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# Accelerating Battery Design Using Computer-Aided Engineering Tools

## Preprint

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and Kandler Smith

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# Accelerating Battery Design Using Computer-Aided Engineering Tools

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**Abstract**—Computer-aided engineering (CAE) is a proven pathway, especially in the automotive industry, to improve performance by resolving the relevant physics in complex systems, shortening the product development design cycle and thus reducing cost, and providing an efficient way to evaluate parameters for robust designs. Most CAE battery models can be enhanced. Academic models include the relevant physics details, but neglect engineering complexities. Industry models include the relevant macroscopic geometry and system conditions, but simplify the fundamental physics too much. Most of the CAE battery tools for in-house use are custom model codes and require expert users. There is a need to make these battery modeling and design tools more accessible to end users such as battery developers, pack integrators, and vehicle makers. Developing integrated and physics-based CAE battery tools can reduce the design, build, test, break, re-design, re-build, and re-test cycle and help lower costs. The National Renewable Energy Laboratory (NREL) has been involved in developing various models to predict the thermal and electrochemical performance of large-format cells and has used in commercial three-dimensional finite-element analysis and computational fluid dynamics to study battery pack thermal issues. These NREL cell and pack design tools can be integrated to help support the automotive industry and to accelerate battery design. Our approach and modeling results are provided in the following paper.

**Keywords**—Lithium-ion battery, electric drive vehicles, modeling, simulation, design tool

## 1. Introduction

Batteries in electric drive vehicles (EDVs), such as hybrid electric, plug-in hybrid, and battery electric vehicles, are critical to achieve the desired fuel economy and affordability needed to significantly impact worldwide gasoline consumption and to reduce greenhouse gas emissions and dependence on oil. However, to do this, the cost, performance, and life of today's batteries must improve. Government entities and industry officials have been investing in product development and manufacturing to produce batteries that meet the desired targets. One approach to accelerate scaling up these batteries from materials to cells to packs and to energy storage systems in vehicles is to use computer-aided engineering (CAE) tools. In many industries, including automotive and combustion engine development, CAE tools have been the proven pathway to:

- Improving performance by resolving the relevant physics in complex systems
- Shortening the product development design cycle, thus reducing cost
- Providing an efficient manner for evaluating parameters for robust design.

It is important to integrate the existing models or newly developed ones into a suite of software tools that can be used by end-users in the industry to design the next generation of batteries faster. CAE for the battery industry needs to mature at par with modeling tools for internal combustion engines, conventional drive trains, and the like to make batteries competitive and affordable for use in advanced vehicles.

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To develop EDV lithium ion batteries, the industry depends on custom-made codes, ad-hoc design approaches, and rules of thumb. The development takes place at various scales, from the angstrom size of molecules and the micron size of electrode layers to the millimeter size of electrode design, centimeter size of cells, decimeter size of modules and packs, and the meter size of packs and vehicles, as shown in Figure 1. Various modeling tools are available and used to predict the behavior of each material, cell, and vehicle.

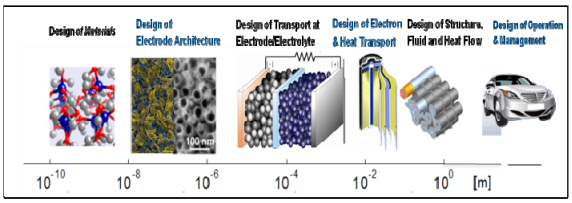


Figure 1: Multiple scales of physics exist in the lithium-ion battery, with various physics interacting across a wide range of length and time scales.

## 2. Background—Modeling at Various Scales

Modeling can be conducted at various levels, including the material level, cell level, pack level, and vehicle level. In an ideal situation, each model level interacts with the other levels, and analysis is performed to provide input to the other levels using input from those levels. However, different level models have been developed by different institutions and written in different programming languages; therefore, it is challenging to make these models interact well together. There is a great need to improve this interaction.

Figure 2 depicts an integrated design tool using a vehicle simulation tool with a battery pack simulation tool that

with a detailed cell-level model embedded in it. The vehicle simulation tool helps identify the requirements for the battery pack, which identifies the size and design of a particular cell. Next, cell-level performance is predicted using different driving profiles, which are converted to battery power profiles using the vehicle simulator. Ambient conditions and battery load are used to identify the temperature rise, which provides feedback on the design of thermal management of the battery pack. The feedback provided could be used to study the impacts of various design parameters such as changes in the size, shape, design, and chemistry of the cell; vehicle size and performance; and the thermal management system.

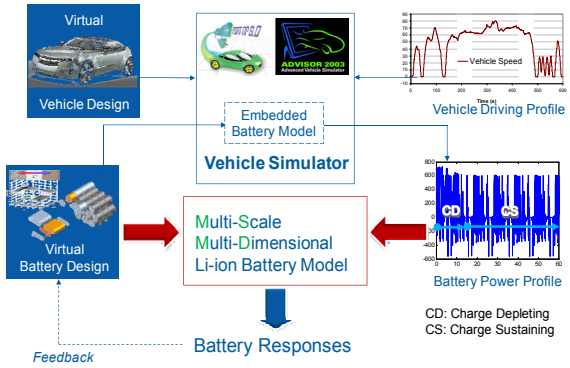


Figure 2: Linking battery cell and pack modeling with vehicle simulations helps study many parameters for designing optimized components.

Optimization can be performed and an initial design of a battery pack and cell could be arrived at for a particular vehicle without conducting any prototyping or testing. Of course, one has to have confidence in these models and design tools; therefore, validation of the models and design tools is critical and must be carried out in parallel with model development.

### 2.1 Cell-Level Modeling

The National Renewable Energy Laboratory (NREL) is the leader in the thermal analysis of batteries and has now added electrochemical modeling capabilities to design large-format cells as the interaction between temperature and electrochemistry becomes paramount with larger format design.

The NREL model captures a three-dimensional aspect of a cell while capturing the electrochemistry as modeled by Dr. John Newman's group. Newman's model captures lithium diffusion dynamics and charge transfer kinetics in porous media; predicts the current/voltage response of a cell; and provides a design guide for thermodynamics, kinetics, and transport across electrodes [1]. The equations cover charge transfer kinetics at a reaction site, species conservation, charge conservation, and energy conservation. Although the model has been very successful for small cells, it is difficult to resolve heat and electron current transport in large cell systems.

Newman's model is often appropriate to predict the behavior of small cells. In large cells, however, particularly for automotive applications, working potential and temperature are non-uniform throughout the cell. The same is true for battery packs consisting of multiple cells. Potential and temperature imbalances cause certain locations of a cell to be cycled more excessively than the rest. The local excess use generates more heat and stress, causing severe localized degradation. Electrical current transfer in non-active conductive components of a cell and heat transfer through a highly anisotropic composite medium in a cell have a critical impact on the performance and degradation of large-format batteries.

Through multi-year efforts supported by the U.S. Department of Energy, NREL has developed a modeling framework for predictive computer simulation of lithium ion batteries, namely the Multi-Scale Multi-Dimension (MSMD) model, which addresses the interplay among the various battery physics in varied scales [2–6]. This paper introduces NREL's MSMD model and demonstrates how the model can be applied to the evaluation and study of large-format cell design. At NREL, Newman's model has been extended to a thermal-electrochemical three-dimensional model using the MSMD (domain) model approach.

### 2.2 Pack-Level Modeling

Designing battery modules and packs needs to take the cell-level models into account but simplifying them for the computational speed. Commercial CAE battery modeling tools have been used primarily for packaging and thermal analysis. Moving beyond thermal modeling, a more complete battery pack CAE tool must be developed to capture the physics related to electrochemistry, thermal, fluid flow, structural, mechanical, and chemical degradation, and finally, exothermic abuse behavior.

The physics of interest for battery CAE include interactions related to charge/discharge processes, localized heat generation, degradation of cell and electrode components, mechanical stress, and heat release during cell abuse and further propagation from cell to cell in a pack. All of these processes must be coupled with temperature, electrical load, and, in some cases, mechanical load on the pack. At the pack level, models must be able to accurately capture cell-to-cell non-uniformity, especially when it impacts system-level behavior and design. Cell-internal non-uniformities are also of interest as they relate to localized heat generation, cooling channel design, and volume expansion.

To design a battery pack that incorporates the implications of selecting a particular chemistry, cell geometry and aspect ratio, particularly the size, location of terminals, cooling methods, driving profiles, and ambient temperature conditions, etc., the existing models and CAE tools need to be further developed and interfaced with the existing cell models. This will be discussed later in this paper.

# 3. Model Description

## 3.1 Overview—Cell Level

The MSMD model approach has achieved computational efficiency for resolving multi-physics interactions occurring over a wide range of length scales by introducing separate solution domains for particle physics, electrode-scale physics, and cell-scale physics. In addition, the MSMD approach provides a modularized framework enabling model flexibility by providing multiple sub-model solver options with various physical/ computational complexities and expandability to add new physics of interest or to drop physics of insignificance or indifference. The successfully integrated MSMD model can expand knowledge on the interplay of different scale battery physics to help speed development of high performing, long lasting, and safe lithium ion batteries for electrified vehicles. Figure 3 shows the modularized hierarchy of structure in NREL's MSMD model.

This modularized approach allows the end-user to pick and choose the desired physics and code for particle, electrode, or cell modeling. The solution technique in each domain depends on the accuracy and fidelity desired. The MSMD approach applies to any electrochemistry, cell shape (cylindrical or prismatic), and electrode configuration (rolled or stacked) with three-dimensional geometries.

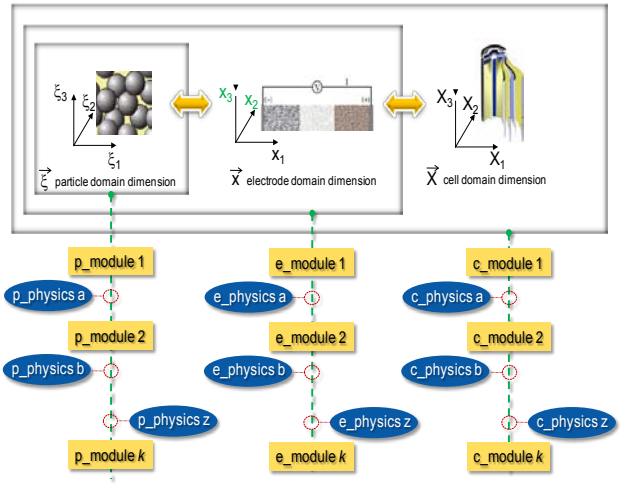


Figure 3: Modularized hierarchy of the model structure in NREL's MSMD approach.

### 3.1.1 Modeling of Large Stacked Prismatic Cells

Large stacked prismatic cells are becoming of increased interest for EDVs. In this case, the impact of macroscopic cell design features such as the number of stacked layers and the electrode area, size, and location of current tabs is explored. The same can be done for a given set of microscopic cell design parameters such as component materials, particle shape and size distribution, electrode loadings, and thickness. Because the cell domain design features are of interest in this model, efficient particle and electrode domain models were chosen for this study. The cell domain model and solver resolve the full three-dimensional geometry of the cells. The electrode domain model was a one-dimension transport model. The spherical particle model was selected to resolve particle domain physics. A state-variable model was used in the solution scheme for particle and electrode domain model solvers to achieve computational efficiency [8]. Figure 4 shows the schematics for the models and solver modules selected for the present study. The equations solved in this study are shown in the appendix.

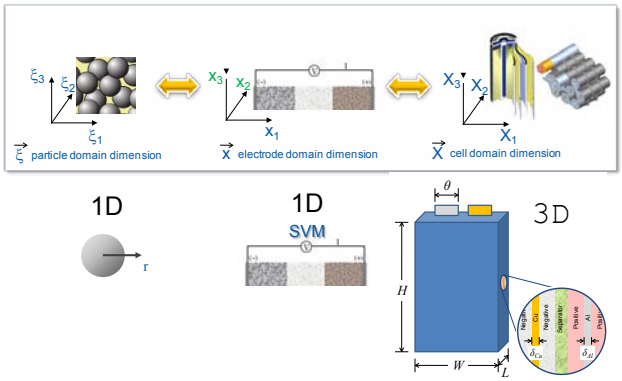


Figure 4: Models and solver modules were selected for this study to evaluate macroscopic designs of large stacked prismatic cells using the MSMD model.

## 3.2 Overview—Pack Level

Computer-aided design (CAD), computational fluid dynamics, and finite element analysis (FEA) software packages are already capable of capturing the complex three-dimensional geometry of battery packs, although they are generally limited in their capability to include battery-relevant physics. For example, FEA models can calculate the stress imposed on various pack components when the pack is exposed to external vibration. They cannot, however, predict localized stresses within the cell stack for a specific electrical cycling condition. The ability to quickly and accurately explore a wide range of thermal, duty cycle, and aging scenarios through computer simulation will substantially reduce battery pack development costs for automotive original equipment manufacturers.

A particular challenge for the battery pack CAE tool is to be able to include the appropriate physics and/or approximations to answer engineering design questions across a range of length scales. To solve the electrochemical-thermal-fluid behavior at the cell or module level, it may be appropriate to fully discretize the cell and flow channel regions with a fine mesh. Direct scaling of the same model to the pack level, however, may not be possible, as the number of volume elements in the mesh could increase more than 100-fold. Timely execution of such a large-scale model may require parallel implementation on a supercomputer. Other alternatives include using reduced order or simplified physics models for individual cells or other pack subcomponents.

## 4. Results and Discussion

### 4.1 Large Stacked Prismatic Cells

To show the utility of battery CAE for designing cells, an example for designing the tab location (Case 1) and aspect ratio (Case 2) for a large stacked prismatic cell are provided for a lithium-ion battery with nickel-cobalt-aluminum (NCA) cathode and graphite anode.

#### 4.1.1 Impact of Tab Location for a 40-Ah Cell (Case1)

Figures 5 and 6 show the example results of an MSMD model of a 40-Ah stacked-cell design with prismatic configuration after discharging the cell at a constant current rate of 200 A for 2 minutes. Two cases were studied, one with positive and negative terminals on the same end (Figure 5), and the other with terminals on both ends (Figure 6). The model predicts the working potential, electrochemical current production, and the resulting temperature. In this case, the temperature near the tabs of the cell with terminals on both sides is about 4°C–5°C higher than in the other cell.

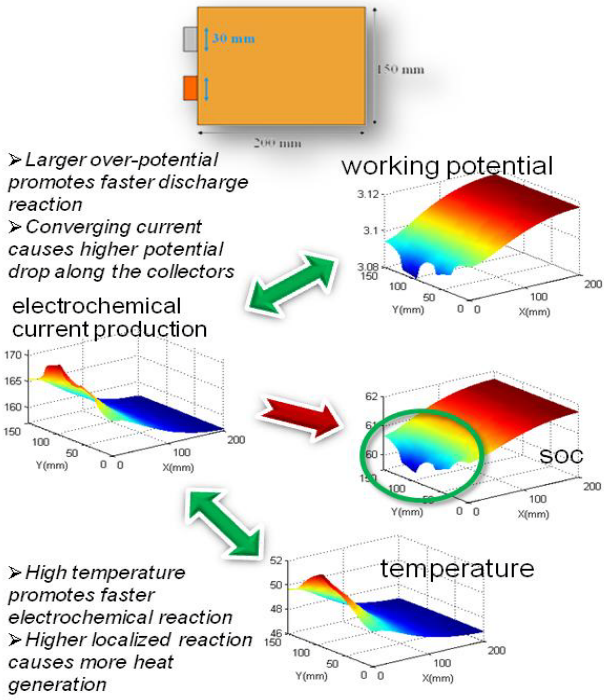


Figure 5: Example results of battery modeling multi-physics interaction for 40-Ah prismatic cells with terminals on the same end after 2 minutes of 200-A constant discharge (compare with Figure 6).

The temperature distribution in the cell with terminals on both ends was much more uniform and thus provides a better way to cool the battery. This stems from the differences in working potential that leads to a different current production and thus temperature distribution, which in turn results in difference in the state of charge (SOC) of each cell. Having this non-uniformity in temperature, current distribution, and SOC in a cell over the many years and cycles expected from the large-format cells could lead to an inconsistent usage of the active material. As a result, the areas close to the tabs in the cell with terminals on the same side can have more usage and potentially degrade faster, as shown by Smith et al. [5].

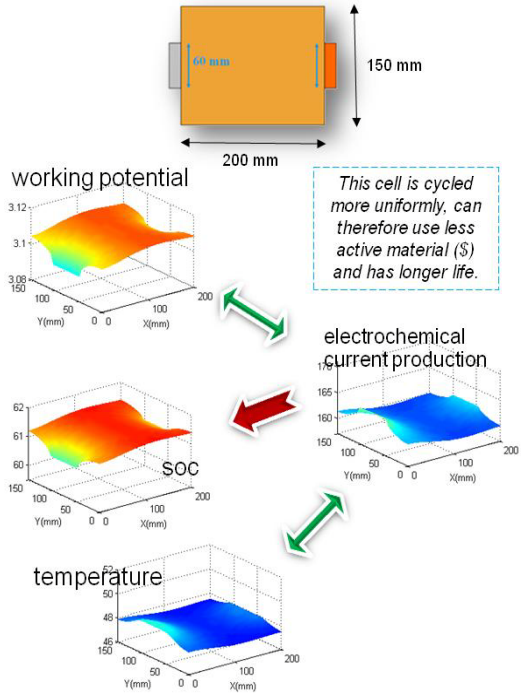


Figure 6: Example results of battery modeling multi-physics interaction for 40-Ah prismatic cells with terminals on both ends after 2 minutes of 200-A constant discharge (compare with Figure 5).

#### 4.1.2 Impact of Aspect Ratio on a 20-Ah Cell (Case 2)

Using a vehicle simulation of a plug-in hybrid electric vehicle (PHEV10), a 20-Ah cell with NCA/graphite chemistry was selected for further analysis. In this study, many parameters, such as current collector thickness ($\delta_{Al}$ = 1.6 x $\delta_{Cu}$), electrode loadings, and electrode thickness, were kept constant while other parameters, such as aspect ratio (H/W), number of electrode layers, and tab width (θ/W), were changed. The initial cell temperature and the air cooling temperature were both assumed to be 30°C. The heat transfer coefficient for all surfaces (tabs and cell surfaces) was assumed to be 20 W/m$^2$/°C. Four alternative designs were considered to deliver the same 20-Ah capacity. Figure 7 shows the different designs. Design 1 (nominal) has terminals on the same end, and design 4 has terminals on both sides. Design 2 is similar to design 1, except it has one-third the capacity of design 1, so three of them should be used in parallel to have the same capacity. Design 2 has three times the surface area of design 1, and design 3 is similar to design 1 except it is thinner and has wider sides to have the same 20-Ah capacity.

The MSMD model was used to simulate the electrochemical and thermal responses of the four designs under a US-06 driving profile for a mid-size sedan PHEV10 design consisting of charge-depleting (CD) and charge-sustaining (CS) driving. The initial SOC of the battery was 90%. The results of the thermal behavior are presented in more detail for the electrochemical behavior in Kim et al. [4] and Smith et al. [6].

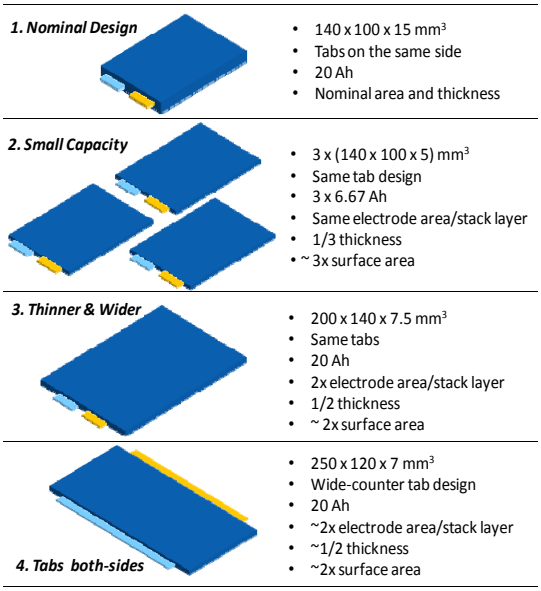


Figure 7: Alternative cell designs were used to study the impact of aspect ratio using the electrochemical-thermal MSMD model.

The results of the thermal response of the four designs to CD and CS profiles are shown in Figure 8. The top graph shows the resulting US-06 power profile for the first 20 minutes of driving (the first 10 minutes is mostly CD). The middle graph shows the average volumetric temperature of each cell design. As can be seen, the thickest cell (design 1) reaches the highest average temperature, while the small-capacity cells (design 2) have the lowest temperature rise. The lower graph shows the temperature difference (maximum – minimum) for the four designs. Design 3 (thin and wide) has the highest temperature difference while design 4 (thin with tabs on both sides) has the lowest. From these analyses, it can be concluded that from the perspective of thermal and electrochemical uniformity and in the attempt to retain the lowest temperature from the three large-format cells, design 4 (thin with tabs on both sides) is the preferred design. Of course, packaging, structural, and cost analyses must be performed to see if design 4 is the optimum cell configuration, which is why it is necessary to perform the battery pack modeling studies using CAE.

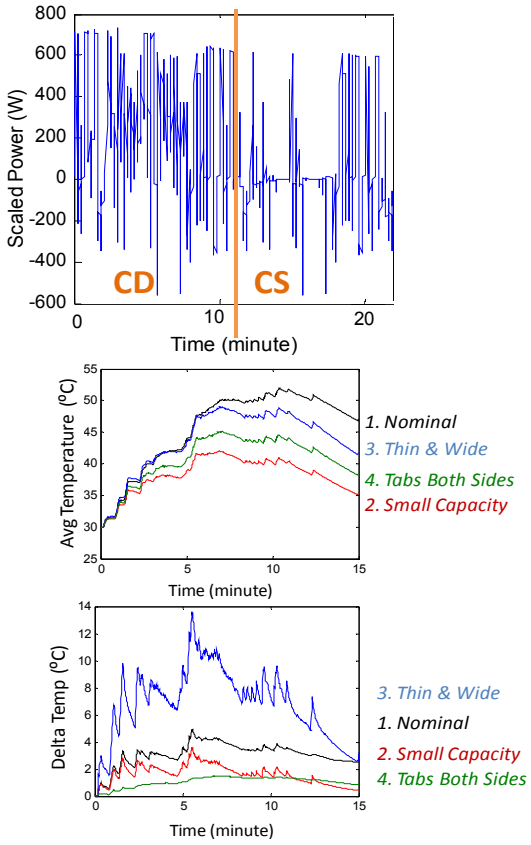


Figure 8: Results of electrochemical-thermal MSMD modeling for four stacked prismatic cells under the US-06 power profile (top graph). Volumetric average temperature rise above initial/ambient temperature of 30°C is shown in the middle graph. The bottom graph shows the temperature difference (maximum – minimum) in each design.

### 4.2. Pack-Level Modeling—Prismatic Cells

The following example provides information from Compact Power, Inc. [7] using CAD, computational fluid dynamics, and FEA software packages for capturing the complex three-dimensional geometry of battery packs. As shown in Figure 9, the cells are prismatic with stacked layers of Mn-spinel/layered mixed cathodes and graphite/amorphous-carbon anodes. The positive and negative terminals are on opposite sides of the cell. The cells are stacked horizontally in a module and then assembled in an air-cooled pack.

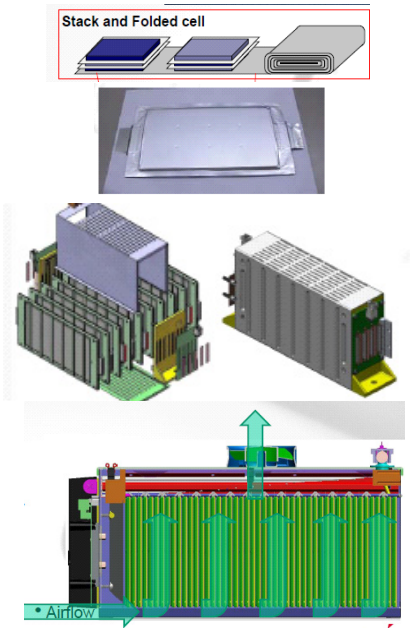


Figure 9: Compact Power, Inc. integrated prismatic cells in an air-cooled pack using existing CAD tools [7].

The cells were assumed to be isothermal for the battery pack studies with the heat source estimated using direct current resistance and the root mean square of the current. To use an integrated approach including electrochemical and thermal performance of cells in CAE tools for a battery pack, further work is needed. The objective of such a pack-level modeling development could include capturing physics and geometry that are important for operation of the energy storage in an EDV environment; achieving good computational efficiency through model reduction, parallelization, etc.; interfacing with commercial software to automate robust design optimization processes; interfacing with appropriate cell-level and (vehicle) system-level models; and encouraging usability by battery non-experts. In addition, it would be beneficial if the battery pack-level CAE tool provided the ability to:

- Rapidly define common cell and battery pack geometries
- Import existing CAD geometries from other commercial packages
- Predict thermal management system performance
- Capture cell-to-cell variations due to parallel/series electrical connections, location in pack, cell manufacturing variability, and degradation at various states of life
- Predict internal cell heat generation and temperature variation
- Evaluate the effects of duty cycle (e.g., aggressive driving, fast charge, etc.)
- Estimate battery pack cost and distribution among various components.

## 5. Conclusion

Non-uniform battery physics, which are more likely to occur in large-format cells, can cause unexpected performance and life degradations in lithium-ion batteries. Robust CAE design tools are needed to evaluate and predict the performance of batteries from material to cell, pack, and vehicle levels. These tools will also shorten the battery design and product development cycle time, thus reducing the battery cost.

The MSMD model was used to evaluate large-format prismatic automotive cell designs by integrating micro-scale electrochemical processes and macro-scale transports. Thin-form factor prismatic cells with a wide counter tab design would be preferable to manage cell internal heat and electron current transport and consequently to achieve uniform electrochemical kinetics across a system.

To transfer and integrate a range of battery modeling tools, various organizations need to collaborate to incorporate existing and new models into software battery modeling suites/tools with the overall goal of shortening the design cycle and optimizing batteries (cells and packs) for improved thermal uniformity, safety, long life, and lower cost.

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Dr. Pesaran leads the energy storage team at NREL. He manages several projects for the Department of Energy and industrial partners, which include thermal testing and analysis of batteries, and modeling and simulation of electric drive vehicles and their energy storage. He received his Ph.D. in thermal engineering from UCLA.


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Dr. Kim's recent research interests in advanced vehicle energy storage system tasks include development of a three-dimensional lithium ion battery thermal abuse model, three-dimensional electrochemical modeling of lithium-ion cells, and modeling hybrid electric vehicle/electric vehicle battery thermal management systems. He holds a Ph.D. in mechanical engineering from Colorado State University.


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Dr. Smith is working in the areas of battery

thermal management and electrochemical modeling. He holds a Ph.D. in mechanical engineering from Penn State. His Ph.D. research developed electrochemistry-based real-time algorithms that enable expanded battery power and energy capability.

## 8. Appendix

The governing equations for battery functional physics in the demonstrated cases shown above are given below. However, model and solver choice in the multi-scale multi-dimension approach can be altered according to the purpose of the model simulation and the domain.

***Particle Domain***

Solid phase diffusion:

$$\frac{\partial c_S}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 D_S \frac{\partial c_S}{\partial r}\right), \; D_S \left.\frac{\partial c_S}{\partial r}\right|_{r=R_S} = \frac{-j^{Li}}{a_S F}$$

Charge transfer kinetics:

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

$$i_o = k(c_e)^{\alpha_a}\left(c_{s,\max} - c_{s,e}\right)^{\alpha_a}\left(c_{s,e}\right)^{\alpha_c}$$

***Electrode Domain***

Charge balance in solid and liquid phases:

$$\nabla\left(\sigma^{eff}\nabla\phi_s\right) - j^{Li} = 0 \text{ , and}$$

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

Transport in electrolyte phase:

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

Heat generation in electrochemically active domain:

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

***Cell Domain***

Temperature:

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

Electric potential in non-active components outside of composite electrodes:

$$\nabla\left(k_e\nabla\Phi\right) + i''' = 0$$

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**14. ABSTRACT** *(Maximum 200 Words)*
Computer-aided engineering (CAE) is a proven pathway, especially in the automotive industry, to improve performance by resolving the relevant physics in complex systems, shortening the product development design cycle, thus reducing cost, and providing an efficient way to evaluate parameters for robust designs. Academic models include the relevant physics details, but neglect engineering complexities. Industry models include the relevant macroscopic geometry and system conditions, but simplify the fundamental physics too much. Most of the CAE battery tools for in-house use are custom model codes and require expert users. There is a need to make these battery modeling and design tools more accessible to end users such as battery developers, pack integrators, and vehicle makers. Developing integrated and physics-based CAE battery tools can reduce the design, build, test, break, re-design, re-build, and re-test cycle and help lower costs. NREL has been involved in developing various models to predict the thermal and electrochemical performance of large-format cells and has used in commercial three-dimensional finite-element analysis and computational fluid dynamics to study battery pack thermal issues. These NREL cell and pack design tools can be integrated to help support the automotive industry and to accelerate battery design.

**15. SUBJECT TERMS**
Li-ion battery; electric drive vehicles; modeling; simulation; design tool

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