

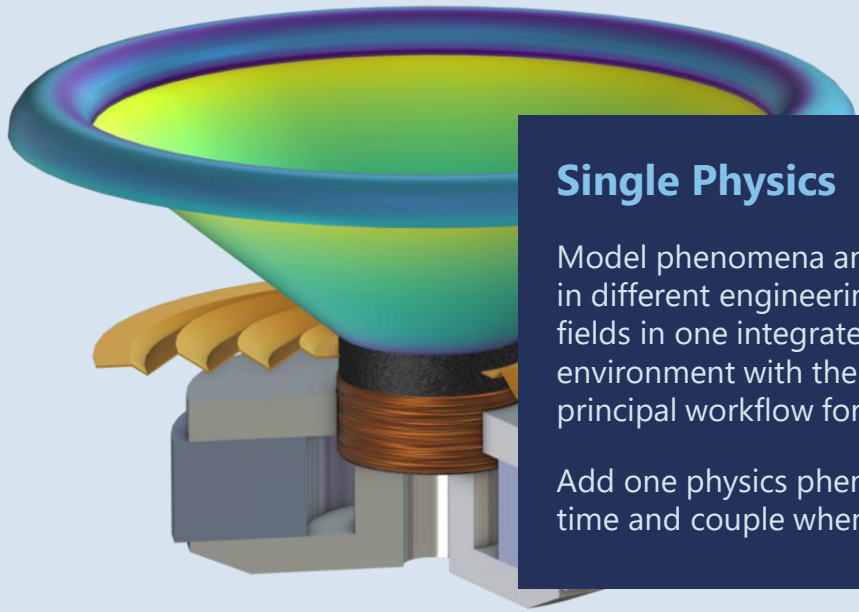
# Optimizing Battery Design with Simulation

Ross Hubble, COMSOL

# COMSOL Multiphysics®

*One software environment, any engineering field.*

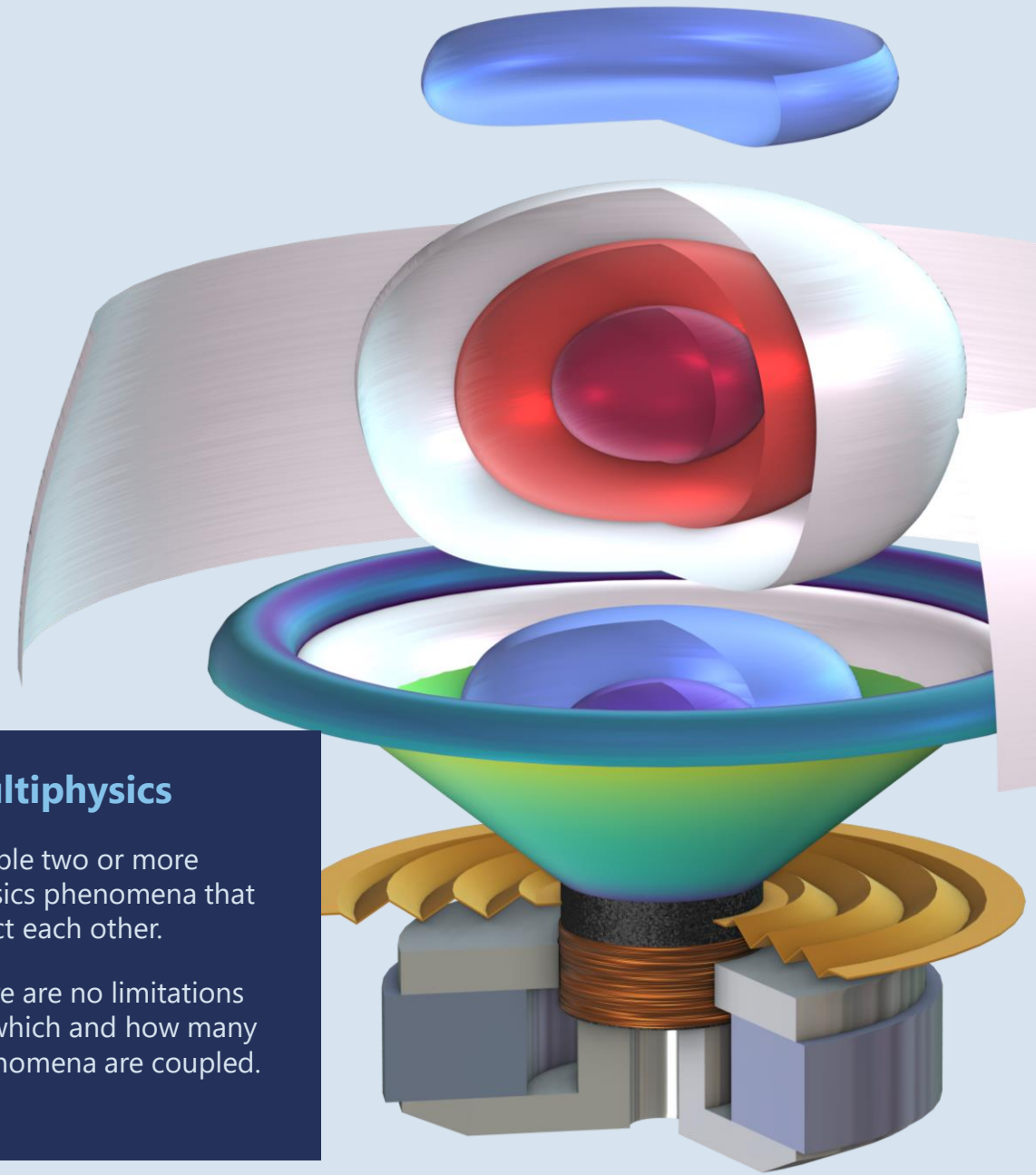
A modeling and simulation platform that provides fully coupled multiphysics and single-physics modeling capabilities.



## Single Physics

Model phenomena and processes in different engineering and physics fields in one integrated environment with the same principal workflow for all areas.

Add one physics phenomenon at a time and couple when you want.



## Multiphysics

Couple two or more physics phenomena that affect each other.

There are no limitations for which and how many phenomena are coupled.

# COMSOL Multiphysics®

*A powerful modeling and simulation platform.*

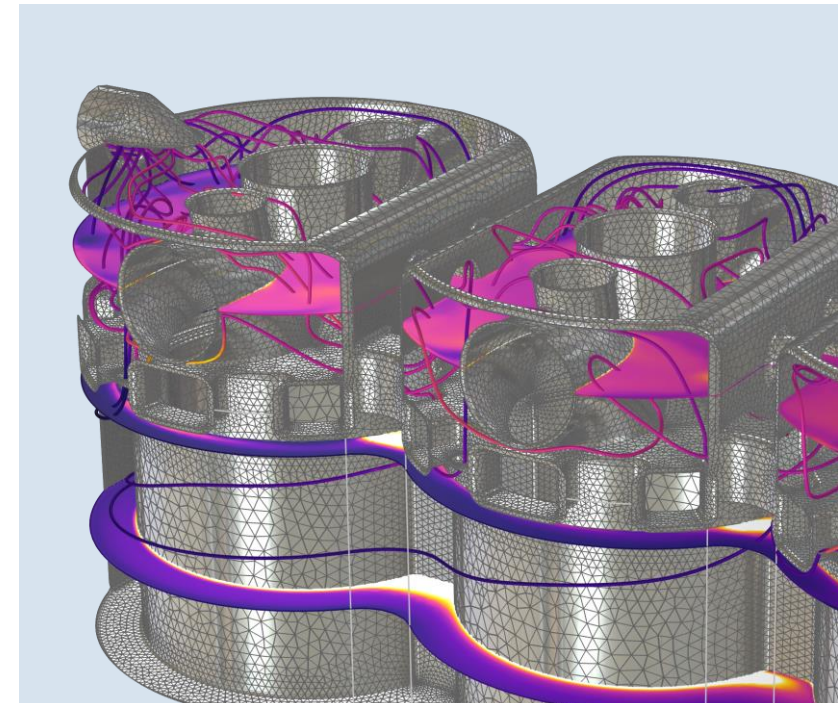
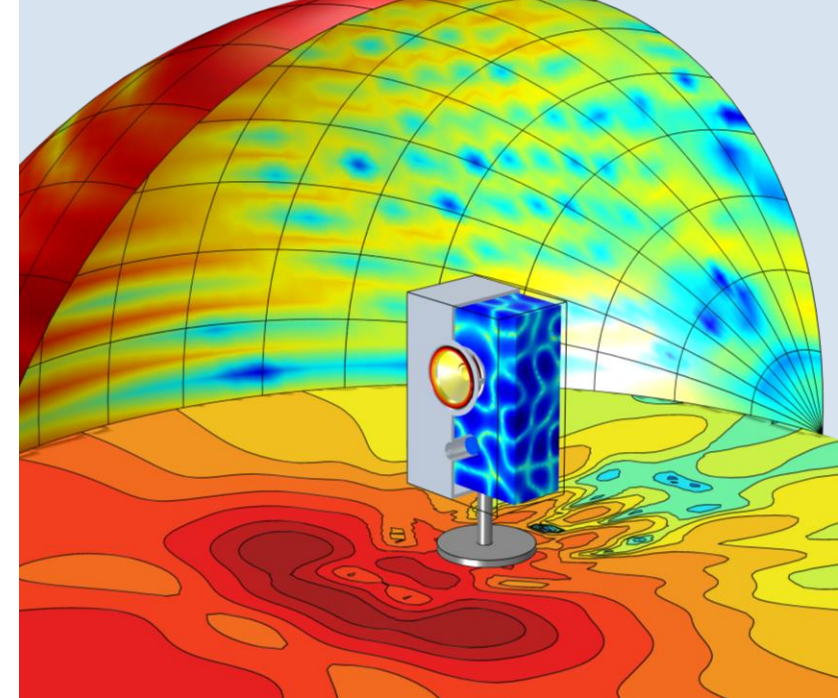
- 35 add-on modules with dedicated user interfaces and tools for modeling and simulation in electromagnetics, fluid flow, heat transfer, structural mechanics, acoustics, and chemical engineering
- 14 interfacing products to connect simulations with spreadsheet, technical computing, CAD, and ECAD
- Based on finite element, boundary element, discontinuous Galerkin, method of lines, and other numerical methods
- Solid, gas, and liquid properties are available in comprehensive material libraries in the platform product and add-on products

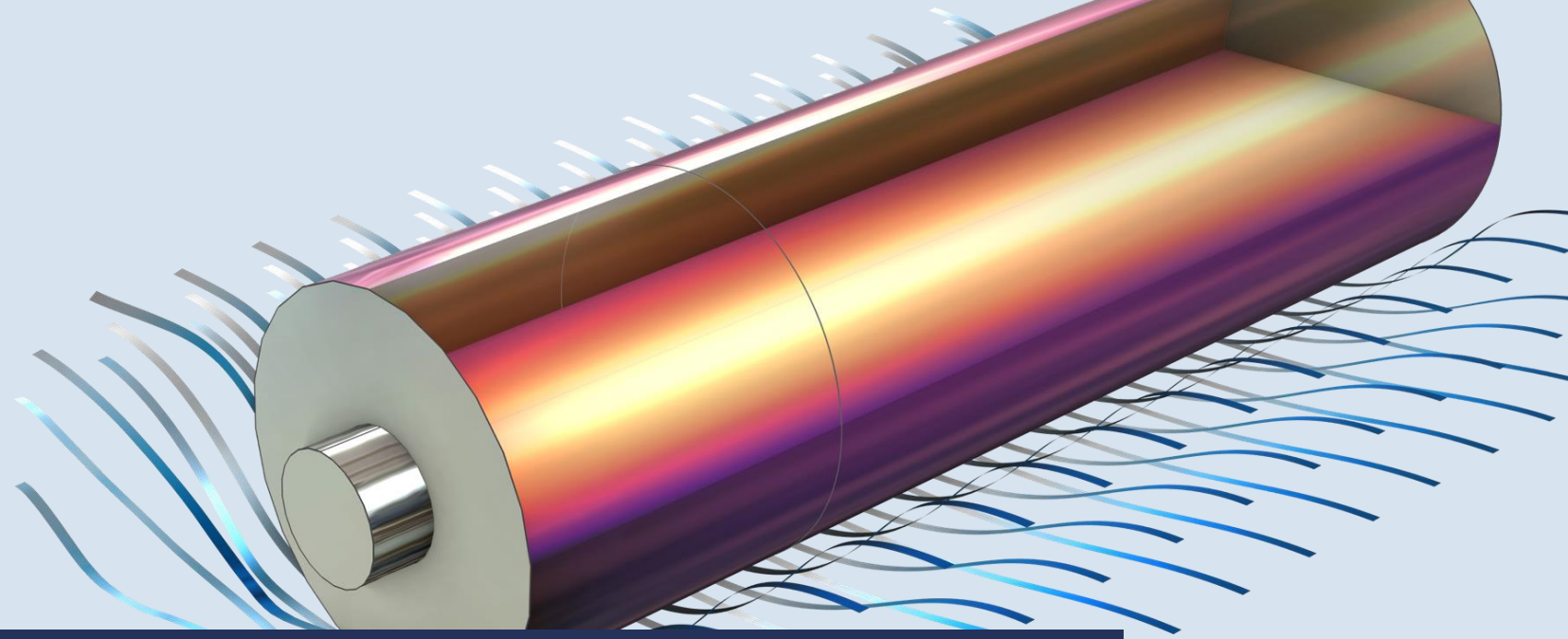
## APPLICATIONS

Build apps with the Application Builder. Compile apps into standalone executable files with COMSOL Compiler™. Host and administer apps with COMSOL Server™.

## MANAGEMENT

Centrally administer and collaborate on models and apps in the Model Manager and Model Manager server.





# Battery Design in COMSOL Multiphysics®

## Battery Design Module

An overview of the functionality for modeling different battery chemistries at different scales and for different purposes.

## Cell Models

- Performance and design
- Capacity fade and aging
- Different levels of fidelity

## Pack Models

- Cylindrical cells
- Pouch cells
- For performance and thermal management

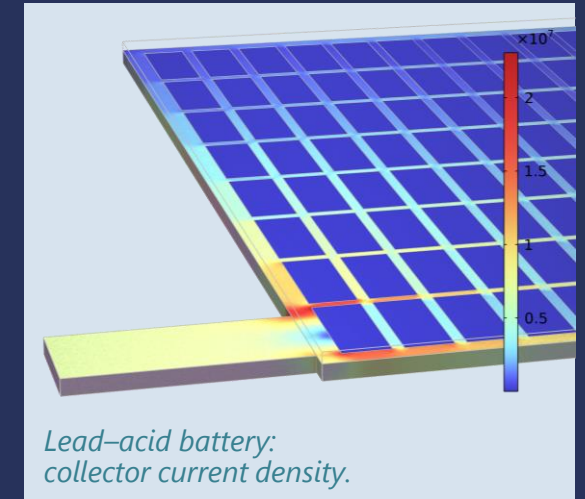
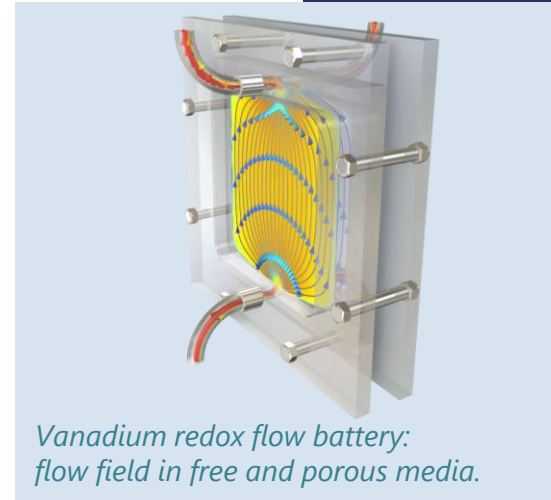
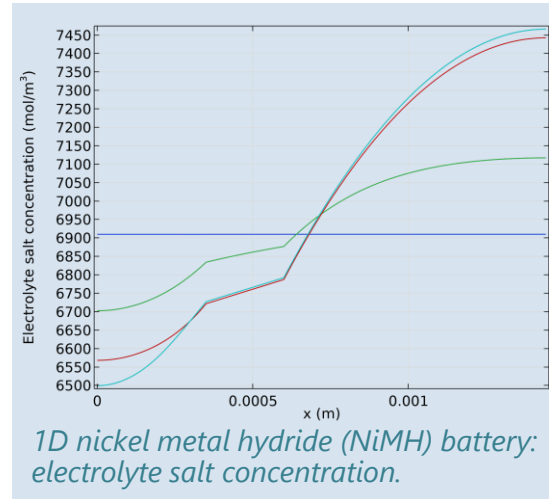
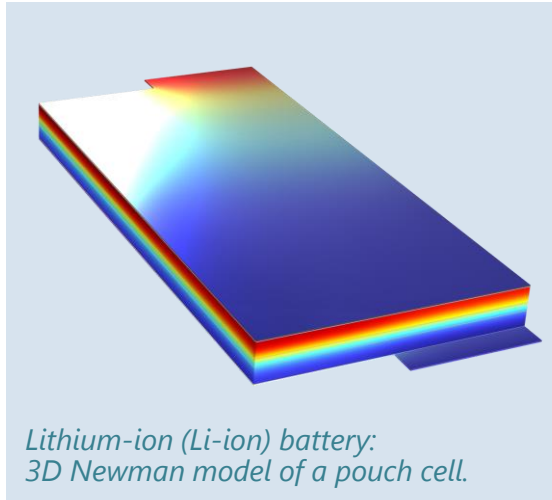
## Thermal Management

- Heat transfer mechanisms
- Electrochemical heat sources
- Short circuits and thermal runaway

## Study Types

- Time dependent
- Cyclic voltammetry, EIS, cycling
- Parameter estimation

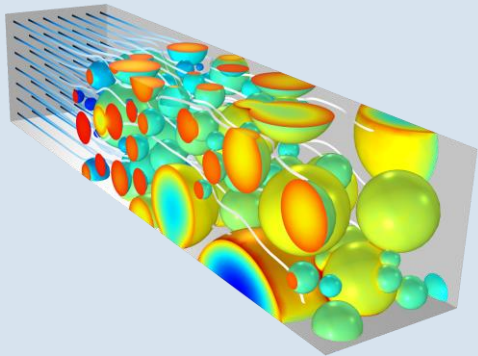
# The Battery Design Module: Chemistries



- Predefined electrochemistry for all major battery chemistries
- Nernst–Planck equations and kinetics for any chemistry, porous or solid electrodes
- Time-dependent, including transient effects, and physics-based EIS\* studies
- Multiphysics: electrochemical heating, fluid flow, and structural mechanics for expansion and contraction during cycling

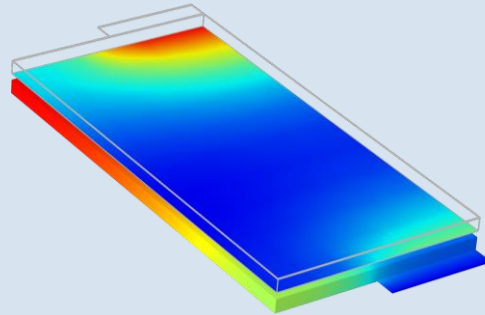
\*EIS = electrochemical impedance spectroscopy

# Battery Model Types in the Battery Design Module



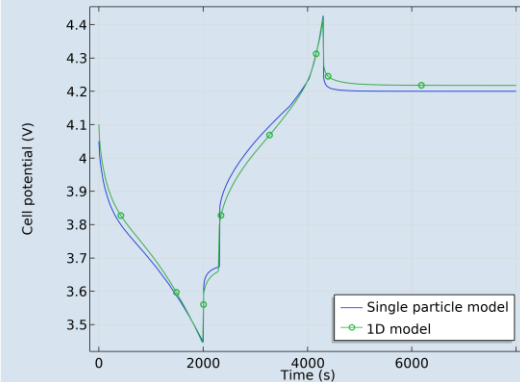
## Heterogeneous Models

- 3D, full geometry, and geometry from tomography
- Transport of all species, kinetics, potentials, etc.
- For fundamental studies of structure, kinetics, mass transport, by-reactions, aging, and more



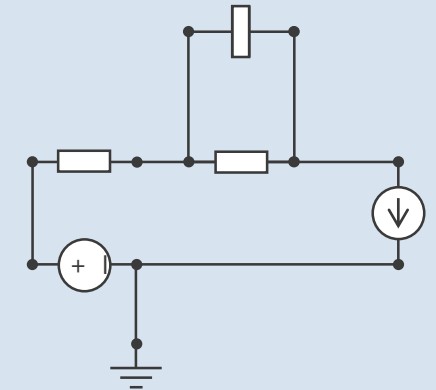
## Homogeneous Models

- 1D to 3D, plus 1D particle diffusion of Li or H, e.g., the Newman model
- Homogeneous electrodes
- For fundamental studies but also for design, performance, aging, and more
- 1D also for battery packs



## Single Particle Models

- 0D, plus 1D particle
- Electrode described with a single "particle"
- Kinetics for each electrode
- For battery packs and systems
- Real-time parameter estimation

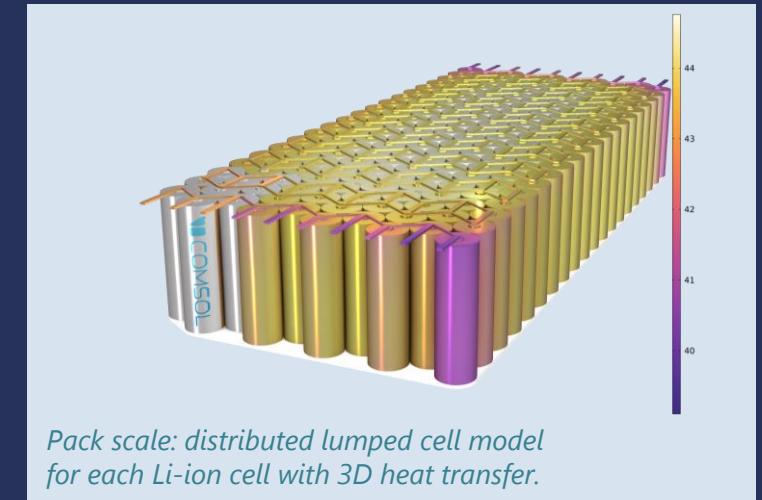
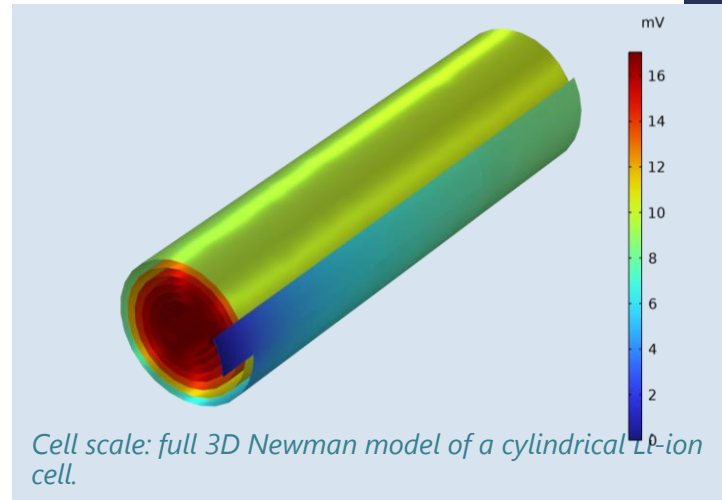
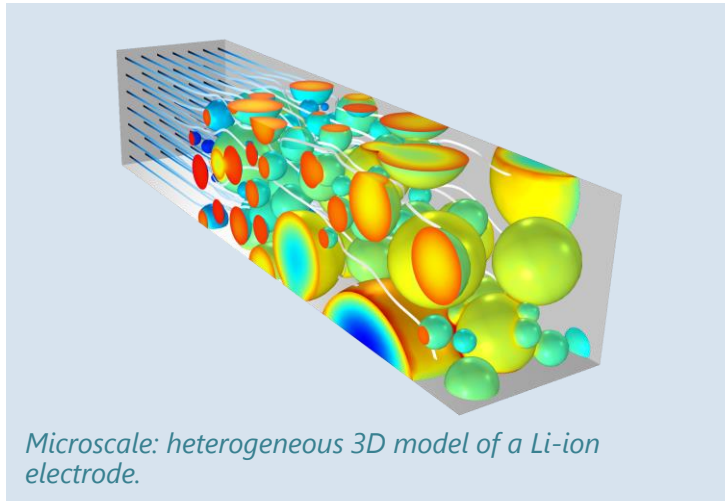


## Equivalent Circuits and Lumped Models

- 0D, plus 1D particle
- Lumped cell parameters
- Computes the SOC\* to determine the OCV\*
- For battery packs and systems
- Real-time parameter estimation

\*SOC = state of charge; OCV = open cell voltage

# The Battery Design Module: Scales



- Modeling from microscale to pack scale
- Full electrochemistry in all scales in 1D, 2D, and 3D
- 1D detailed electrochemistry or 0D lumped cell models for modeling many cells at the pack scale, e.g., for thermal management models
- Time-dependent studies, including transient effects, charge–discharge cycles, and EIS\* studies for all scales and chemistries

\*EIS = electrochemical impedance spectroscopy

# Battery Chemistries

## Newman model for Li-ion cells:

- Models the electrolyte concentration and intercalating species (Li), as well as electrolyte and electrode potentials
- Aging effects, SEI, and effects of expansion and contraction during cycling

pouch\_cell\_utilization.mph - COMSOL Multiphysics

File Home Definitions Geometry Materials Physics Mesh Study Results Developer

Application Builder Model Manager Component 1 Add Component Parameters Parameters Case Definitions Build All Import LiveLink Add Material Lithium-Ion Battery Add Physics Build Mesh Mesh 1 Compute Study 1 Add Study

Workspace Model

Model Builder

pouch\_cell\_utilization.mph (root)

- Global Definitions
  - Parameters 1
  - Default Model Inputs
  - Materials
- Component 1 (comp1)
  - Definitions
  - Geometry 1
    - Materials
      - Aluminum (mat1)
      - Copper (mat2)
      - Graphite, LiC6 MCMB (Negative, Li-ion Battery)
      - LMO, LiMn2O4 Spinel (Positive, Li-ion Battery)
      - LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat)
    - Lithium-Ion Battery (lion)
      - Electrolyte 1
      - No Flux 1
      - Insulation 1
      - Initial Values 1
      - Separator 1
      - Poros Electrode - Negative
        - Particle Intercalation 1
        - Poros Electrode Reaction 1
      - Poros Electrode - Positive
        - Electrode 1
      - Electric Ground 1
      - Electrode Current 1
      - Initial Cell Charge Distribution 1
    - Multiphysics
  - Mesh 1
- Study 1
  - Parametric Sweep
    - Step 1: Current Distribution Initialization
    - Step 2: Time Dependent
  - Solver Configurations
  - Job Configurations
  - Results

Settings

Poros Electrode

Equation

Show equation assuming: Study 1, Current Distribution Initialization

$$\nabla \cdot \mathbf{J}_l = R_l, \quad R_l = -\sum_m \frac{v_{Li+m} i_{v,m}}{F} + R_{l,src}$$

$$\nabla \cdot \mathbf{i}_l = i_{v,total} + Q_l$$

$$\nabla \cdot \mathbf{i}_s = -i_{v,total} + Q_s$$

$$\mathbf{J}_l = -D_{l,eff} \nabla c_l + \frac{i_l t_{\pm}}{F}$$

$$\mathbf{i}_l = -\sigma_{l,eff} \nabla \phi_l + \left( \frac{2\sigma_{l,eff} RT}{F} \right) \left( 1 + \frac{\partial \ln f}{\partial \ln c_l} \right) (1 - t_{\pm}) \nabla \ln c_l$$

$$\mathbf{i}_s = -\sigma_{s,eff} \nabla \phi_s$$

$$D_{l,eff} = \epsilon_l^{1.5} D_l, \quad \sigma_{l,eff} = \epsilon_l^{1.5} \sigma_l, \quad \sigma_{s,eff} = \epsilon_s^{1.5} \sigma_s$$

$$i_{v,total} = \sum_m i_{v,m} + i_{v,d}$$

Model Inputs

- Coordinate System Selection
- Electrolyte Properties
- Electrode Properties
- Particle Properties
  - Intercalating particles
- Poros Matrix Properties
  - Electrode volume fraction:  $\epsilon_s$  epss\_neg 1
  - Electrolyte volume fraction:  $\epsilon_l$  1-epss\_neg 1
  - Effective Transport Parameter Correction
    - Electrolyte conductivity: Bruggeman
    - Electrical conductivity:

Graphics Electric Potential

C\_rate(2)=4 1 Time=630 s Volume: Electric potential (V) Volume: Electric



# Battery Chemistries

## Other examples

Lead Acid

Nickel Metal Hydride

Lithium-Sulfur, Li-S

Nickel-Cadmium, NiCd

Zinc-Silver Oxide, Zn-AgO

Zinc-Bromine, Zn-Br

znbr\_flow\_battery.mph - COMSOL Multiphysics

File Home Definitions Geometry Sketch Materials Physics Mesh Study Results Developer

Application Builder Model Manager Component 1 Add Component Parameters Pi a= Variables f Functions Pi Parameter Case Build All Import LiveLink Add Material Tertiary Current Distribution, Nernst-Planck Add Physics Build Mesh Mesh 1 Compute Study 1

Workspace Model Definitions Geometry Materials

Model Builder

- znbr\_flow\_battery.mph (root)
  - Global Definitions
    - Parameters 1
    - Default Model Inputs
    - Materials
  - Component 1 (comp1)
    - Definitions
    - Geometry 1
      - Materials
      - Tertiary Current Distribution, Nernst-Planck (tcd)
        - Electrolyte 1
        - No Flux 1
        - Insulation 1
        - Initial Values 1
        - Separator 1
        - Porous Electrode - Negative
        - Porous Electrode - Positive
        - Electric Ground 1
        - Electrode Current 1
        - Internal Electrode Surface 1
        - Inflow 1
        - Outflow 1
        - Initial Values 2
      - Global ODEs and DAEs - Tank Model (ge)
      - Multiphysics
      - Mesh 1
    - Study 1
      - Parametric Sweep
      - Step 1: Current Distribution Initialization
      - Step 2: Time Dependent
      - Solver Configurations
      - Job Configurations
      - Results

## Settings

### Porous Electrode

#### Equation

Show equation assuming:

Study 1, Current Distribution Initialization

$$\nabla \cdot \mathbf{J}_i + \mathbf{u} \cdot \nabla C_i = R_{i,\text{tot}}, \quad R_{i,\text{tot}} = \sum_m R_{i,m} + R_{\text{dl},i} + \epsilon_i R_i$$

$$\nabla \cdot \mathbf{i}_l = \epsilon_l F \sum_i z_i R_i + Q_l + i_{v,\text{total}}$$

$$\nabla \cdot \mathbf{i}_s = -\epsilon_s F \sum_i z_i R_i + Q_s - i_{v,\text{total}}$$

$$\mathbf{J}_i = -D_{i,\text{eff}} \nabla C_i - z_i u_{m,j,\text{eff}} F C_i \nabla \phi_i$$

$$\mathbf{i}_l = -\sigma_{l,\text{eff}} \nabla \phi_l$$

$$\mathbf{i}_s = -\sigma_{s,\text{eff}} \nabla \phi_s$$

$$D_{i,\text{eff}} = \epsilon_i 1.5 D_i$$

$$\sigma_{l,\text{eff}} = \epsilon_l 1.5 \sigma_l$$

$$\sigma_{s,\text{eff}} = \epsilon_s 1.5 \sigma_s$$

$$i_{v,\text{total}} = \sum_m i_{v,m} + i_{v,\text{dl}}$$

#### Model Input

#### Coordinate System Selection

#### Convection

#### Diffusion

#### Migration in Electric Field

Mobility:

Nernst-Einstein relation

$$u_{m,j} = \frac{D_j}{RT}$$

Charge number:

Z<sub>cBr2</sub> 0

Electrolyte material:

Domain material

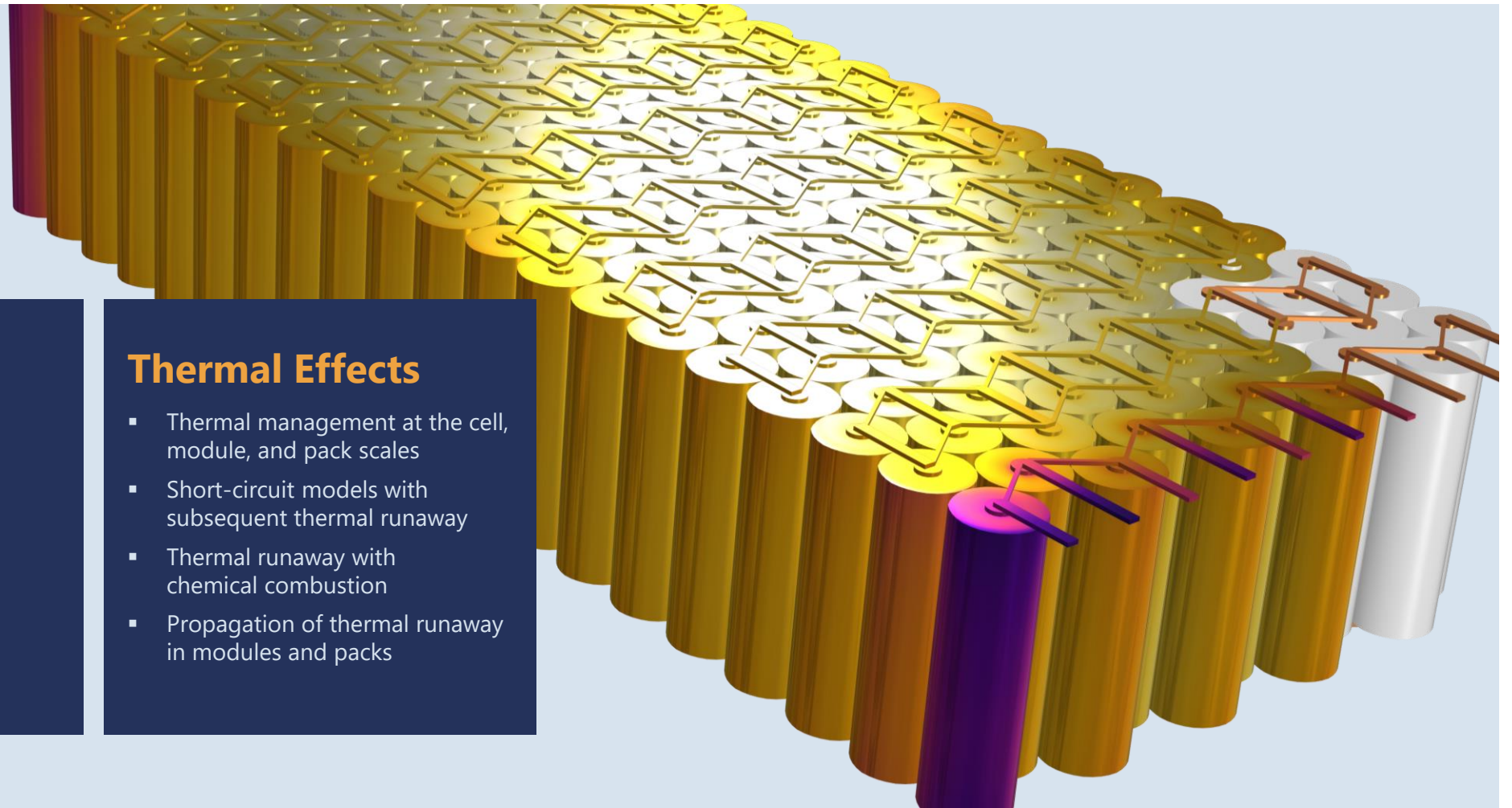
# Aging and Thermal Management

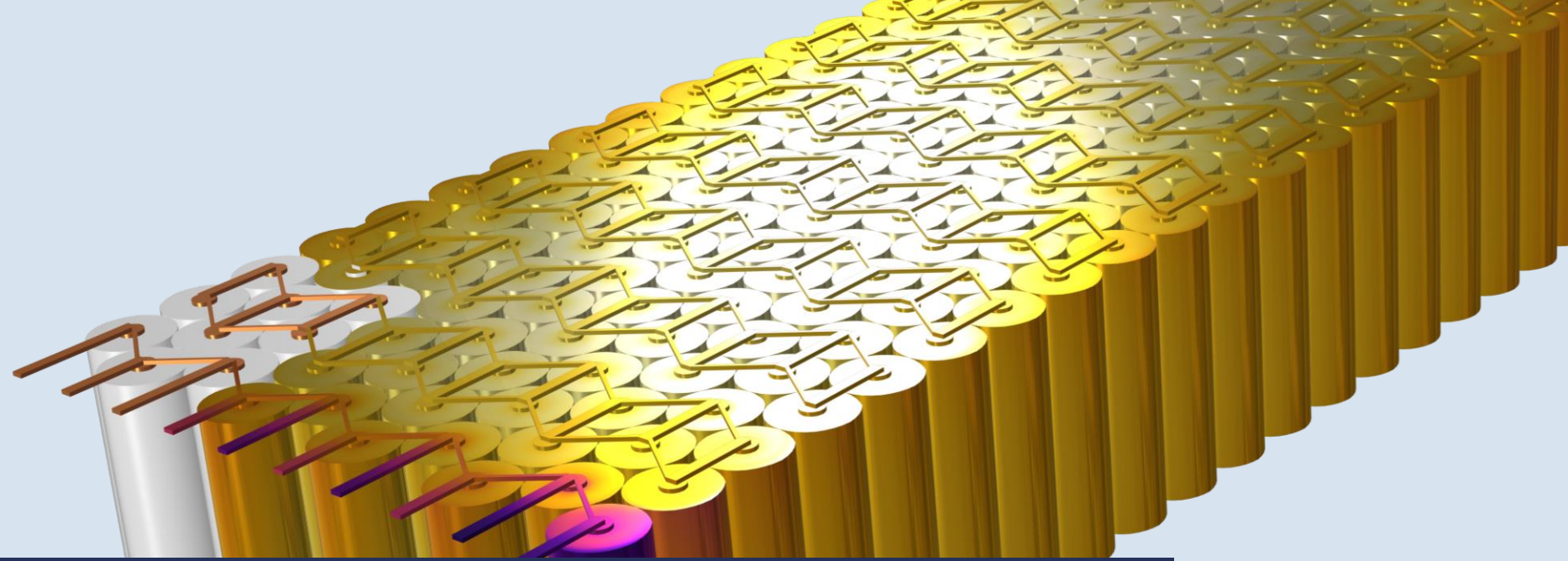
## Capacity Fade and Aging

- Plating and short circuits
- Gas evolution
- Side reactions and loss of surface area
- Loss of electrolyte
- SEI formation
- Mechanical degradation, e.g., crack formation

## Thermal Effects

- Thermal management at the cell, module, and pack scales
- Short-circuit models with subsequent thermal runaway
- Thermal runaway with chemical combustion
- Propagation of thermal runaway in modules and packs





# Modeling of Heat Generation and Heat Transfer

## Cooling

- Avoids excess SEI (Li-ion) formation and gassing
- Slows down deterioration of materials

## Hot Spots

- Lead to accelerated aging
- Increase risk for thermal runaway

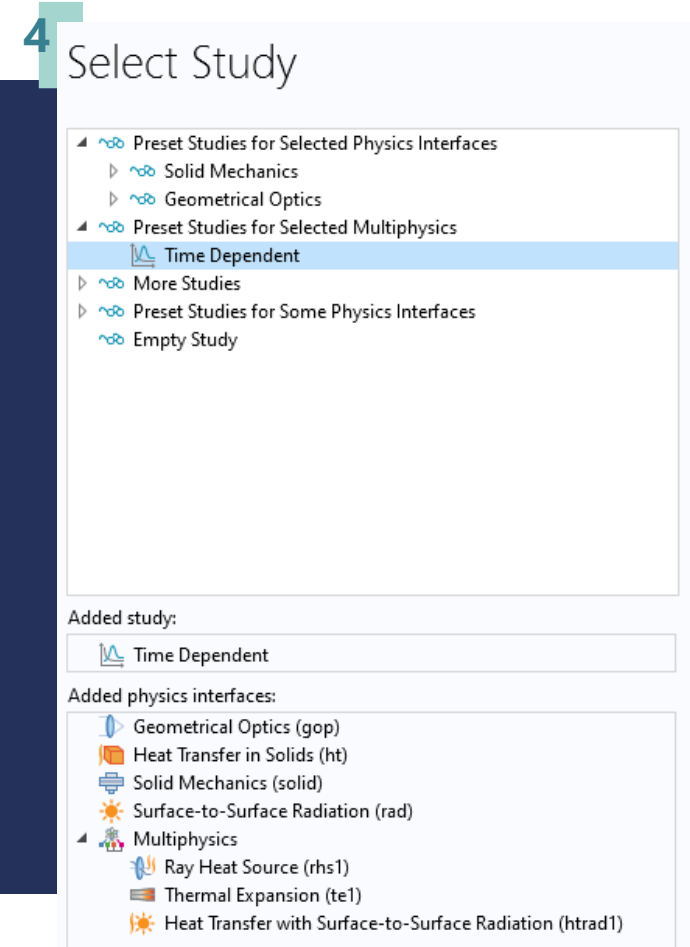
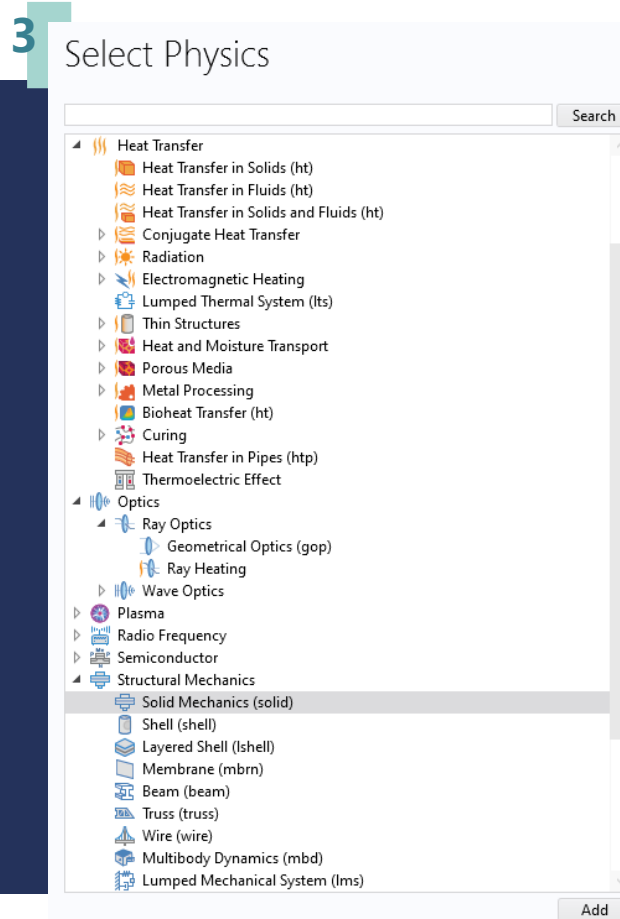
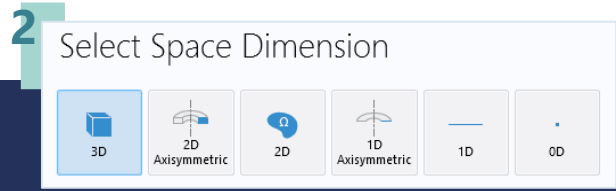
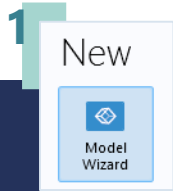
## Startup from Cold

- Low-temperature operation may result in lithium plating
- Low temperature yields low electrolyte conductivity and poor performance

## Worst Case

- Find maximum temperature during misuse
- Avoid thermal runaway

# Demonstration

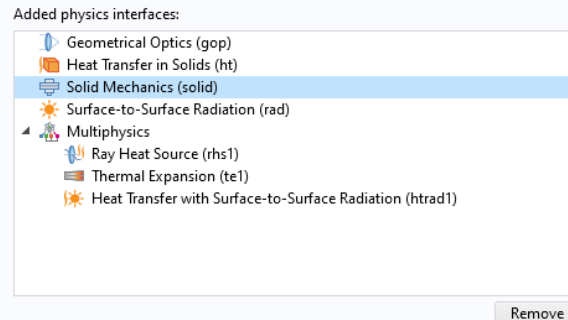


## THE FIRST STEP

# The Model Wizard

When creating a new model, the Model Wizard assists with selecting:

- Dimension (3D, 2D, 1D, or 0D)
- Physics interface(s) from the physics list
- Study for the physics interfaces



1. Select *Model Wizard*.
2. Select space dimension.
3. Select physics interfaces.
4. Select study.

## Application Builder and Model Manager

Click the respective button to switch to the Application Builder or Model Manager.

## Model Builder Window

The model tree, with the associated toolbar buttons, gives you an overview of the model. The modeling process can be controlled from context-sensitive menus.

## Settings Window

Shows the settings for the node that is selected in the model tree.

## Ribbon

Controls for all steps of the modeling process.

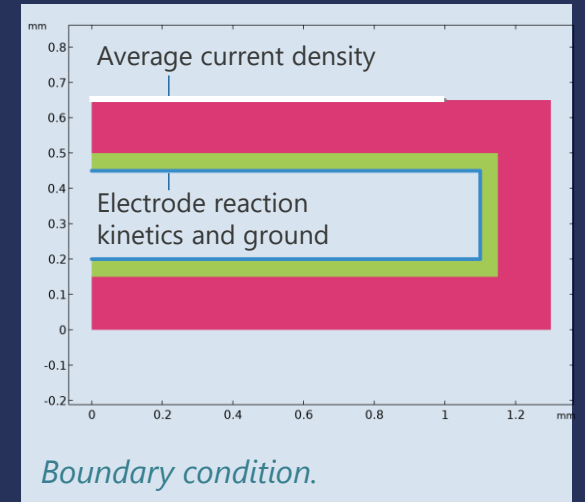
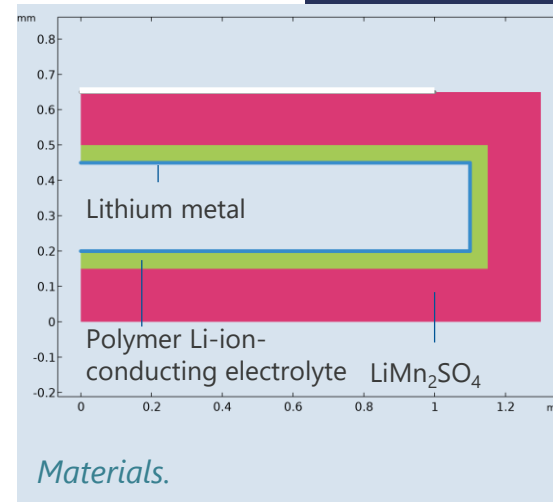
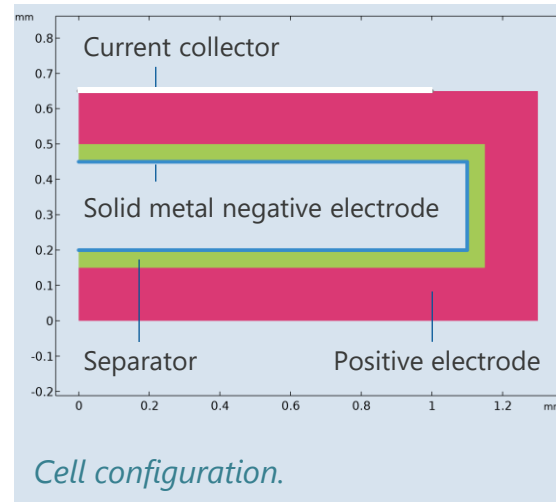
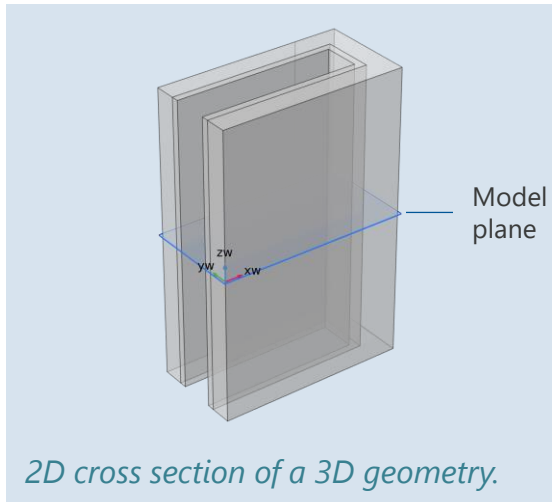
## Graphics Window Toolbar

## COMSOL Desktop® Model Builder

The screenshot displays the COMSOL Desktop Model Builder interface for a model named "pouch\_cell\_utilization.mph".

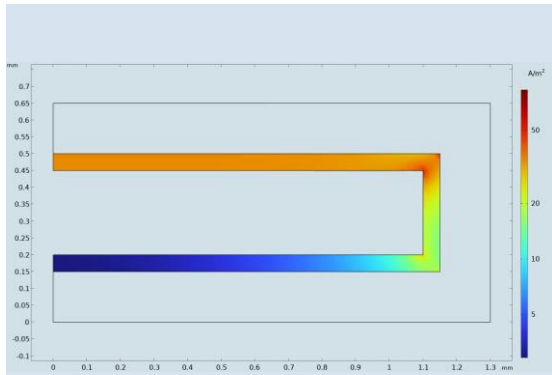
- Ribbon:** The top ribbon contains tabs for File, Home, Definitions, Geometry, Materials, Physics, Mesh, Study, Results, and Developer. The Physics tab is active, showing options for Lithium-ion Battery, Add Physics, Build Mesh, Compute, Study, Add Study, Potential in the Collectors and Tabs, Add Plot Group, Windows, and Reset Desktop.
- Model Builder Window:** The left pane shows the model tree for "pouch\_cell\_utilization.mph (root)". It includes Global Definitions (Parameters 1, Default Model Inputs, Materials), Component 1 (comp1) with sub-items for Definitions, Geometry 1, Materials (Aluminum, Copper, Graphite, LMO, LiPF6), Lithium-ion Battery (lithion) with sub-items for Electrolyte 1, No Flux 1, Insulation 1, Initial Values 1, Separator 1, Porous Electrode - Negative, Porous Electrode - Positive, Electrode 1, Electric Ground 1, Electrode Current 1, Initial Cell Charge Distribution 1, and Multiphysics. Below the tree is a small 3D preview of the battery cell.
- Settings Window:** The middle pane shows settings for the selected "Electrode Utilization in a Large Format Lithium-ion Battery" node. It includes fields for Title, Description, Author, Computation time, Expected, Last, and Thumbnail. A description is provided: "Large lithium-ion batteries are widely deployed in electric vehicles and for stationary energy storage applications. In the (stacked) pouch battery cell design, all current exits the cell on the cell collector tabs; and as the cell size and power increases, the voltage gradients in the highly conductive metal foil..."
- Graphics Window:** The right pane displays a 3D surface plot of "Electric Potential (mV)". The plot shows a color gradient from blue (low potential) to red (high potential) across the battery cell layers. The axes are labeled in meters (m). A color bar on the right indicates the potential scale from 0 to -9.187 mV, with a multiplier of  $\times 10^{-11}$ . The plot title is "C\_rate(2)=4.1 Time=0 s".
- Information Window:** The bottom pane shows the Messages, Progress, Log, and Probe Table 1 tabs.

# Model Definition

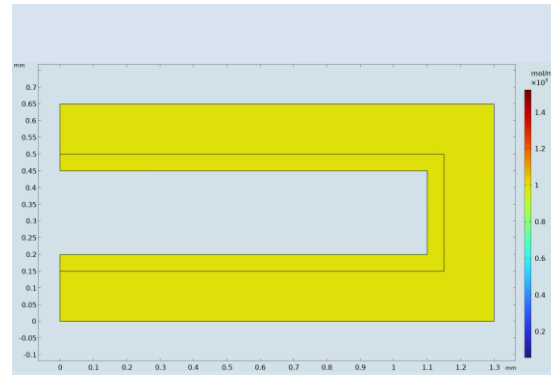


- Full Newman model for the Li-ion battery positive electrode
- Half-cell model with solid negative electrode and LMO porous positive electrode
- Material properties from the Battery Design Module material library
- Current density applied at the current collector corresponds to 1C
- Butler–Volmer kinetic expression at the lithium metal boundary
- Time-dependent study

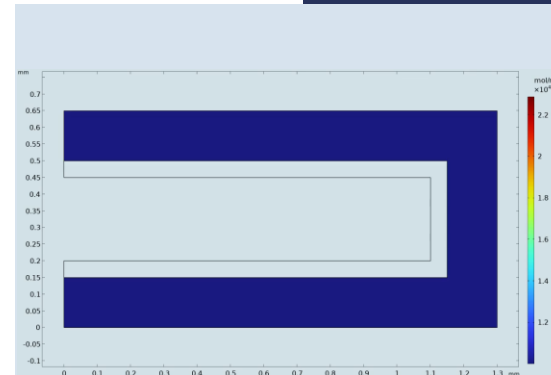
# Model Results



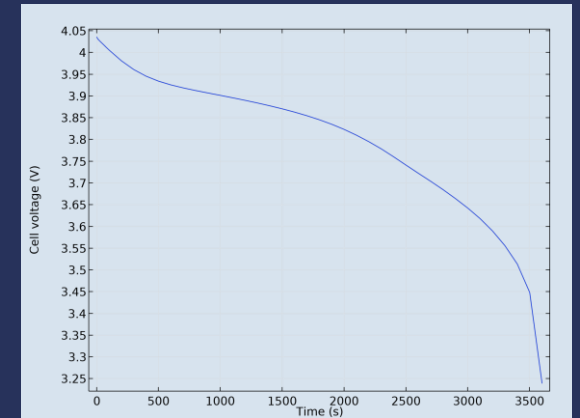
Animation of the current density in the electrolyte.



Animation of the lithium salt concentration in the electrolyte and pore electrolyte.



Animation of the lithium concentration in the particles in the positive electrode.



Cell voltage vs. time.

- The positive electrode initially discharges in the regions close to the current collector, *i.e.* the upper rectangular part
- As the lithium concentration is depleted, the regions further away from the current collector are discharged
- In this case, the position of the current collector requires that the model is at least 2D for the cell to be modeled accurately



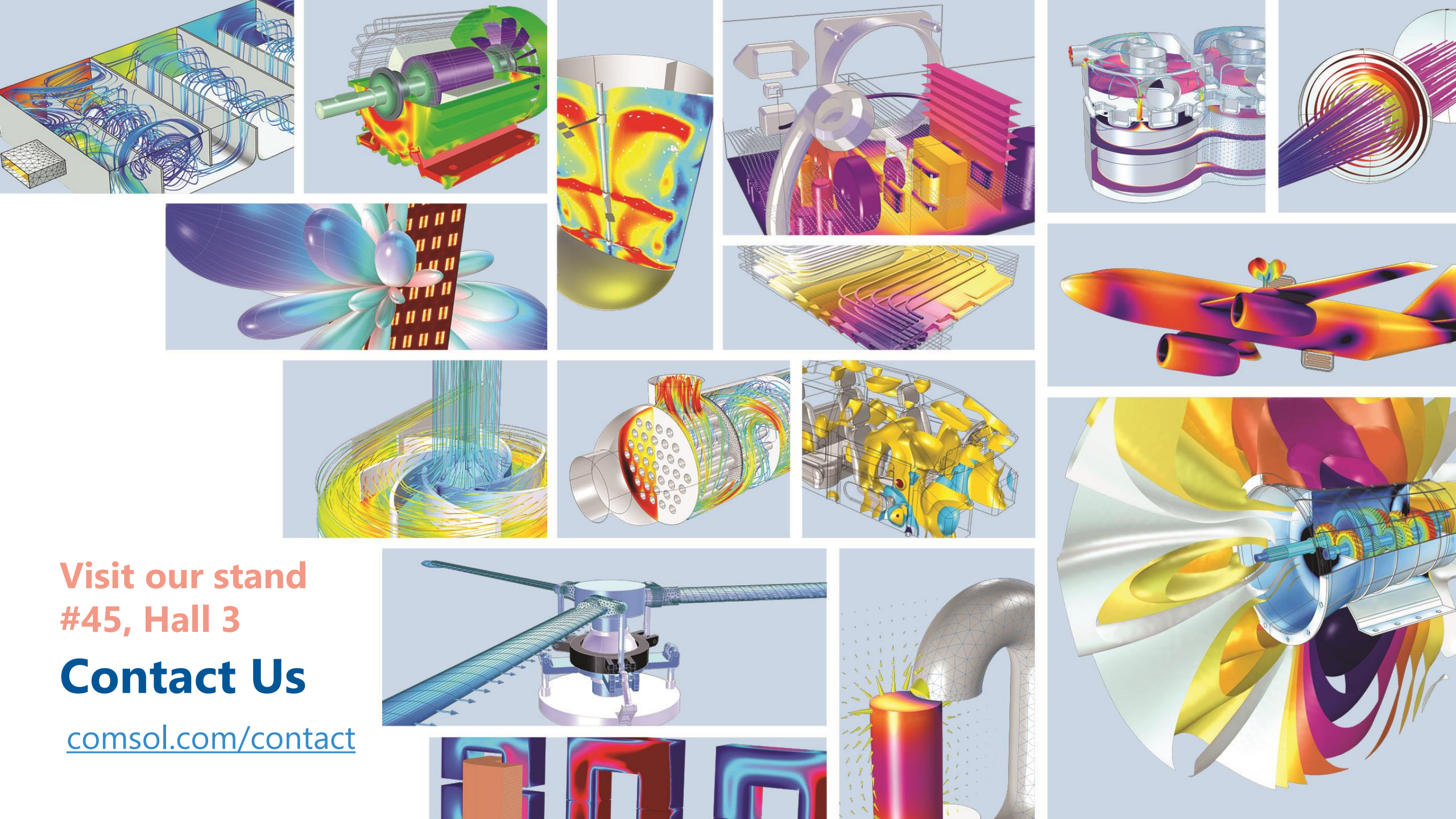
# Concluding Remarks

## Modeling with the Battery Design Module

- Battery interfaces and a material library for most battery chemistries
- Ability to enter any battery chemistry
- CAD import, built-in CAD, great meshing tool, unlimited evaluation, and visualization
- Straightforward modeling workflow, just like for all types of modeling and simulation areas

The screenshot displays the COMSOL Multiphysics software interface for a battery model simulation. The main window is titled "pouch\_cell\_utilization.mph - COMSOL Multi". The interface is divided into several sections:

- Model Builder:** Shows the hierarchical structure of the model, including Global Definitions, Component 1 (comp1), and Lithium-Ion Battery (lion). The Lithium-Ion Battery section is expanded, showing various physics and material settings.
- Settings:** Displays the configuration for the "pouch\_cell\_utilization.mph" model. Key settings include:
  - Protection:** Editing and running are not protected.
  - Used Products:** COMSOL Multiphysics and Battery Design Module.
  - Unit System:** SI.
  - Presentation:** Title: "Electrode Utilization in a Large Format Lithium-Ion Battery". Description: "Large lithium-ion batteries are widely deployed in electric vehicles and for stationary energy storage applications. In the (stacked) pouch battery cell design, all current exits the cell on the cell collector tabs; and as the cell size and power increases, the voltage gradients in the highly conductive metal foil..."
  - Author:** COMSOL
  - Expected:** (Empty field)
  - Last:** 9 min 23 s
- Graphics:** Shows a 3D visualization of the battery cell with a color-coded utilization map. The title is "Probe Plot 1" and the equation is  $C\_rate(2)=4$  1 Time=0 s. The visualization shows a cross-section of the battery cell with a color gradient from blue (low utilization) to red (high utilization). The x-axis is labeled "m" and ranges from 0 to 0.1.



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