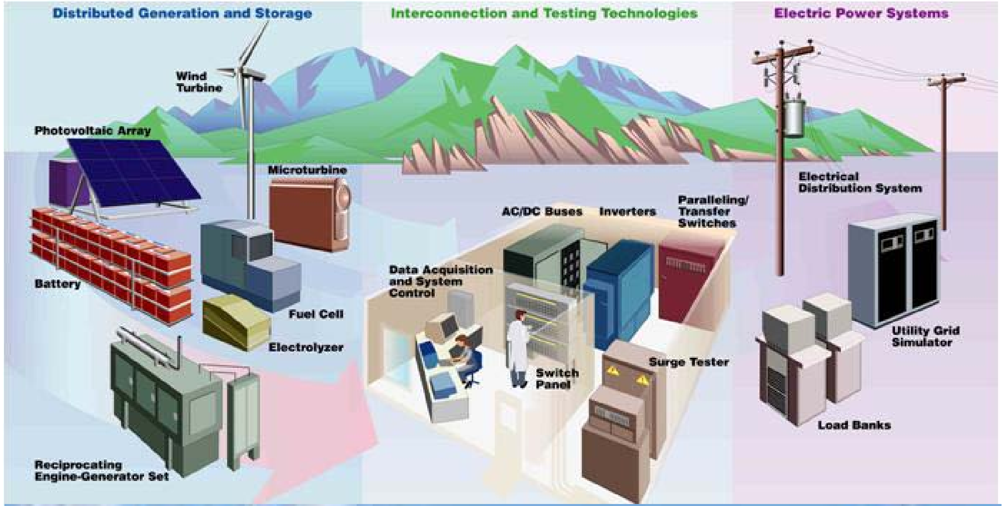


Phase 2: Verify Performance
Conduct Long-Term Testing

- Subject the aged batteries to the expected use profile and conditions of the second use application to verify performance and degradation predictions and lifetime valuations

- Lab testing for precise control of conditions

- Field testing for final demonstration



NREL's Distributed Energy Resources Test Facility could serve as a venue for this phase

Phase 3: Facilitate Implementation of Second Use Projects

- **Disseminate study findings** to inform the market of the potential profitability of the second use of traction batteries
- **Provide validated tools and data** to industry
- **Develop design and manufacture standards** for PHEV/EV batteries that facilitate their reuse
- **Propose regulatory changes** to encourage the reuse of retired traction batteries in other applications

Planned Work – Battery Second Use

- NREL is currently seeking partners to investigate the reuse of retired PHEV/EV traction batteries to reduce vehicle cost and emissions as well as our dependence on foreign oil.
- A Request for Proposal (RFP) was issued in April 2010 seeking a subcontractor to accomplish the aspects of this effort.
  - You can find RFP No. RCI-0-40458 at www.nrel.gov/business_opportunities - current solicitations.
  - Proposals are due near the end of May 2010 (extended to early June 2010).
  - If you have questions regarding the RFP, please contact Kathee Roque at Kathee.Roque@nrel.gov.
- A workshop to solicit industry feedback on the entire process is also being planned.
- Aged batteries will be tested in 2-3 suitable second-use applications.
- Hope to answer the questions, “Do PHEV/EV batteries have any value for other application? What are the barriers?”

Concluding Remarks

- Computer-Aided Engineering for Automotive Batteries
  - DOE is supporting efforts to bring industry and National Labs together to develop a suite of software tools for accelerating the design of cells and packs.
    - A new program has been initiated to bring all the modeling together
  - NREL has multiple modeling tools and will be collaborating with partners to integrate them for industry use.
    - NREL will be issuing RFPs for collaboration in this area
- Secondary Use of PHEV and EV Batteries
  - DOE is supporting efforts to evaluate the second use of retired lithium ion batteries to identify if second use batteries could reduce the initial cost of PHEV and EV batteries.
  - NREL is involved technically and will collaborate with partners.
    - NREL has issued an RFP for collaboration