Mathematical Modeling as a Tool for Understanding Lithium-Ion Batteries in Electric Vehicles

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Why Battery Modeling?

- Modeling & Simulations can improve the design of cells and modules by identifying limitations in a design
- Modeling allows simulation of performance at relevant operating conditions or at relevant failure-modes

Origins and Use

- First published in the early 1990s, battery modeling is based on electrochemical and thermodynamic concepts and is used to:
  - » Predict cell voltage during different operating conditions
  - » Study thermal management in batteries

Cell Chemistry*	
Positive electrode	$LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$
Electrolyte	1.2 M LiPF6 in EC:EMC (3:7)
Separator	Celgard 2325
Negative electrode	Li_xC_6
Capacity	21 Ah
Size	140x240x7 mm

**Note*: The simulations in Figures 2-4 are based on the cell chemistry specified in the table above.*

What's in a Model?

- Equations and Mathematical Properties Describing Battery Processes
- Values of Properties Obtained through Carefully Designed Experiments and based on Theoretical Models

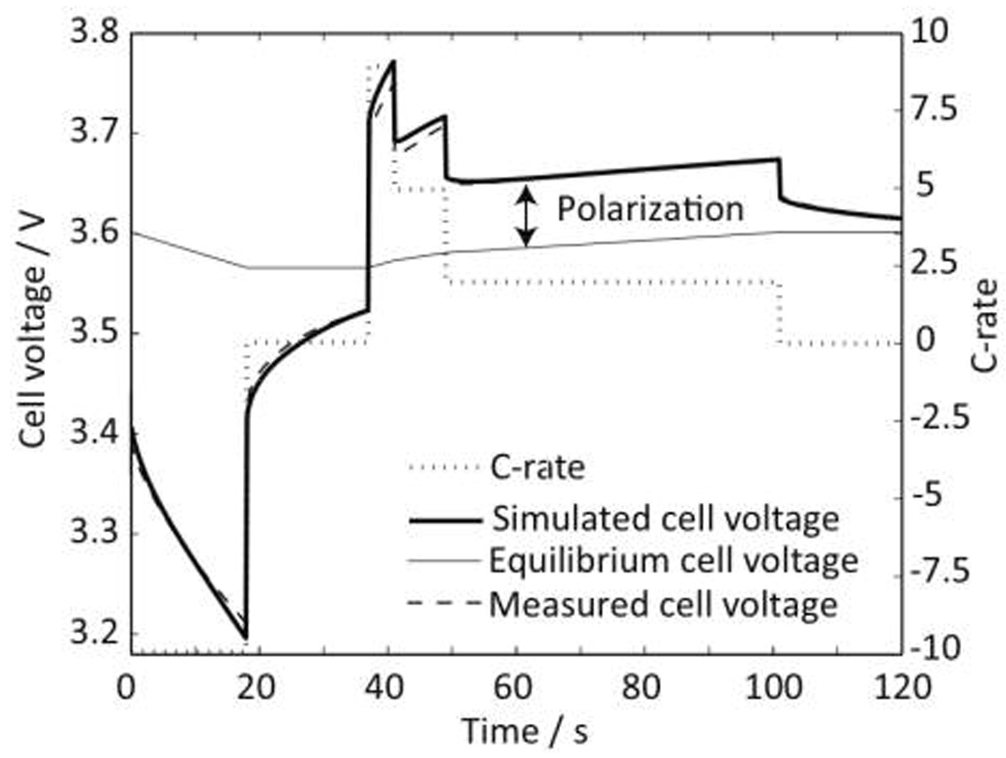

Figure 1
Analysis of the Polarization in a Li-Ion Battery Cell by Numerical Simulations
Nyman et al. , *J. Electrochem. Soc. 157, A1236 (2010)*

Modeled Processes

- Electronic Current Conduction
- Ionic Charge Transport
- Mass Transport in the Electrolyte
- Material Transport of Lithium within the Electrodes
- Butler-Volmer Electrode Kinetics
- Heat Generation due to Joule Heating
- Heat Transfer by means of Conduction and Convection

Temperature Distribution Inside Cell

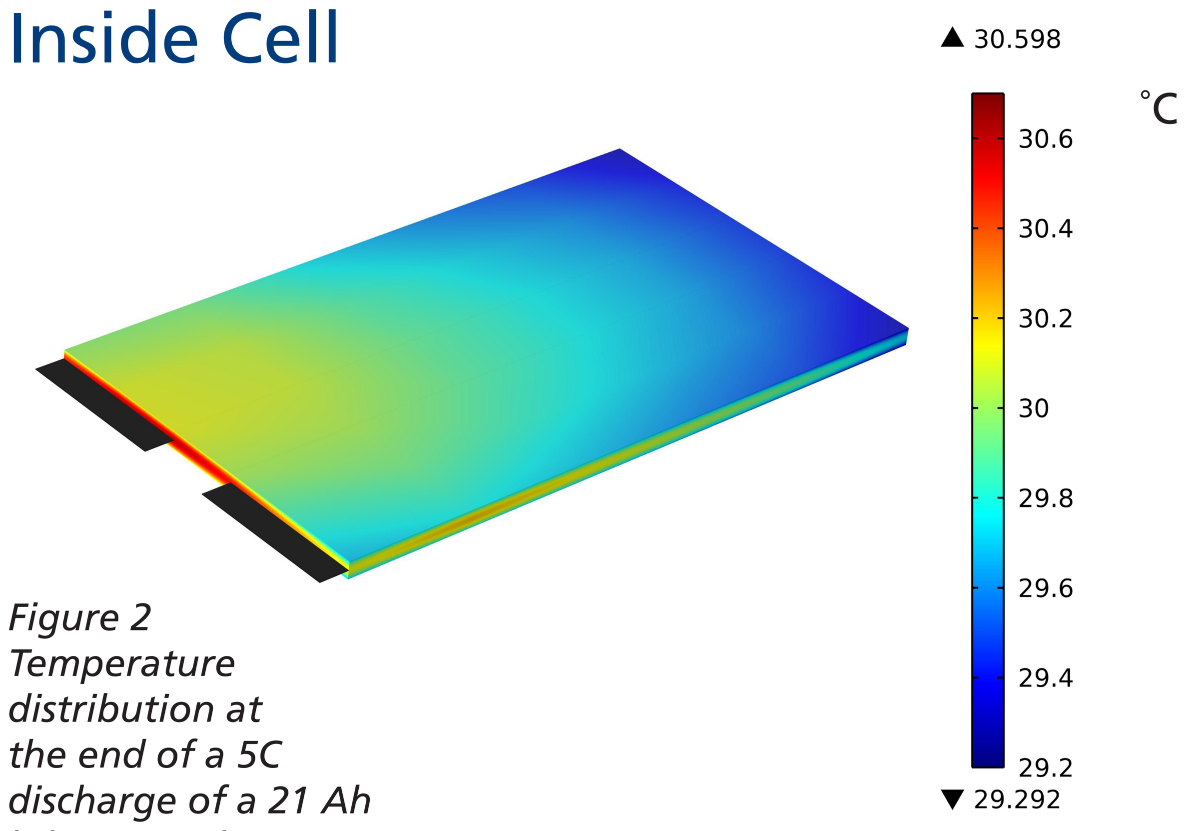

Figure 2
Temperature distribution at the end of a 5C discharge of a 21 Ah lithium-ion battery

Maximum Temperature as a Function of C-rate

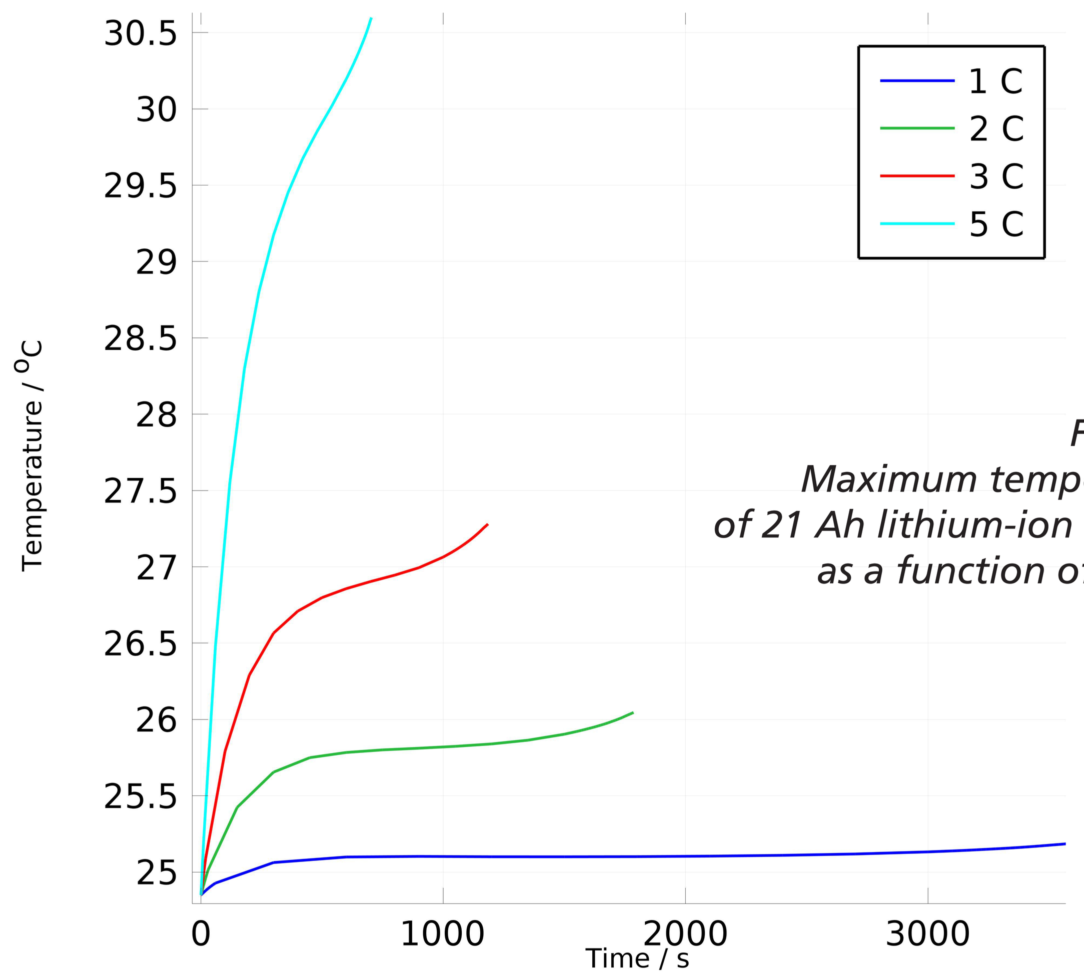

Figure 3
Maximum temperature of 21 Ah lithium-ion battery as a function of C-rate

Thermal Management System Model

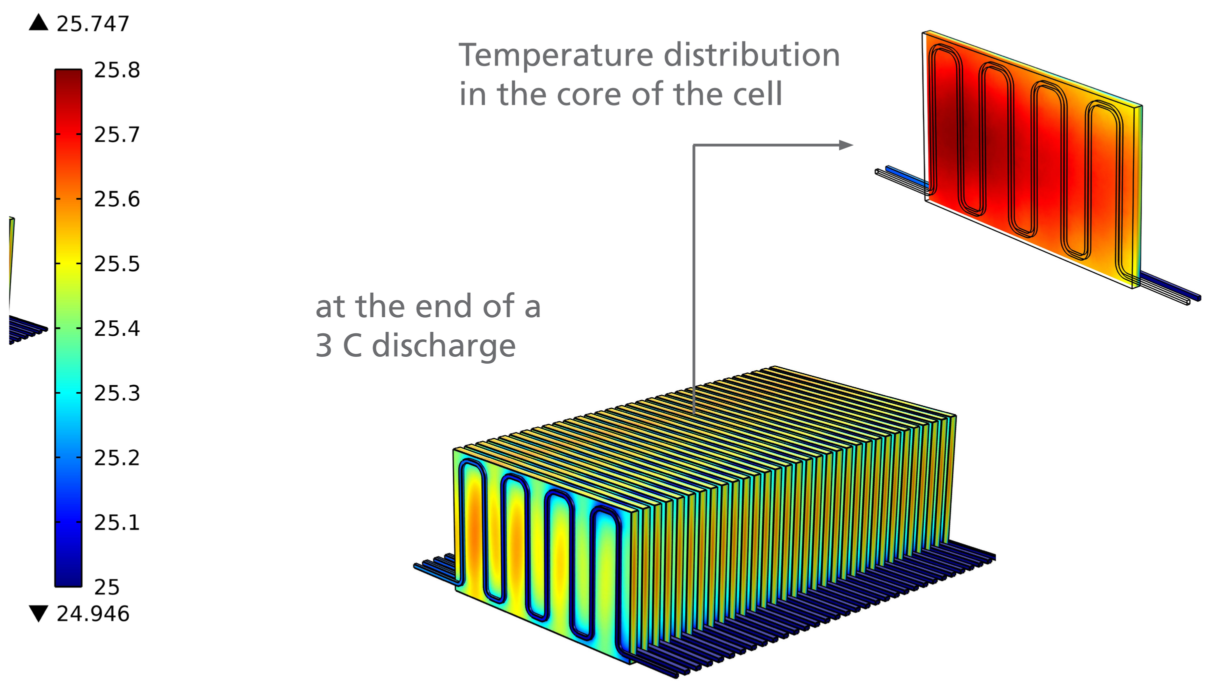

Figure 4
Temperature distribution on the surfaces of the cells and in the cooling channels

Measuring a Decline in Performance

- Lithium-Ion Batteries Lose Capacity & Internal Resistance Increases Over Time
- Reactions responsible for this can be included in a performance model, and simulation can be used to:
  - » estimate battery life under different operating conditions, and
  - » design and control operating conditions to avoid accelerated aging

Concluding Remarks

Mathematical Modeling + Reverse Engineering + Experimental Testing

- Evaluates the safety and performance of a battery cell and its applications
- Enhances understanding of the interaction between battery processes
- Knowledge saves time and cost

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