Thermal & Electrochemical Simulation Of Battery Pack Systems
CD-adapco Battery Modeling Technology

**Micro-structure Electrochemistry**
- Virtually test SEM produced electrode geometry

**Cell Design Tool**
- Build physics based models of electrode pairs and couple them to the cells physical construction
- Use the provided database of materials to construct virtual cells and test their performance

**Module & Pack Analysis**
- Flow, thermal & Electrochemistry analysis of complex power systems
- Study detailed spatial effects at cell, module & pack level

**Overall System Design**
- Interface Module & Pack analyses with complex power train system models
- Embed physics based or empirical models into power train systems models

*Provides previously unseen spatial effects within electrodes*  
"Design" next generation electrodes
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Micro-structure Electrochemistry

- A genuinely unique tool which predicts the spatial distribution of ions and potential within an arbitrary, multi-phase microstructure region
  - Electric Potential in solid and electrolyte regions
  - Salt concentration in electrolyte
- Concentration of Li in active parts of electrode

Use STAR-CCM+ CAD tool to improve binder’s network realism
A VARTA LIC 18650 WC LiCoO2 battery was segmented by FIB-SEM and reconstructed**. A 21 million cell finite volume mesh was created including active material, secondary conductive phase and electrolyte fluid phase*.

*Presented at Solid State Electrochemistry Workshop 2013 held at Heidelberg

**Hutzenlaub et al. 2012 Three-Dimensional model development for lithium intercalation electrodes, J. Power Sources 185(2)

Three-dimensional electrochemical Li-ion battery modelling featuring a focused ion-beam scanning electron microscopy based three-phase reconstruction of a LiCoO2 cathode, Hutzenlaub et.al. Electrochimica Acta - 2014

“Primary use is the design of next generation battery electrodes”
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**Pouch**

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Cell Design Tool

- A comprehensive design environment which links a physics based electrochemistry model with a sizing program, enabling the electrochemical and physical design of a cell to be studied.

- Building any shapes – Stack, wound prismatic & wound cylindrical.

- Performance degradation – Calendar Aging Model
  - Run a 1 year aging simulation.
  - Compare “Initial” with “aged” cell performance.
Discharge Response

- Sanyo LiNi0.33Mn0.33Co0.33O2 18650 cell (2.05Ahr)
- Cells disassembled and physically characterized
- C/5 to 2C discharge rate

- Errors within 6.5% over total discharge
- Errors within 2.8% over 60% SOC window

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CAEBAT Work – Single Cell Analysis

*Johnson Controls Inc. VL6P cell (6Ahr)*
- Detailed flow, thermal & electrochemistry model created in STAR-CCM+
- Cell model features electrode discretization
- Liquid cooled installation
- US06 drive cycle derived load applied to model

The authors would like to acknowledge JCI’s contribution to the testing work within the CAEBAT project and also their approach to this collaborative project, specifically Brian Sisk and Kem Obasih.

The authors would also like to acknowledge the Department of Energy’s co-funding of this project, specifically Dave Howell & Brian Cunningham as well as NREL’s Energy Storage team, specifically Ahmad Pesaran & Kandler Smith.
CAEBAT Work - Module Analysis

Johnson Controls Inc 12 cell module

- Detailed flow, thermal & electrochemistry model created in STAR-CCM+
- 12 cell module, each with electrode discretization
- Liquid cooled system
- Transient electrical/thermal boundary conditions

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Overall System Design
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- Link to system design software
  - Matlab Simulink & AMEsim dominant
- Example – AMEsim hybrid vehicle system coupled to electro-thermal module model
- Equivalent circuit battery model representation
- Driving a NEDC cycle
Overall System Design

- Increased fidelity of Battery model
- Changing voltage > varying current
- Point Temperatures vs Integrated/average Temperatures
Example Thermal Abuse Modelling

- Full Pack CAD Representation
- Circuit layout
- CAD representation: cell internals
- CAD representation: cell internals
- CAD representation: Jelly rolls
- Maximum Jelly Roll Temperature

Simulation of abuse tolerance of lithium-ion battery packs
A three-dimensional thermal abuse model for lithium-ion cells
Conclusion

With access to a wide range of length scales
And to high-fidelity performance models
Combined with multi-physics
It is possible to simulate complex systems from material to full EV assembly
And complex problems such as drive cycles tests, abuse etc…

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