Development of Computer-Aided Design Tools for Automotive Batteries

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General Motors R&D Center

Date: June 17, 2014

Project ID # ES119

Overview

Timeline

- Start – June 2011
- Finish – Dec 2014
- 75% Complete

Budget

- Total project funding: $7.1 M
  - DOE - $ 3,540 K
  - Contractor – $ 3,540 K
- Funding received
  - FY 12: $ 1,488 K (6/11 – 12/12)
  - FY 13: $ 1,267 K (1/13 – 12/13)
  - Total: $2,755 K
- Funding for FY 14
  - $785 K

Barriers

- Barriers
  a) Lack of validated computer-aided engineering tools for accelerating battery development cycle
  b) Complexity of multi-scale, multi-physics interactions
- Targets -shorten time and cost for design and development of EDV and HEV battery packs

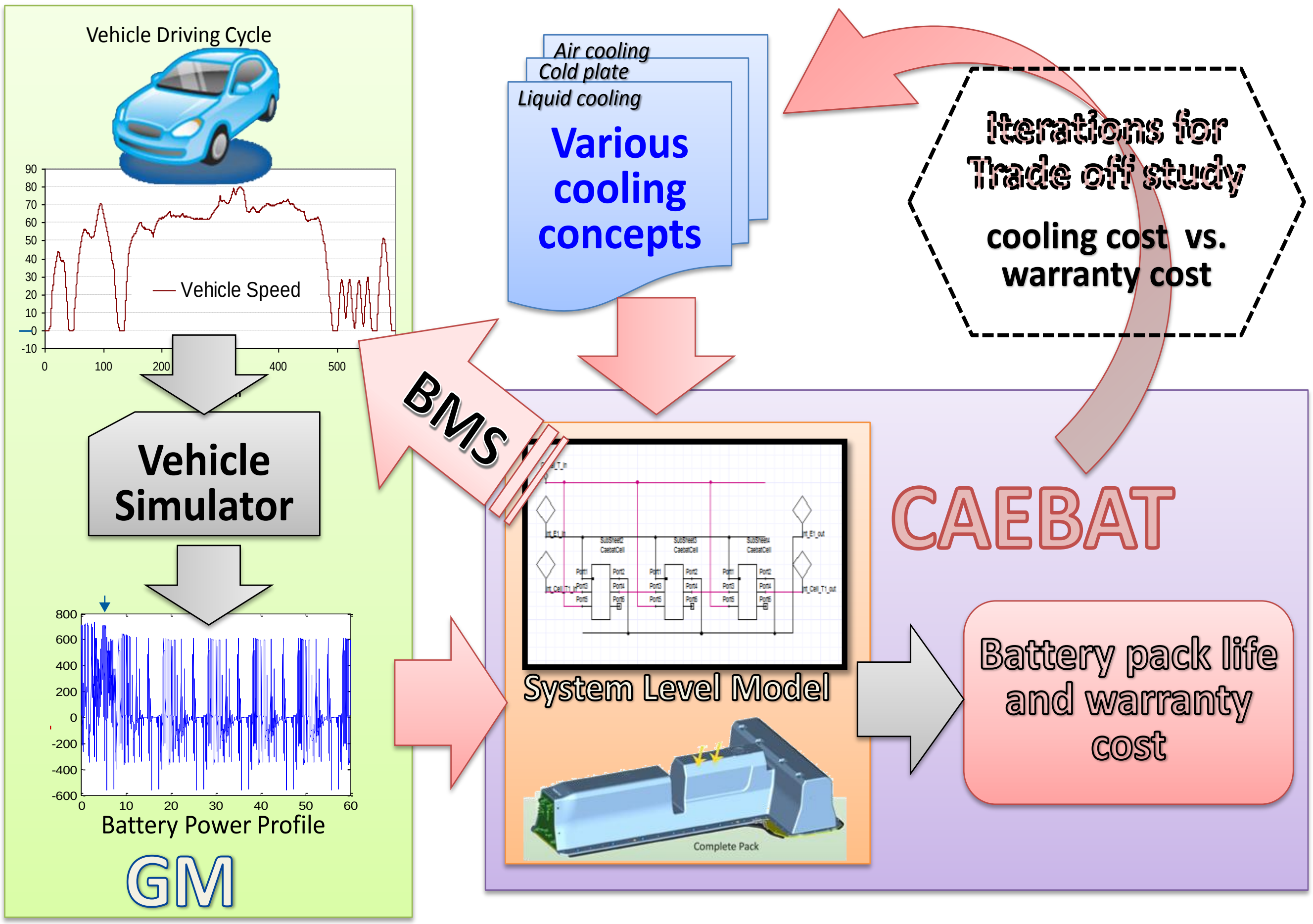
Partners

- GM : End user requirements, verification/validation, project management
- ANSYS : Software dev. and commercialization
- ESim : Cell level sub models, life model
- NREL : Technical monitor

Project Lead: GM R&D Center

Funding provided by Dave Howell of the DOE Vehicle Technologies Program . The activity is managed by Brian Cunningham of Vehicle Technologies.
Subcontracted by NREL, Gi-Heon Kim Technical Monitor

Project Relevance/Objectives: faster design cycles and optimize batteries (cells and packs) for improved performance, safety, life, and low cost.



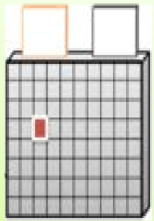
- Address multi-scale, multi-physics interactions
- Provide flexibilities
- Expandable framework
- Validate models

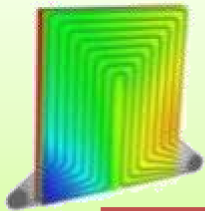
Ability to provide trade off studies between various cooling concepts and the battery pack life.

Milestones

Month /Year	Milestone or Go/No-Go Decision	
Feb-2013	Go/No-Go decision: Deliver the cell level simulation tool. The cell level model includes three sub models and a scale coupling based on MSMD approach.	Complete
June-2013	Milestone: Validation of the cell level model. Deliver the first pack level model. The pack level model includes a system level capability with reduced order models (ROM).	Complete
Sept-2013	Milestone: System level simulation software tool was delivered. LTI (Linear Time Invariant) system level ROM model approach has been validated in comparison with the full field simulation results.	Complete
Dec-2013	Go/No-Go decision: Official public release of ANSYS (version 15) that includes user defined electrochemistry models that allows user to apply their own models while utilizing FLUENT's battery framework.	Complete
Jan-2014	Milestone: System level model without ROM was completed and validated compared to the full field simulation and the test data. Demonstrated System simulations for US06 drive cycle. Demonstrated LTI ROM for US06 drive cycle.	Complete
Dec - 2014	Milestone: Develop CAE process automation for the pack level simulations. Implement cycle life and abuse models. Incorporate NREL's multi-particle model. Incorporate the Open Architecture Software interface. Deliver the final pack level design tools.	On track

Project Approach





Cell Level Model (Full field simulation)

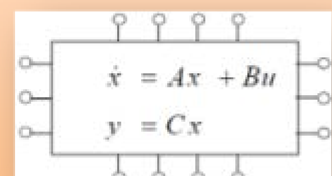
- Full field simulation based on CFD and electrochemistry model
- Cell level performance including various cooling concepts

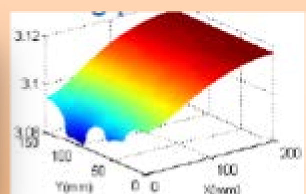
Pack Level Model

Co-simulation

Reduced-Order Models

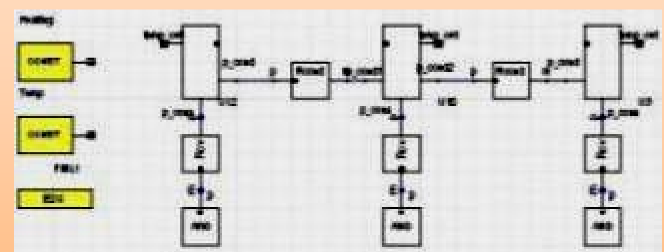
- Reduced order models for flow and thermal analysis at the pack level





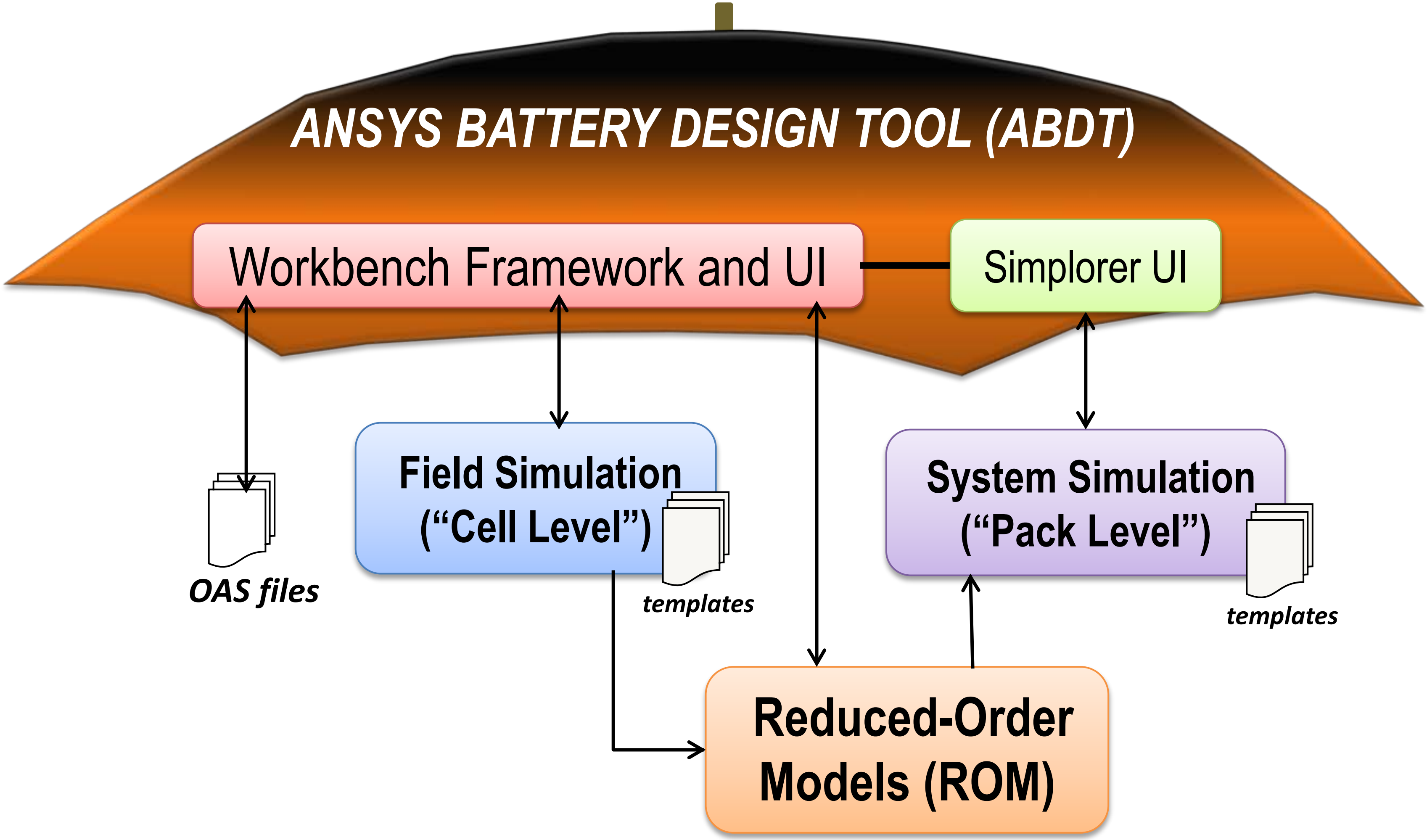
System Level Model

- Construct a “linear” or “non-linear” system simulation model from the full pack simulation model



Strategy is to offer a wide range of methods allowing analysts to trade off computational expense vs. resolution

Roadmap for Battery CAE Tools

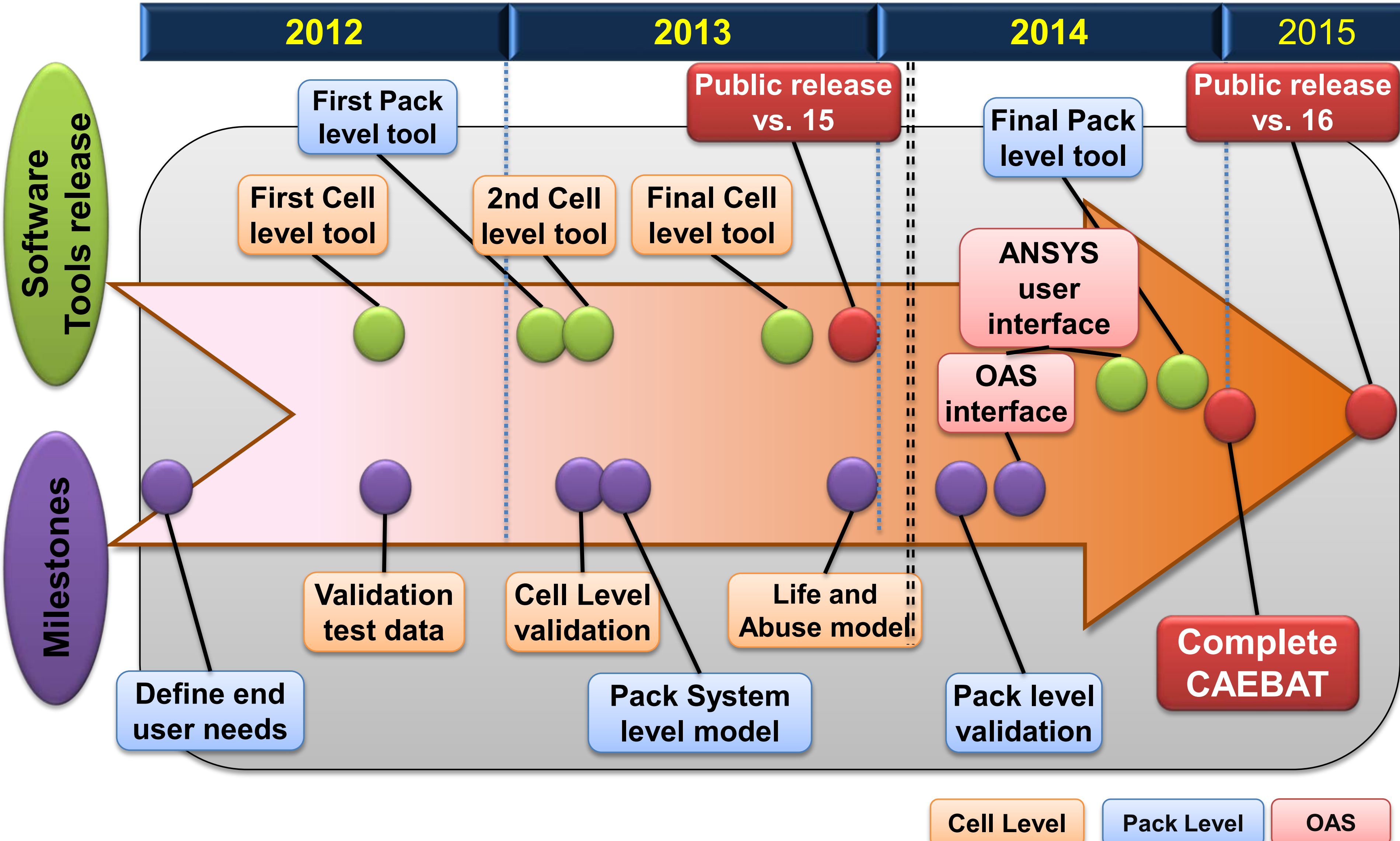


ABDT is the "umbrella" over all capabilities, including the graphical user interface (UI) that automates/customizes battery simulation workflow, leveraging ANSYS commercial products.

Technical accomplishments

- The ANSYS Battery Design Tool (ABDT) has been developed by utilizing the ANSYS Workbench Framework. This framework facilitates the integration of existing applications with external tools to create a seamless workflow.
- Model validation is completed for the cell level and module level and is on-going for the production pack level.
- Physics based cycle life model has been developed based on a P2D model for the LG cell and a simpler version of equivalent-circuit model (ECM) was derived for a potential cycle life model.
- NREL has developed a udf (user defined function) for multiple particle/multiple active material models for GM team.
- Linear ROM model developments are on target.
  - LTI system level model approach has demonstrated for practical simulations of the entire pack for both air and a liquid cooling.
- Explored the non-linear ROMS such as POD/DEIM (Proper Orthogonal Decomposition / Discrete Empirical Interpolation Method) for simulating nonlinear realistic battery packs.

Project Timeline

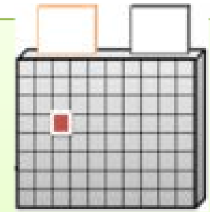


Validation of CAEBAT Tools

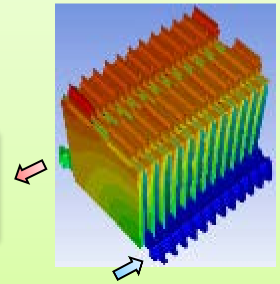
Cell/Module

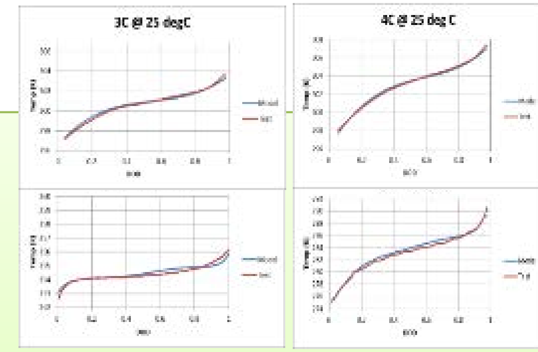
Full Field Simulation

Cell



Module



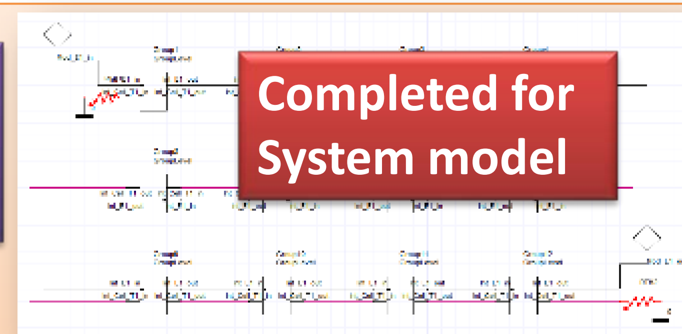


Completed for Cell and Module level

Pack/Module

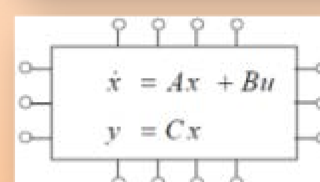
System Level Simulation

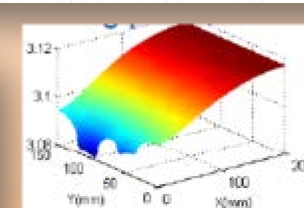
System model without ROM

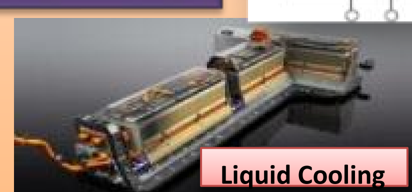


Completed for System model

System model with ROM

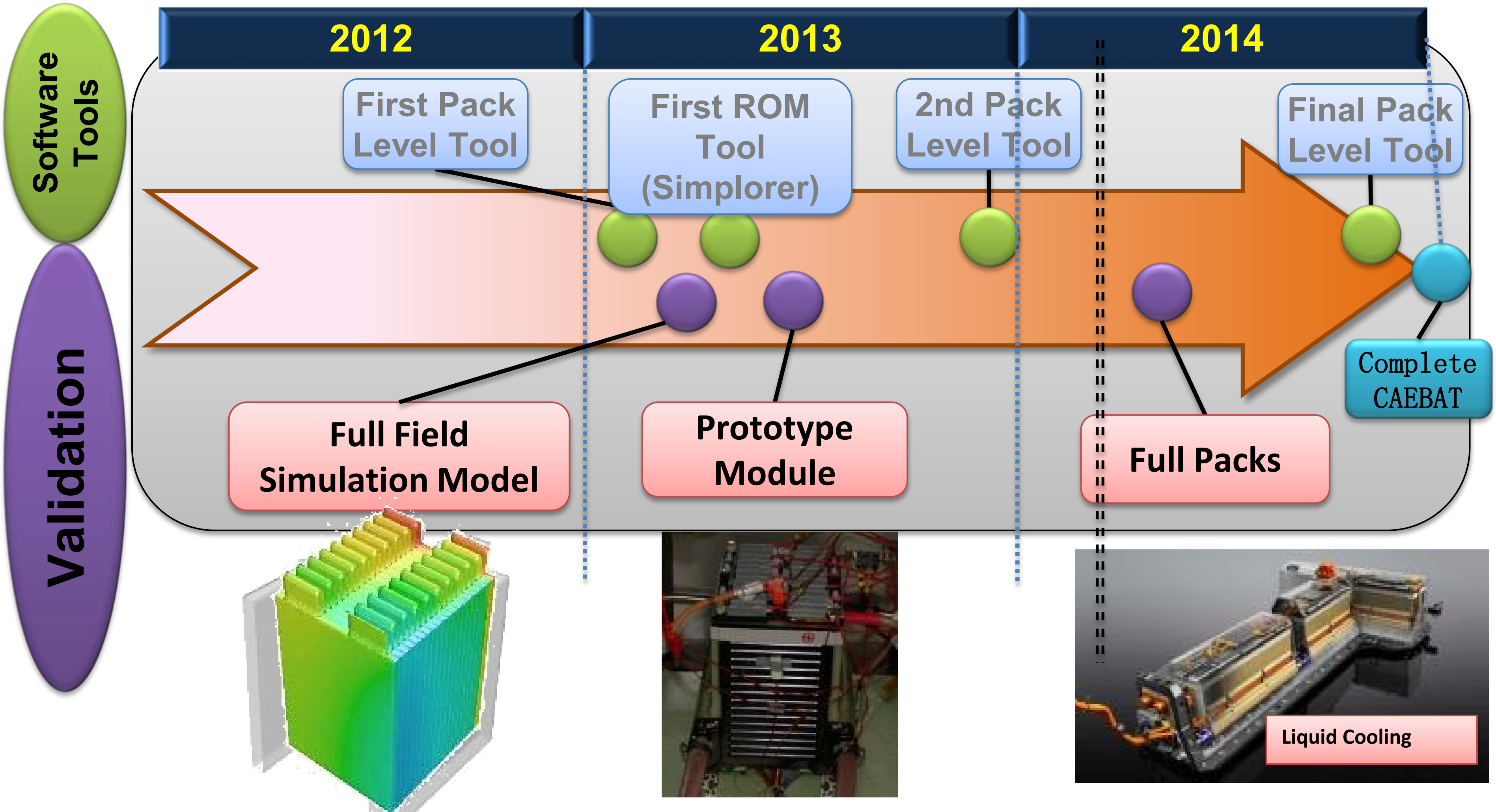






On target

Pack Level Validation Time Line



To validate the system level models with ROM models.

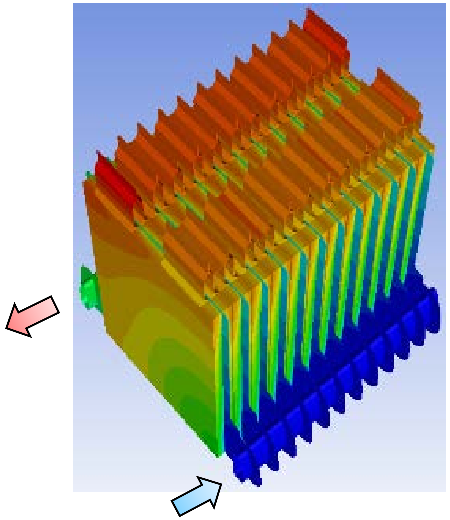
To validate for both full field and the system level simulation.

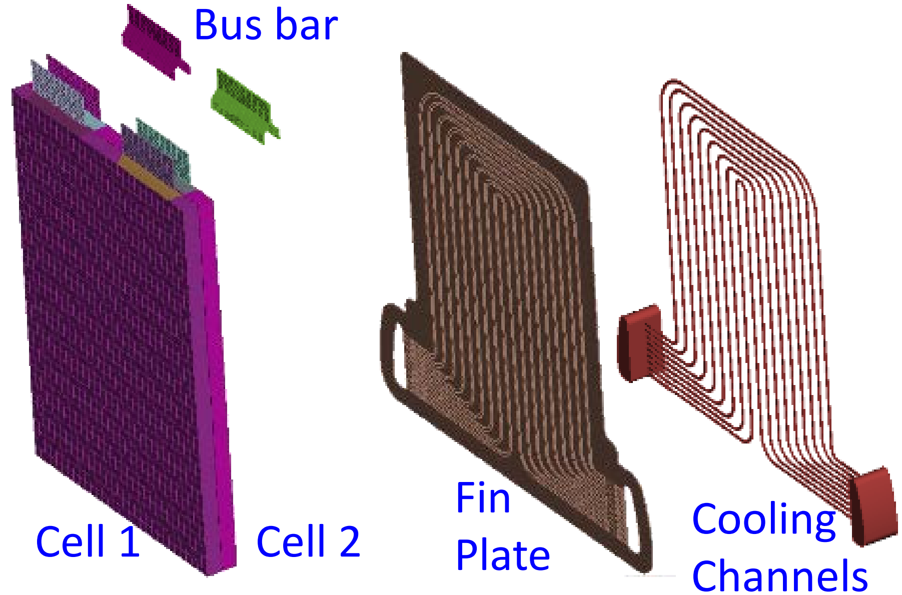
To validate for system level simulations

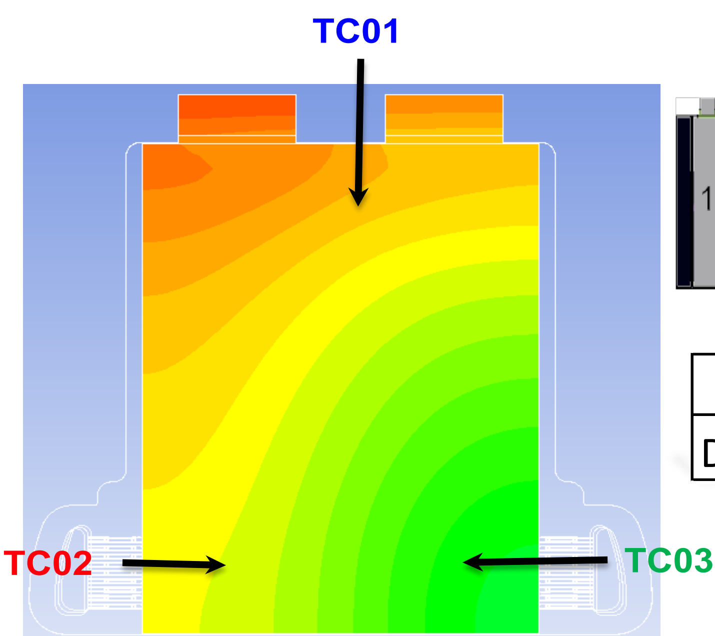
Validation of Full Field Simulation

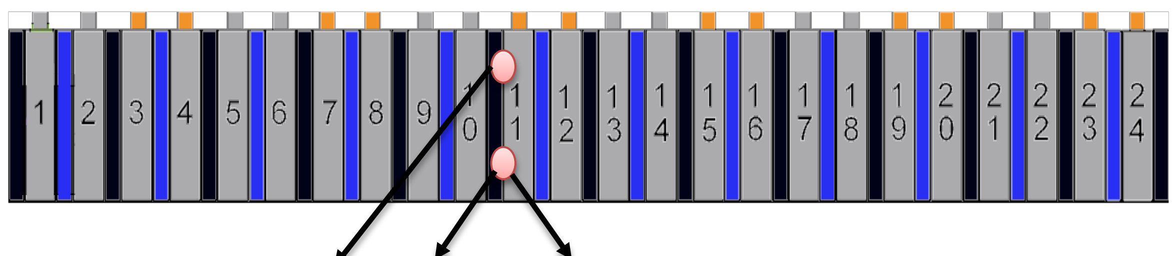
24 cell prototype

Temperature Profiles





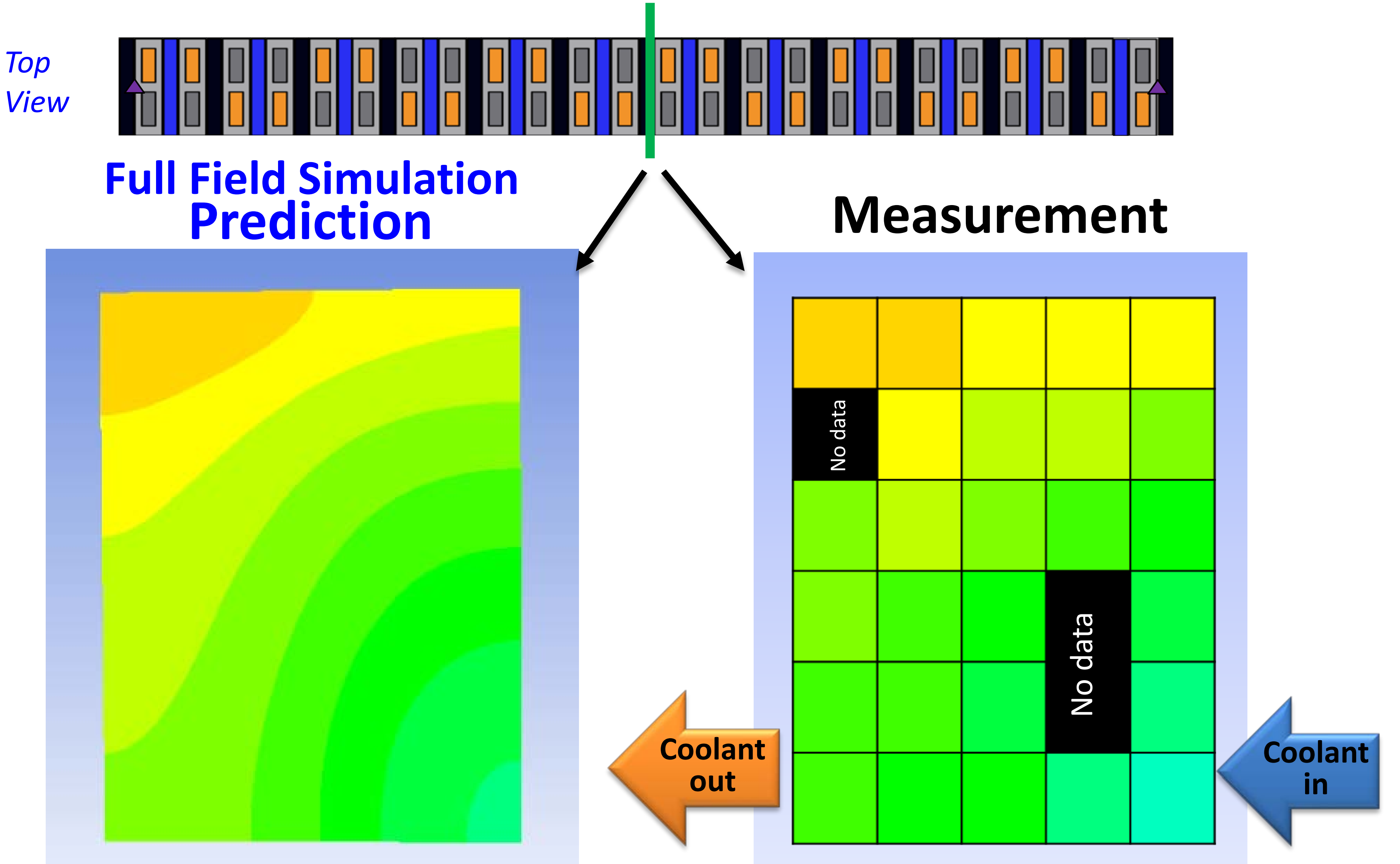




	TC #01	TC #02	TC #03
Diff, ^{o}C	0.8	0.3	-0.7

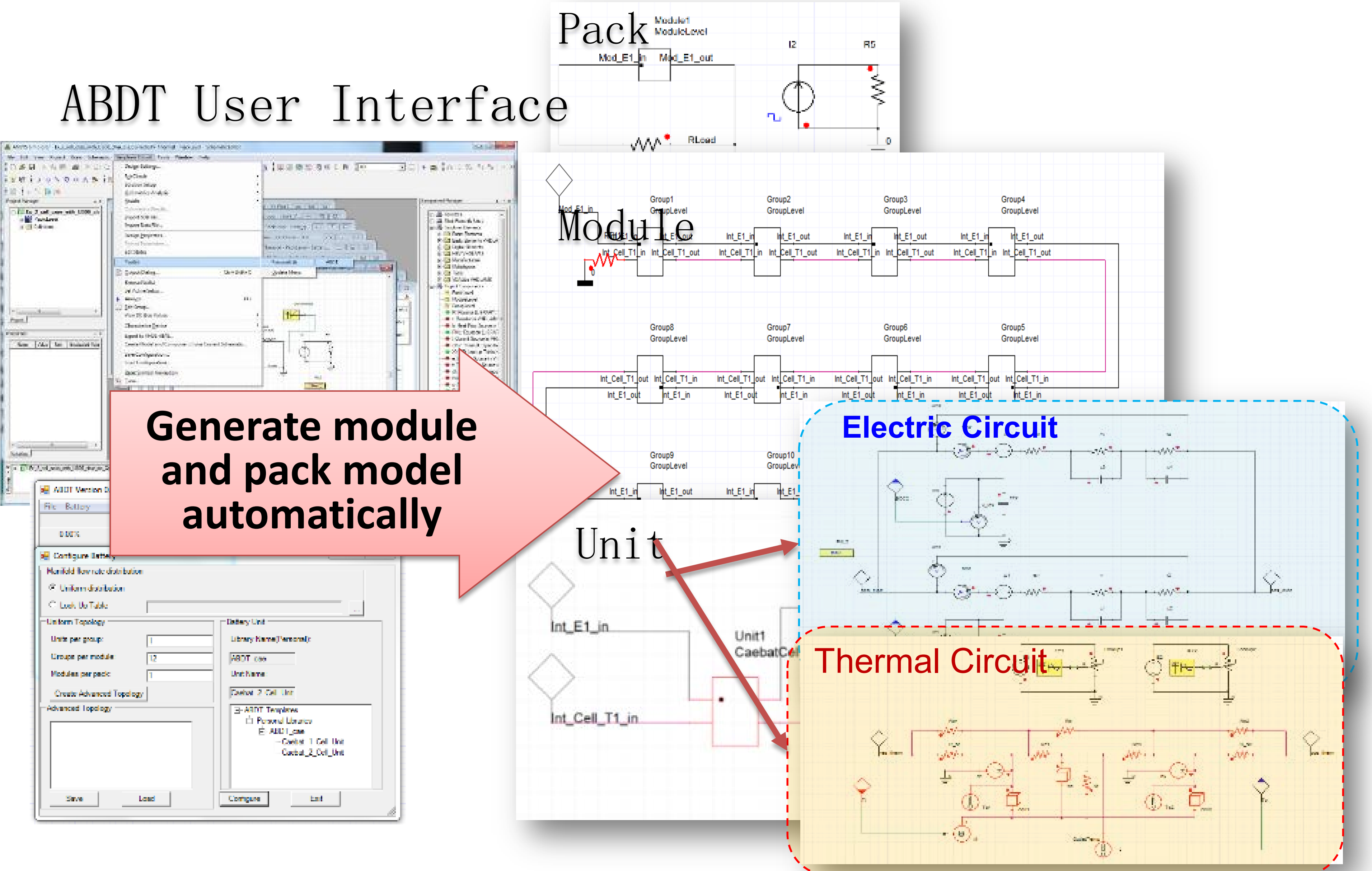
A 24 cell module validation test set up for full field simulation against test data for high-frequency pulse charge-discharge.

Validation for 24 Cell Module

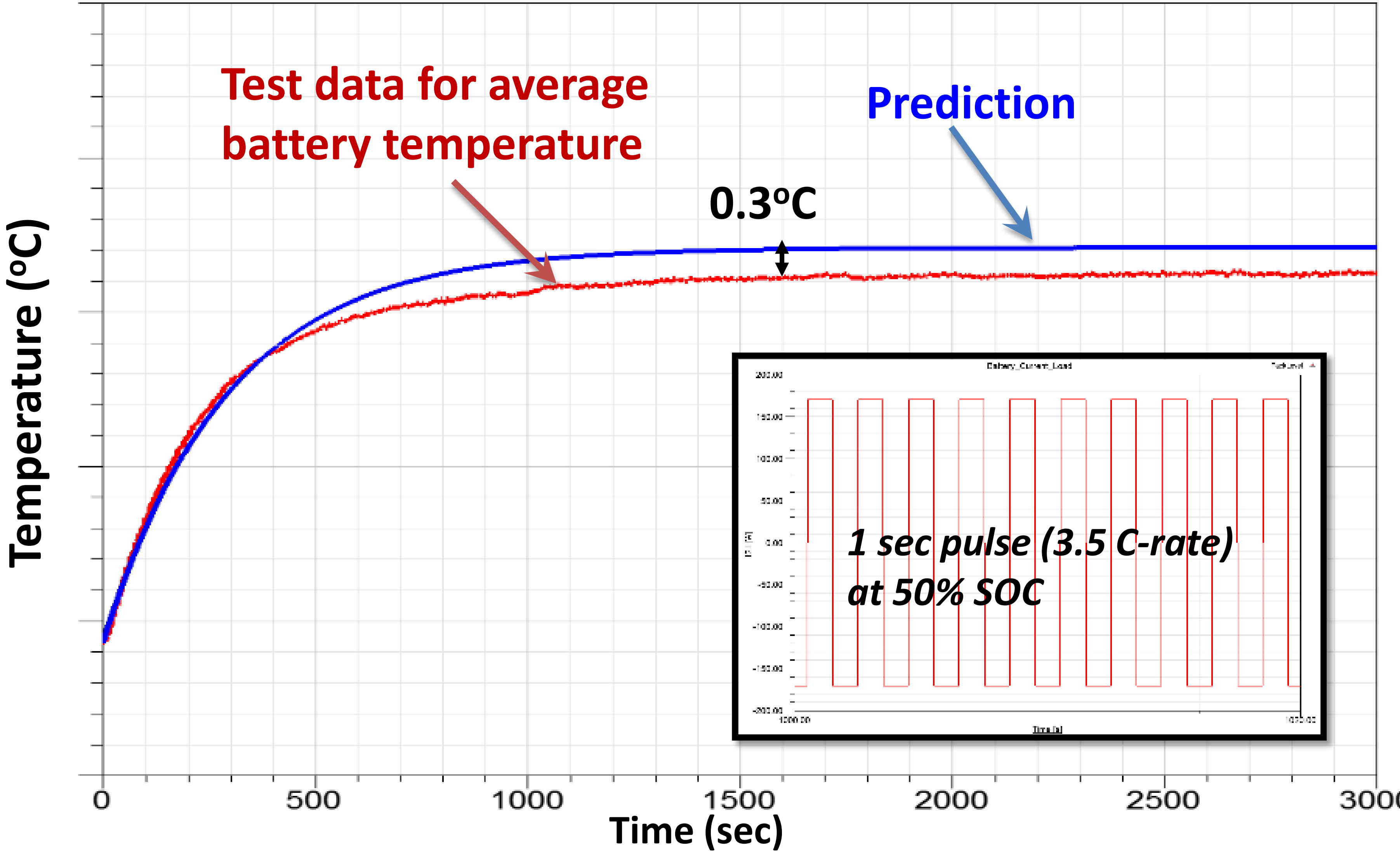


Maximum difference between the prediction and the measurement is within 1 ^{O}C.

System Simulation for 24 Cell Module

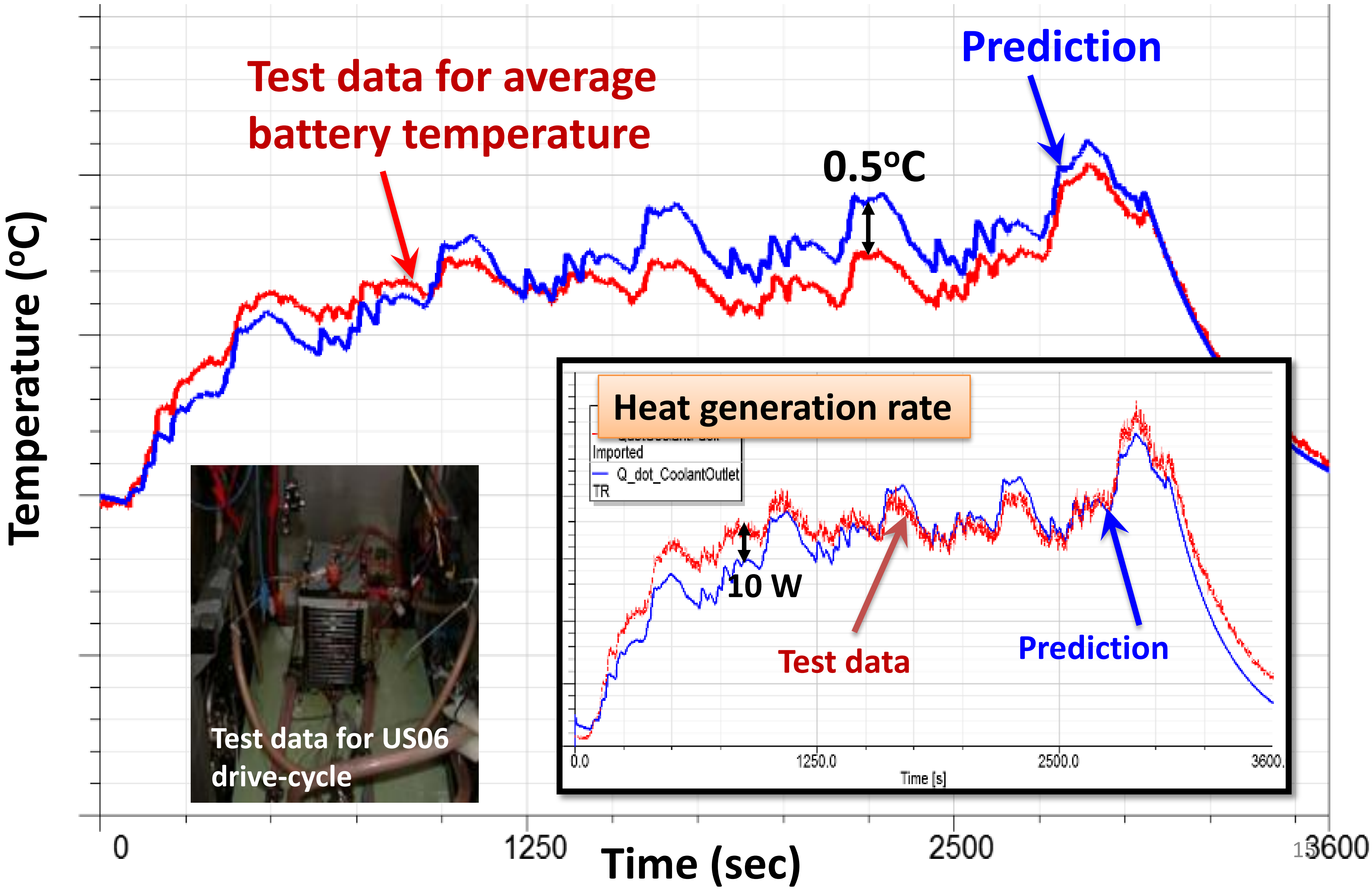


Validation of System Simulation

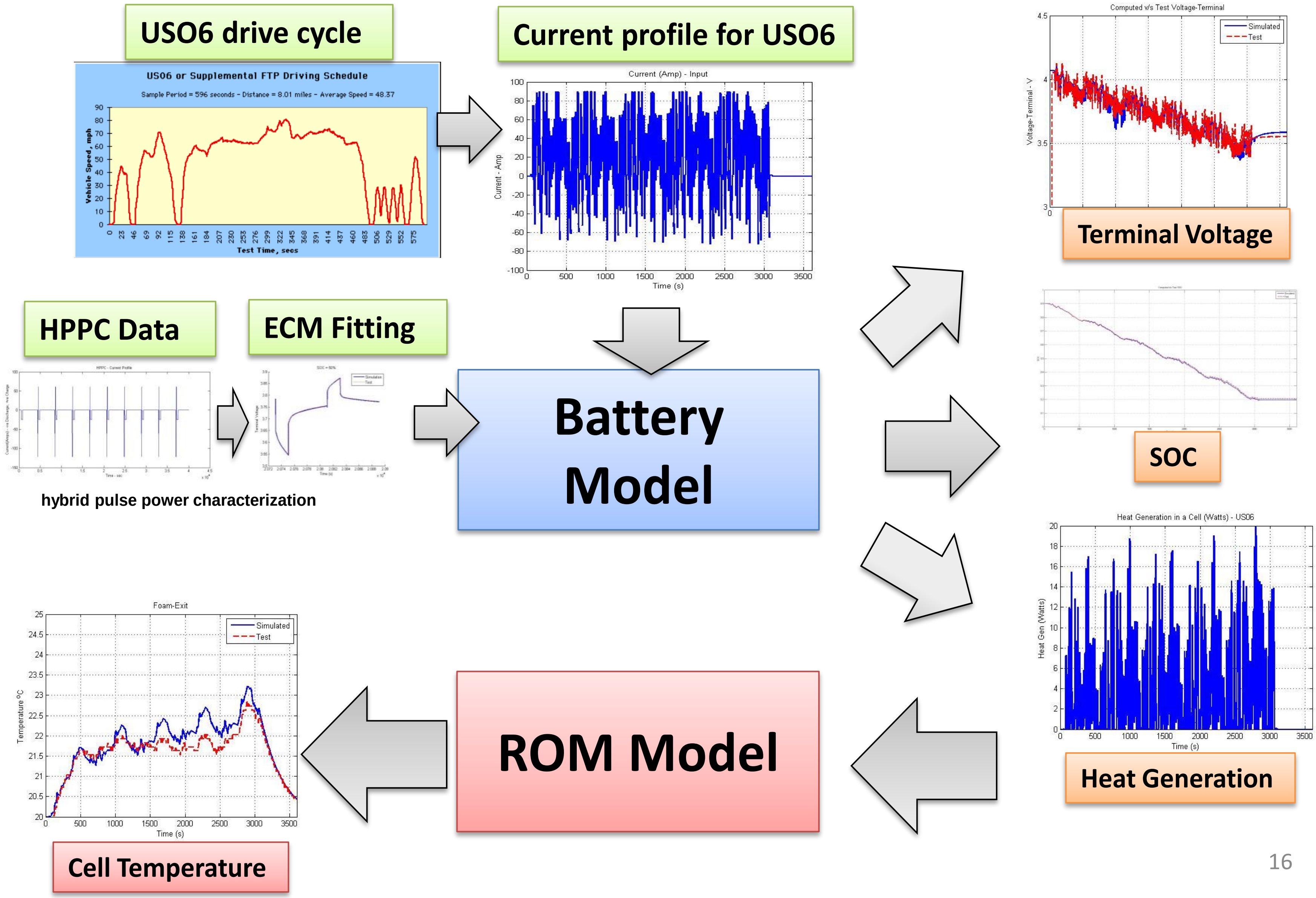


System simulation without ROM reproduced electric and thermal characteristics which are comparable to the test data

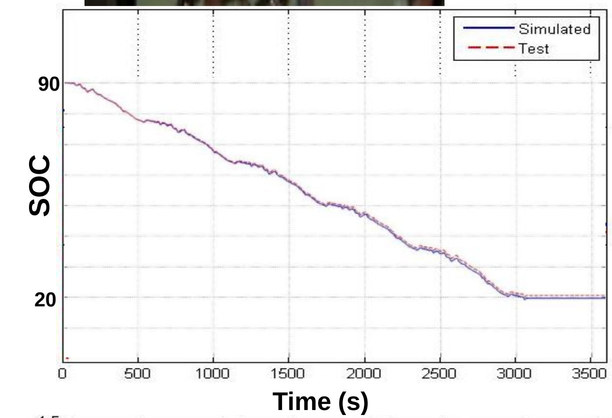
Validation of System Simulation for USO6 drive cycle

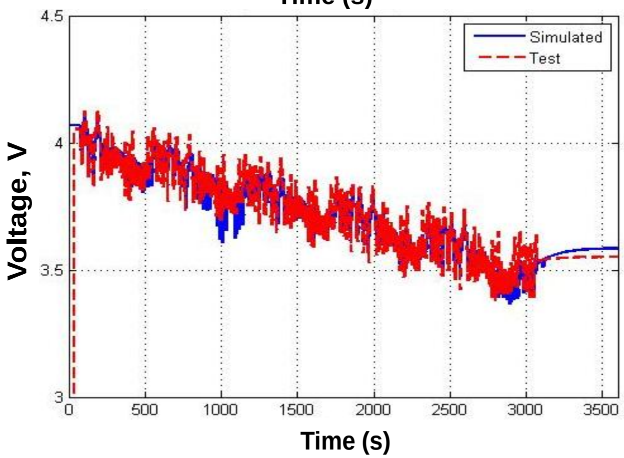


LTI ROM System-Modeling approach for Battery Thermal Simulation

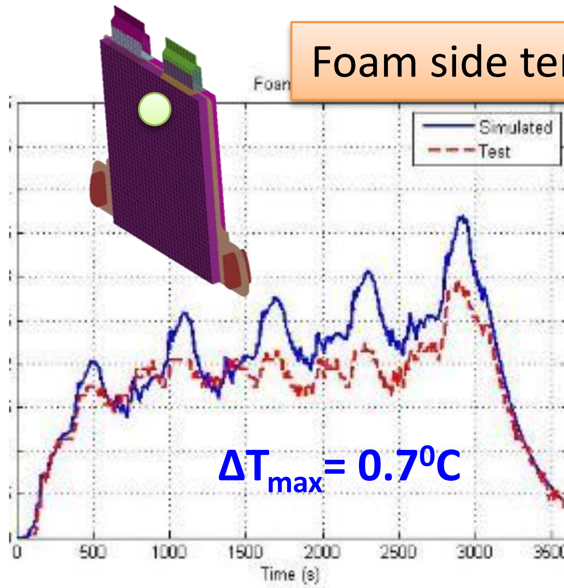


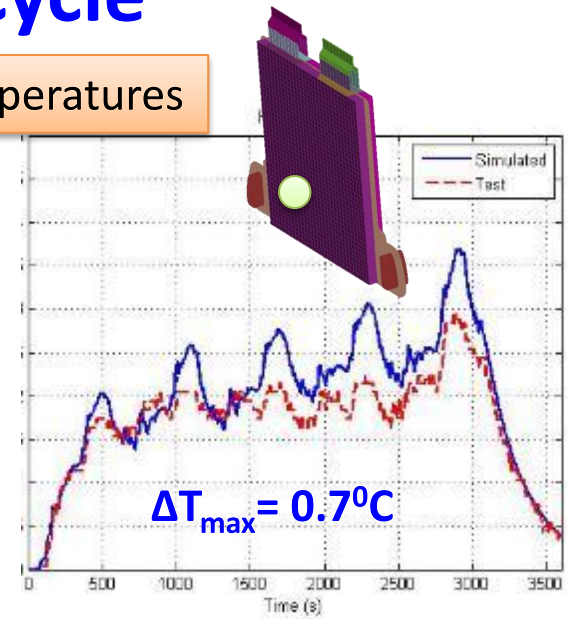
Comparison between the model and the test data for US06 Drive-Cycle



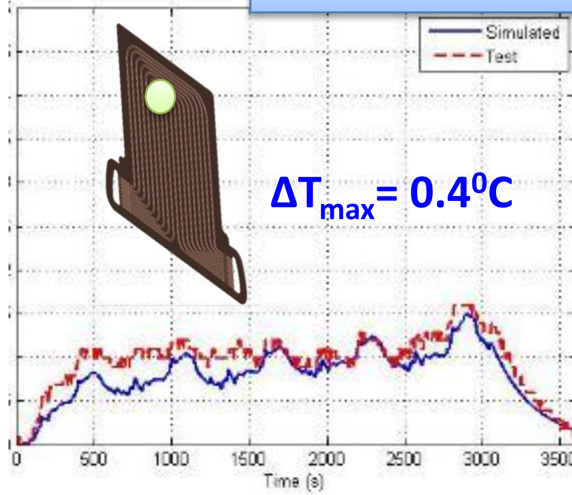


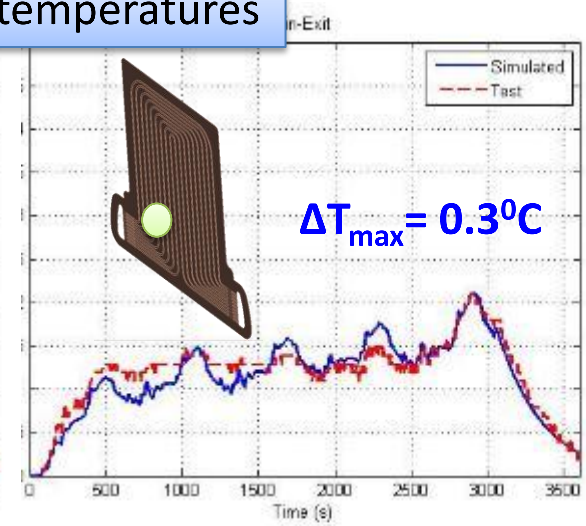
Foam side temperatures





Cooling fin side temperatures





Collaborations

GM(Sub contract)

GM R&D (Project Lead)

- Collaborate with ANSYS/ESIM/NREL
- Pack level strategy
- ROM verification & validation
- Pack level validation

GM Battery CAE Group

- Perform math model verification and cell level validation
- Set vehicle requirements for cell and pack design
- Perform vehicle level validation under various driving schedules

GM Canada Group

- Perform test for cell level performance data and cycle life test

ANSYS (Sub to GM)

- Develop flexible frame work for multi-physics models
- Integrate cell/pack level simulation capability
- Process automation & OAS

Esim (Sub to GM)

- Physics based cell aging model for capacity fade and cell life

NREL (Prim)

- Provide project technical direction (Gi-Heon Kim, Tech monitor)
- Provide Cell chemistry model for multiple particle/active materials

ORNL (Sub to NREL)

- Open Architecture Software

- GM has interacted with all the team members, ANSYS, ESIM, ORNL, and NREL.
- Last couple years we had weekly progress meetings with ANSYS, ESIM and NREL.
- FY 2014, we has planned to have bi-weekly meetings to check the progress.
- GM team has provided 4 Quarterly reviews each year to NREL and DOE.

Future Work

Remainder of FY14

- Thermal abuse/runaway model has been developed and will be implemented in the 2nd Q to handle the thermal propagation in the pack.
- Practical cell cycle life models have been defined and it is planned to be included in 3rd Q. The physics based cycle life model will be implemented 4th Q.
- Complete workflow automation for LTI/LPV ROM process.
- Implement models for multiple active/particle materials.
- Pack level verification, validation, and demonstration.
- Complete battery-specific graphical user interface (ABDT)
- Complete a standard data-exchange interface based on specifications from the OAS Workgroup

Summary

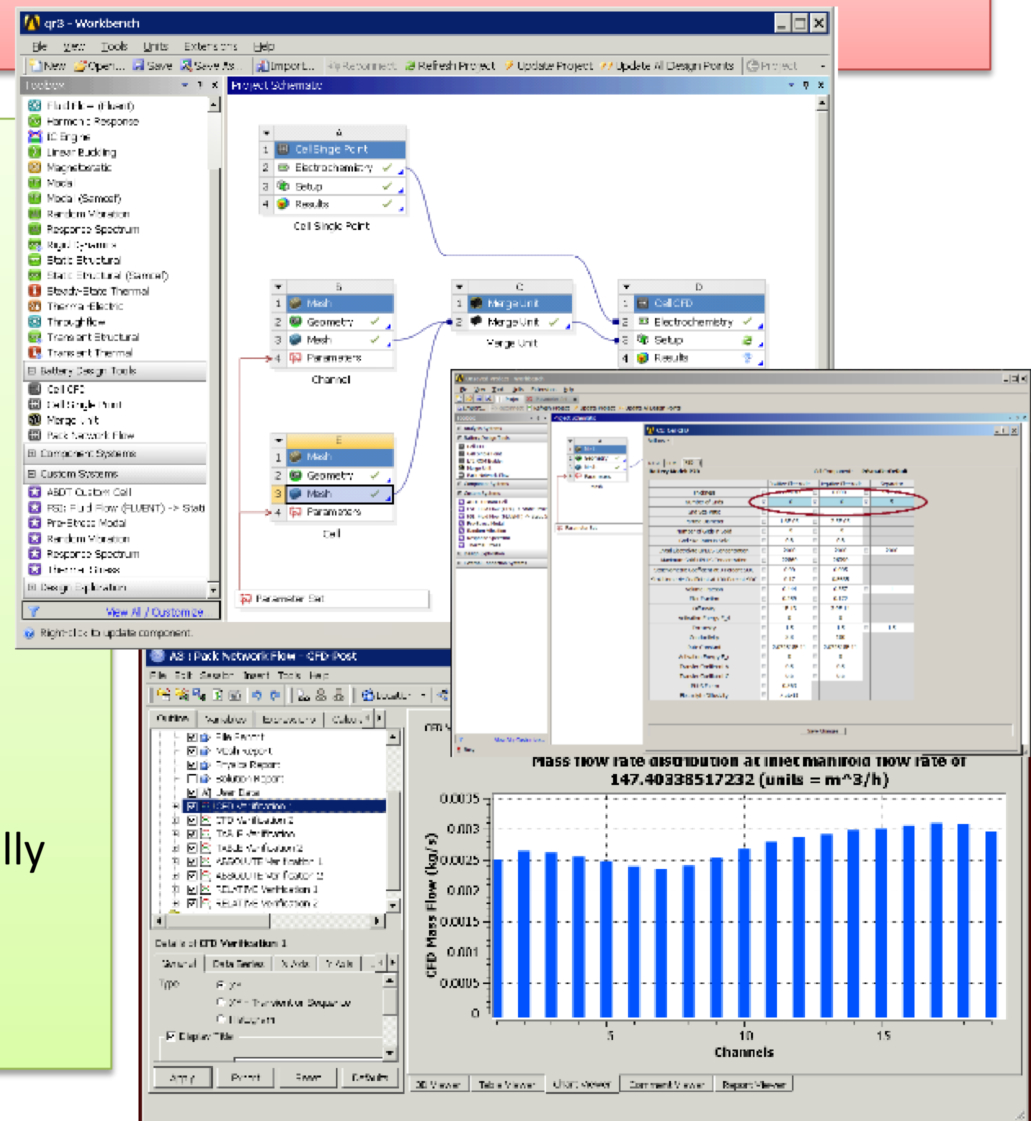
- **Several software deliverables for the cell level tools.**
  - NREL's MSMD framework is implemented in FLUENT with three electrochemistry sub-models, 2Q 2013.
  - Cell level validation was completed, 3Q 2013.
  - Developed user defined electrochemistry models that allows user to apply their own models while utilizing FLUENT's battery framework, 4Q 2013.
  - **The major release of FLUENT Version 15 in December 2013 contains NREL's MSMD battery model further developed jointly by GM and ANSYS.**
- **First pack level software tool was delivered to GM, NREL, and ESim**
  - Auto electrical connection by detecting the cell configurations in the pack.
  - Code is completely parallelized, 2Q 2013.
- **Cycle life test completed with 30% capacity fade.**
  - Cycle life test at an elevated temperature is in progress and to be completed in 4Q 2014.
  - Physics based cycle life model has been developed and to be implemented in 4Q 2014.
- **Pack level validation is completed for a 24 cell module.**
  - Full field simulation was validated in 4Q 2013.
  - System level model was completed and validated compared to the full field simulation and the test data and comparisons are satisfactory 1Q 2014.
  - LTI system level ROM model approach has been validated in comparison with the full field simulation results 2Q 2013.
  - Demonstrated for USO6 driving cycles and validated in 4Q 2013 and 1Q 2014.

Sustainable Software Tool (CAEBAT)

Support of DOE CAEBAT

The automotive industry requires CAE design tools that include the following capabilities.

- **Modular:**
  - —Integrate physics and chemistry in a computationally efficient manner.
- **Provide Flexibilities:**
  - —Provide a platform to enable various simulation strategies.
- **Provide Expandable Framework:**
  - —Enable future users to easily add new physics of interest.
  - —OAS-compatible.
- **Validated :**
  - —Ensure model predictions agree with experimental data by performing carefully designed experiments.
- **Easy to use**



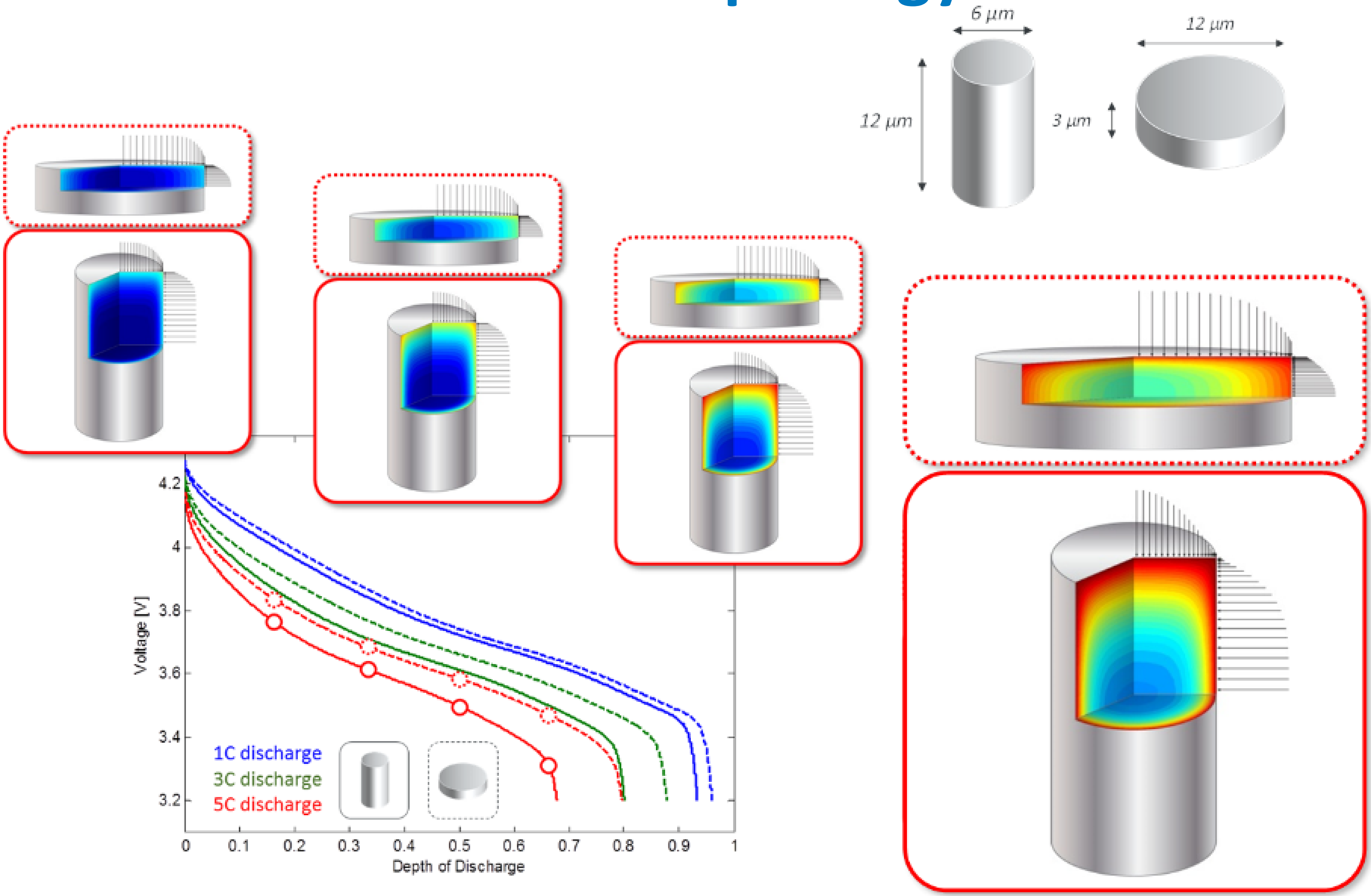
Technical Back-Up Slides

Why Multi-Particle Model?

Multiple Particle Model Uses

- Two-cathode and Two-anode cells are going into **production vehicles**
- OCVs of two cathode materials, their diffusion mechanisms are different causing **highly nonlinear HPPC response** that even 6P or 8P models were not able to capture
- Developing an **equivalent single electrode** is turning out to be a challenge for certain chemistries
- Diffusion coefficients and other time constants are functions of SOC, charge vs. discharge
- **Physics-based degradation models** for multiple particle models need to be developed – long term
- **Battery cell manufacturers** are interested in evaluating effect of particle size distribution (skewness, variance) on material utilization, performance (P/E ratio) using virtual methods – experimental techniques take years to assess

Electrode Particle Morphology



Implementation of NREL's Multi-particle Model in ANSYS/Fluent using MSMD Protocol

- **ANSNS**: It will be a demonstration of expandability and flexibility of the model architecture that ANSYS/Fluent adopted in the project.
- **GM**: GM is interested in using the model with multiple particle, multiple active material features. GM CAE and Battery Algorithms teams are ready to apply these models.
- **DOE/NREL**: NREL's developments can be quickly available to EV industries through CAEBAT program products.
- **Public Benefit**: This would be a good success story of delivering expertise in national lab to a direct use of EV industry using the DOE's CAEBAT product outcomes.

Reformulation of Deshpande's model

- **The model equations in original form**

$$\frac{d\overline{Q}}{dN} = 2BAL_{\mathrm{SEI}}^{0}\left(1-CN\right)^{\frac{m}{2-m}} - B\left(1+2l_{\mathrm{cr}}\rho_{\mathrm{cr}}a_0\right)\frac{1}{2}K_{\mathrm{th}}\left(N\right)^{-1/2} - 2BA\sum_{i=1}^{N-1}\left[1-C\left(N-i\right)\right]^{\frac{m}{2-m}}\frac{1}{2}K_{\mathrm{th}}\left(N-i\right)^{-1/2}$$

$$A = l_{\mathrm{cr}}\rho_{\mathrm{cr}}\left[\sigma_{\theta,\max} b\sqrt{\pi a_0}\right]^m k \qquad \sigma_{\theta,\max} = -\frac{1}{15}\frac{E\Omega}{(1-v)}\left(\frac{i_{\mathrm{s}}R_{\mathrm{s}}}{FD_{\mathrm{s}}}\right) \qquad B = \frac{n_{\mathrm{SEI}}F\rho_{\mathrm{SEI}}4\pi R_{\mathrm{s}}^2}{3600\left[\mathrm{s}\cdot\mathrm{hr}^{-1}\right]M_{\mathrm{SEI}}Q_0} \qquad C = -\frac{2-m}{2}k\left[\sigma_{\theta,\max}b\sqrt{\pi a_0}\right]^m a_0^{\left(\frac{m-2}{2}\right)}$$

a_0	depth of a pre-existing crack $[\mathrm{m}]$
D_{s}	diffusion coefficient of the solute in the solid phase $\left[\mathrm{m}^2\cdot\mathrm{s}^{-1}\right]$
E	Young's modulus of electrode material $\left[\mathrm{N}\cdot\mathrm{m}^{-2}\right]$
F	Faraday's constant $\left[\mathrm{C}\cdot\mathrm{mol}^{-1}\right]$
i_{s}	current over electrode particle surface $\left[\mathrm{A}\cdot\mathrm{m}^{-2}\right]$
k, m	Paris' law parameter
K_{th}	SEI thickness growth parameter
l_{cr}	depth of a pre-existing crack $[\mathrm{m}]$
L_{SEI}^{0}	initial SEI thickness $[\mathrm{m}]$
M_{SEI}	molecular weight of compounds constituting SEI $\left[\mathrm{g}\cdot\mathrm{mol}^{-1}\right]$
n_{SEI}	number of lithium atoms per SEI molecule formed
Q_0	capacity after formation cycle $[\mathrm{Ah}]$
Q_0	capacity at N^{th} cycle $[\mathrm{Ah}]$
$\overline{Q}$	fractional cell capacity
R_{s}	radius of the spherical electrode particle $[\mathrm{m}]$
ρ_{SEI}	density of SEI film $\left[\mathrm{g}\cdot\mathrm{m}^{-3}\right]$
ρ_{cr}	number of cracks per unit area of the particle $\left[\mathrm{m}^{-2}\right]$
$\sigma_{\theta,\max}$	maximum tangential stress $\left[\mathrm{N}\cdot\mathrm{m}^{-2}\right]$
Ω	partial molar volume of the solute $\left[\mathrm{m}^3\cdot\mathrm{mol}^{-1}\right]$

The parameter values in Deshpande's model vary with materials and electrode designs; so a life model should involve the validation of the capacity fade equation

- **The reformulated model equations**

$$\frac{d\overline{Q}}{dN} = b_1\left(1-b_2N\right)^{-b_3} - b_4\left(N\right)^{-1/2} - b_5\sum_{i=1}^{N-1}\left[1-b_2\left(N-i\right)\right]^{-b_3}\left(N-i\right)^{-1/2}$$

where $b_1 = 2BAL_{\mathrm{SEI}}^{0} \quad b_2 = C \quad b_3 = \dfrac{m}{m-2} \quad b_4 = B\left(1+2l_{\mathrm{cr}}\rho_{\mathrm{cr}}a_0\right)\dfrac{1}{2}K_{\mathrm{th}} \quad b_5 = BAK_{\mathrm{th}}$

The parameter vector is defined as $\underline{\mathbf{b}} = \left[b_1 \quad b_2 \quad b_3 \quad b_4 \quad b_5\right]$

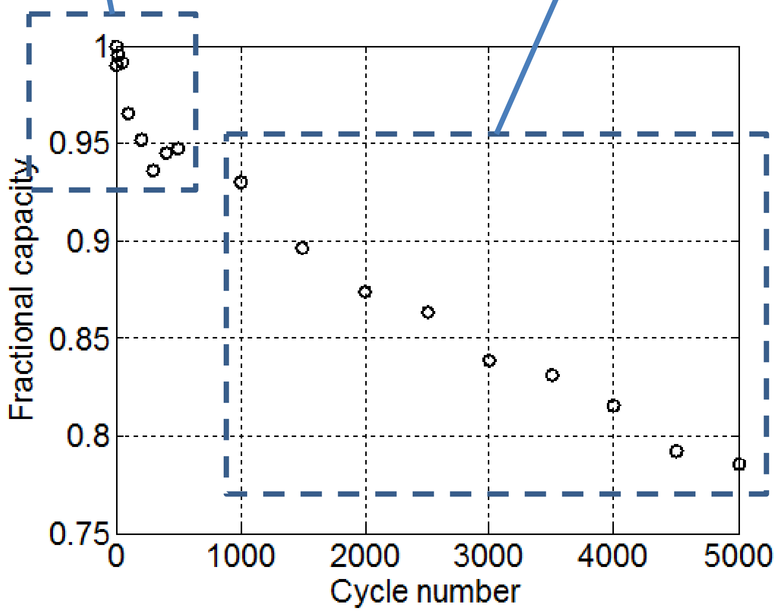
The capacity fade equation can be expressed as $\dfrac{d\overline{Q}}{dN} = \mathrm{f}\left(\underline{\mathbf{b}}, N\right)$

The extrapolatability of Deshpande's model

To check the extrapolatability of Deshpande's model, there should be more OPCAP data points during the initial cycling stage (i.e, the first 500 cycles) than during the later stage (i.e. >500 cycles); therefore, we generated synthetic data with random noise (± 0.01 in fractional capacity) where nine OPCAPs (BOL, cycle #10, 20, 50, 100, 200, 300, 400, and 500) were included during the first 500 cycles.

The "finished cycles" (the first 500 cycles)

The "future cycles" (>500 cycles)



The synthetic data with noise

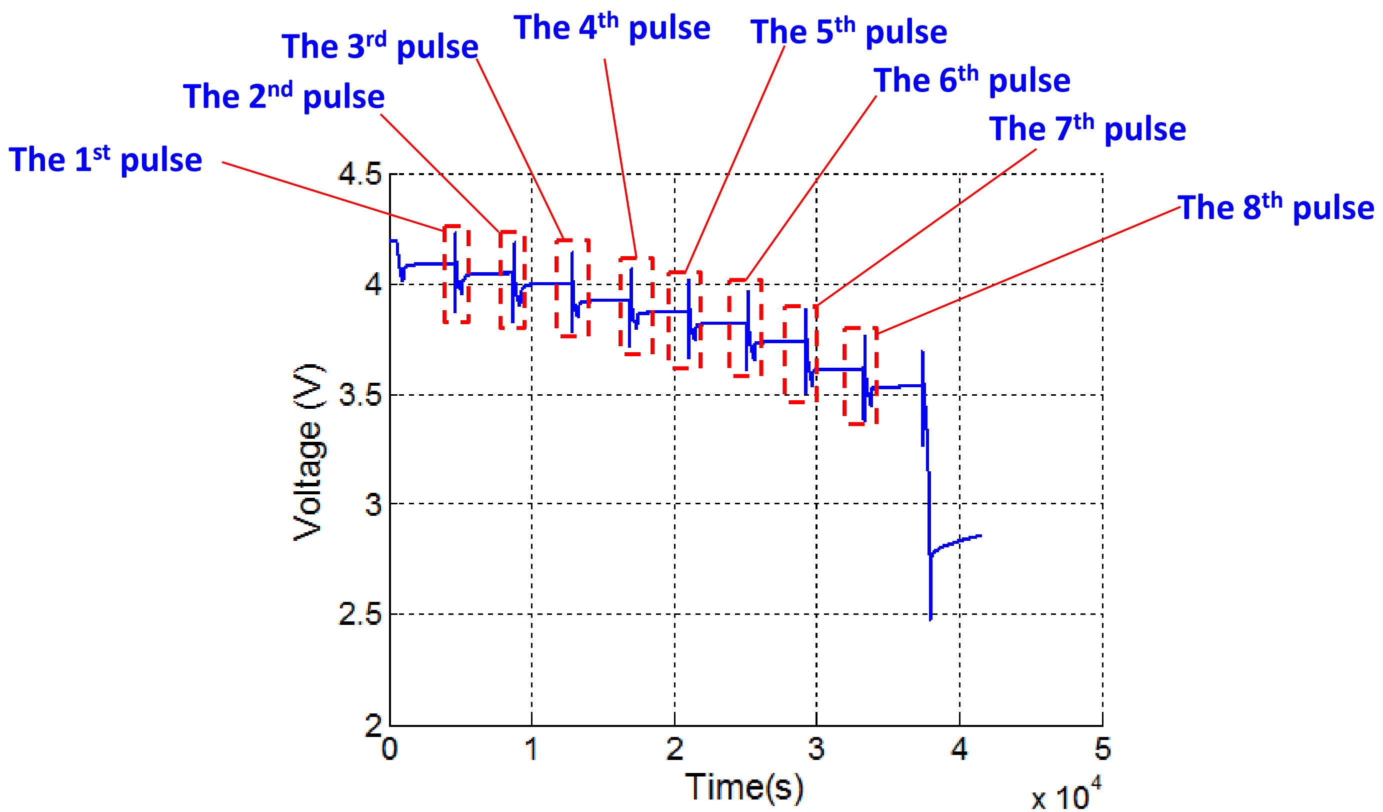
Fit Deshpande's model to the synthetic capacity data at "finished cycles"

Run the model with the parameter values obtained in the previous step and extend the simulation to the "future cycles"

Compare the model predictions and the synthetic data values at the "future cycles"

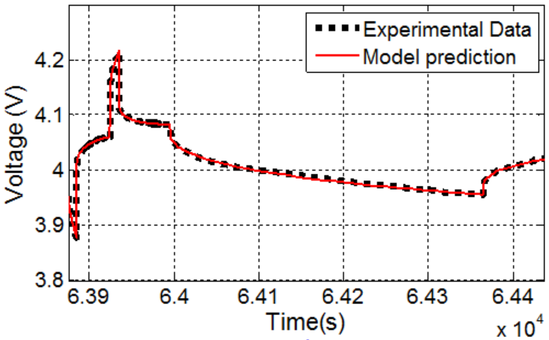
The Periodic HPPC measurements

- Before each OPCAP check, the HPPC of the cell was measured.
- In each HPPC, 9 pulses were made at different SOC, and the first 8 pulses were chosen to be used for model validation

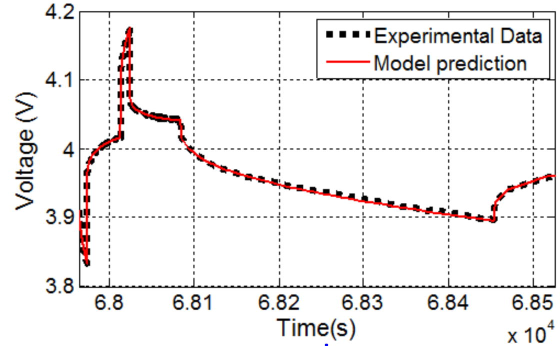


The HPPC voltage profile

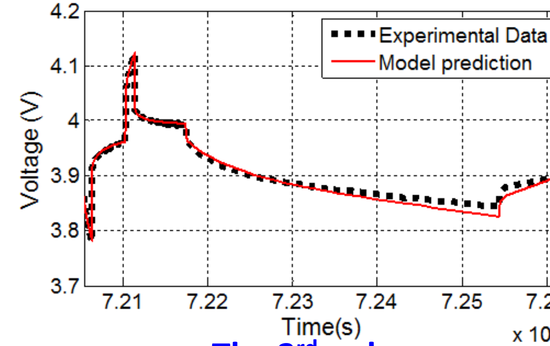
Fitting ECM to HPPC at BOL



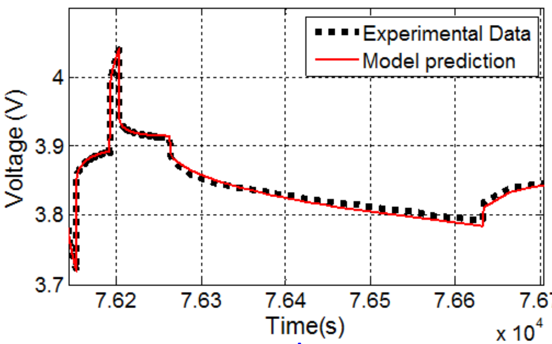
The 1st pulse



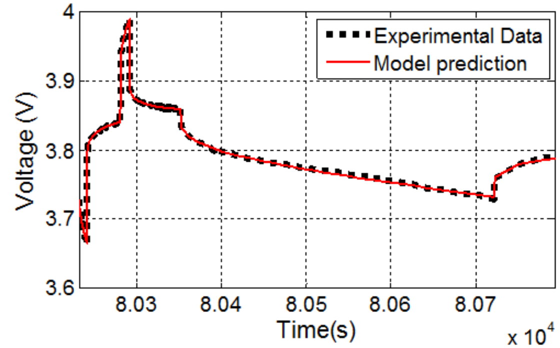
The 2nd pulse



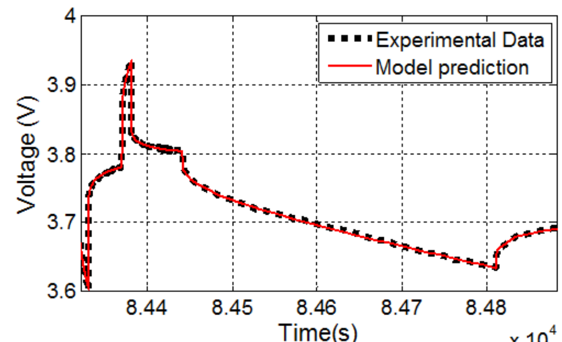
The 3rd pulse



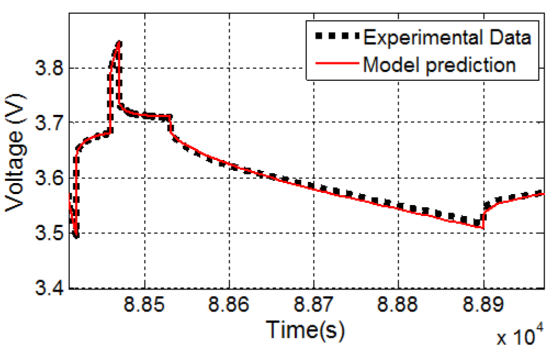
The 4th pulse



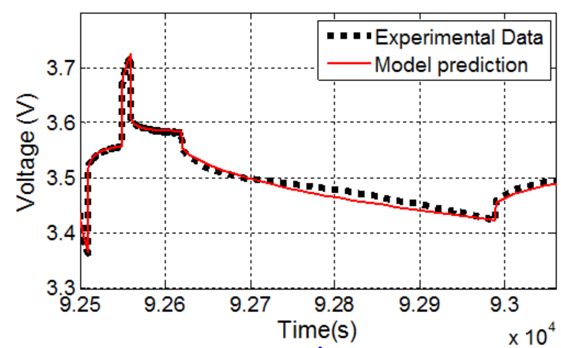
The 5th pulse



The 6th pulse

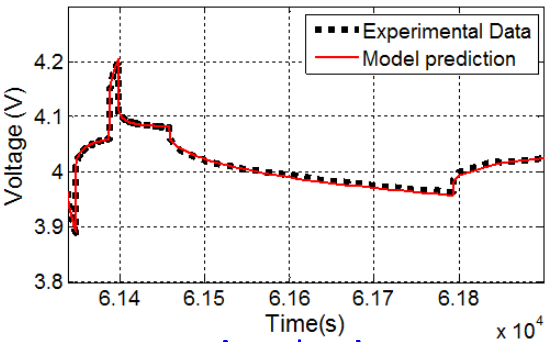


The 7th pulse

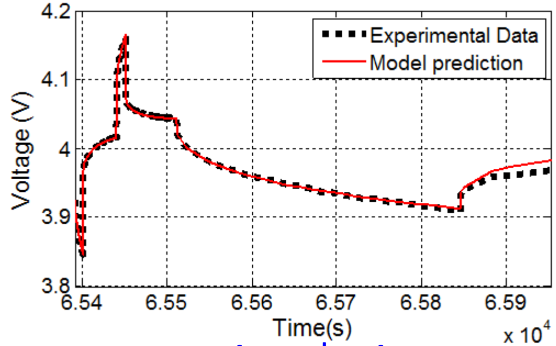


The 8th pulse

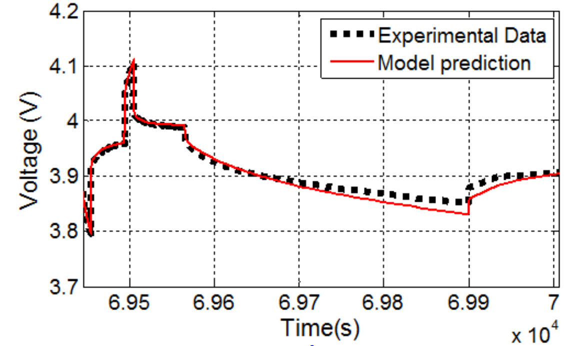
Fitting ECM to HPPC at 1000th cycle



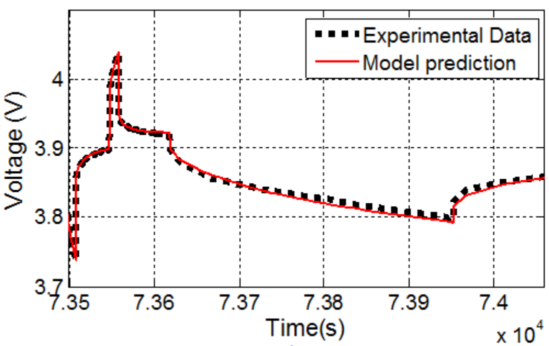
The 1st pulse



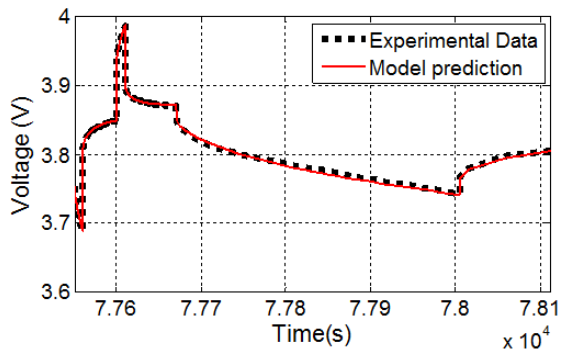
The 2nd pulse



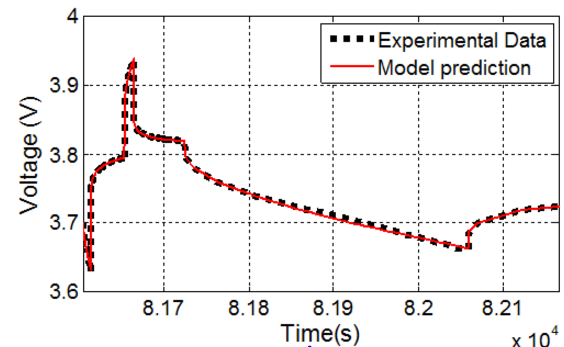
The 3rd pulse



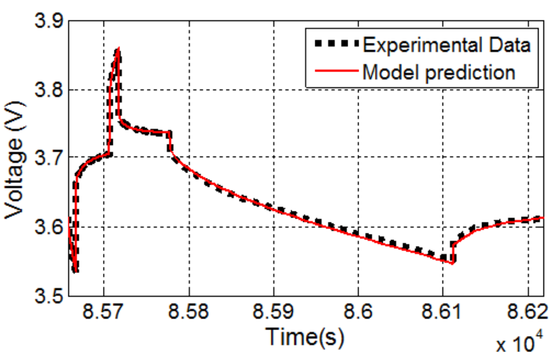
The 4th pulse



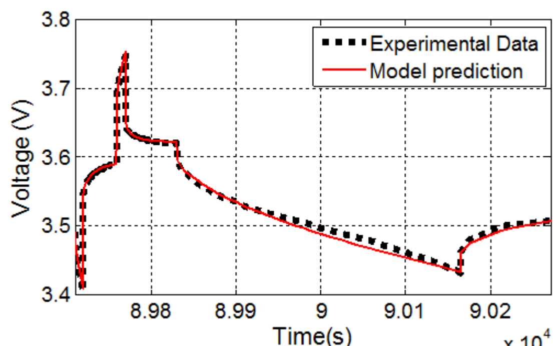
The 5th pulse



The 6th pulse

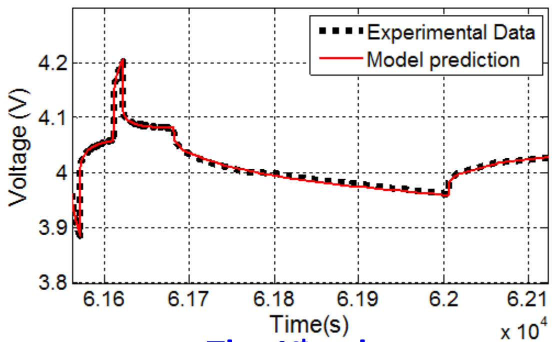


The 7th pulse

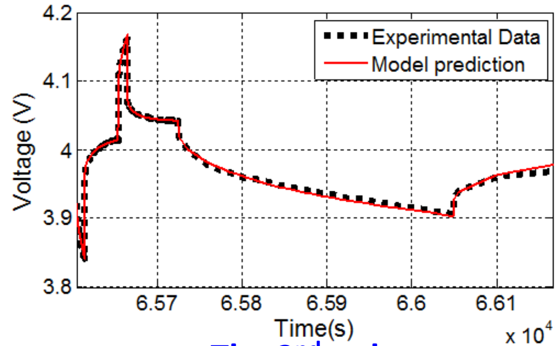


The 8th pulse

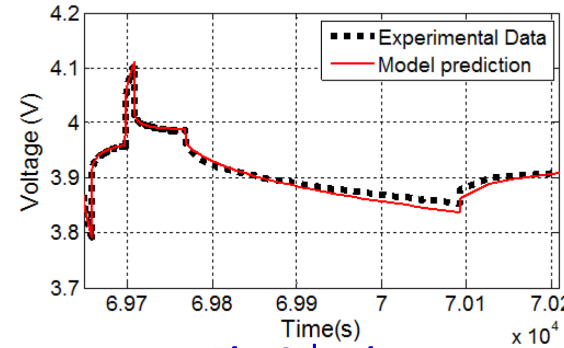
Fitting ECM to HPPC at 2000th cycle



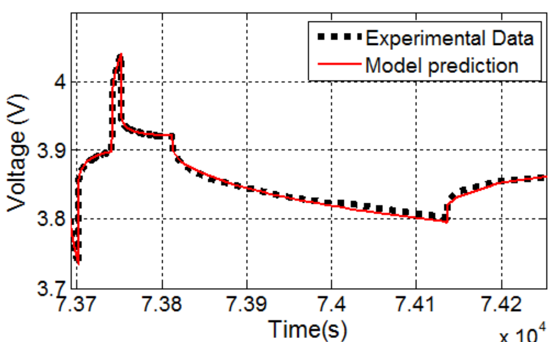
The 1st pulse



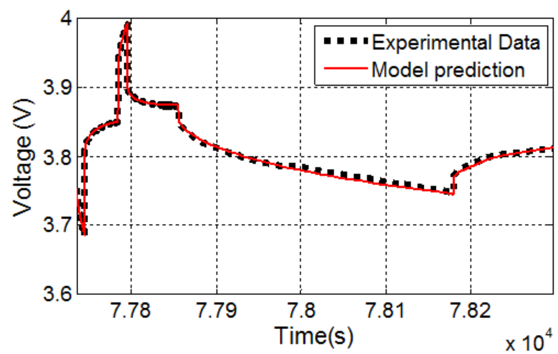
The 2nd pulse



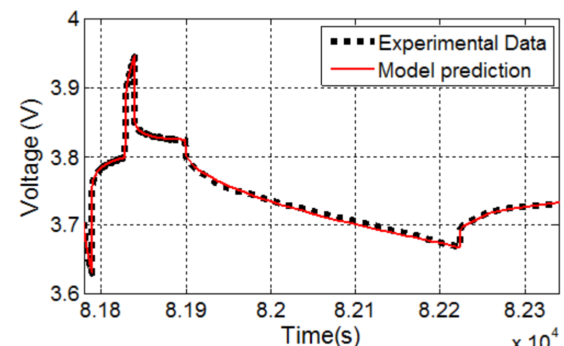
The 3rd pulse



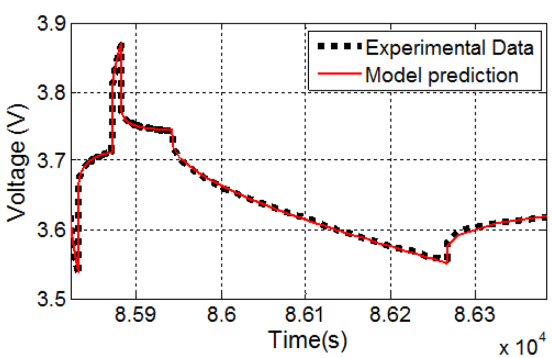
The 4th pulse



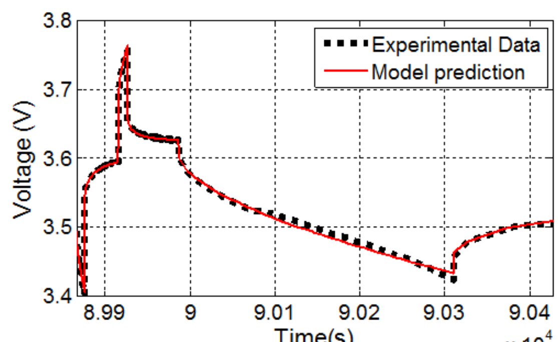
The 5th pulse



The 6th pulse



The 7th pulse



The 8th pulse

Publications/Presentations

1. *Taeyoung Han, Gi-Heon Kim, Lewis Collins, "Multiphysics simulation tools power the modeling of thermal management in advanced lithium-ion battery systems," ANSYS Quarterly magazine "Advantage", 2012*
2. *Taeyoung Han, Gi-Heon Kim, Lewis Collins, "Development of Computer-Aided Design Tools for Automotive Batteries-CAEBAT," Automotive Simulatiuon World Congress (ASWC), Detroit, October 2012.*
3. *Xiao Hu, Scott Stanton, Long Cai, Ralph E. White, "A linear time-invariant model for solid-phase diffusion in physics-based lithiumion cell models.," Journal of Power Sources 214 (2012) 40-50.*
4. *Xiao Hu, Scott Stanton, Long Cai, Ralph E. White, "Model order reduction for solid-phase diffusion in physics-based lithium ion cell models," Journal of Power Sources 218 (2012) 212-220.*
5. *Meng Guo, Ralph E. White, "A distributed thermal model for a Li-ion electrode plate pair," Journal of Power Sources 221 (2013) 334-344.*
6. *Ralph E White, Meng Guo, Gi-Heon Kim, "A three-dimensional multi-physics model for a Li-ion battery", Journal of Power Source, 2013.*
7. *Saeed Asgari, Xiao Hu, Michael Tsuk, Shailendra Kaushik, "Application of POD plus LTI ROM to Battery Thermal Modeling: SISO Case, to be presented in 2014 SAE World Congress.*
8. *Ramesh Rebba, Justin McDade, Shailendra Kaushik, Jasmine Wang, Taeyoung Han, "Verification and Validation of Semi-Empirical Thermal Models for Lithium Ion Batteries ," to be presented in 2014 SAE World Congress.*
9. *Meng Guo, Ralph E. White, "A distributed thermal model for a Li-ion electrode plate pair," Journal of Power Sources 250 (2014) 220-235.*