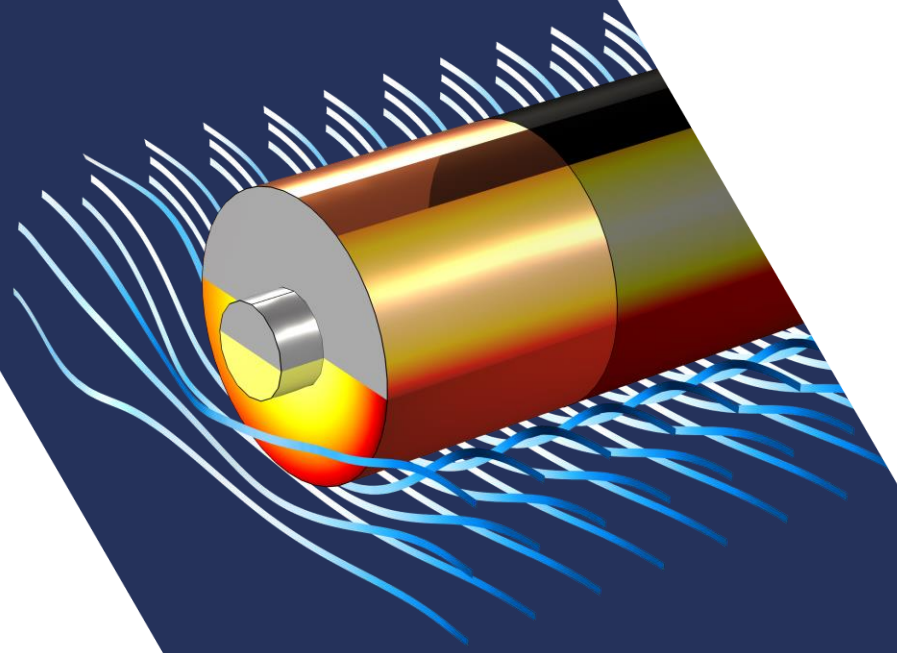


Optimizing Battery Design with Simulation

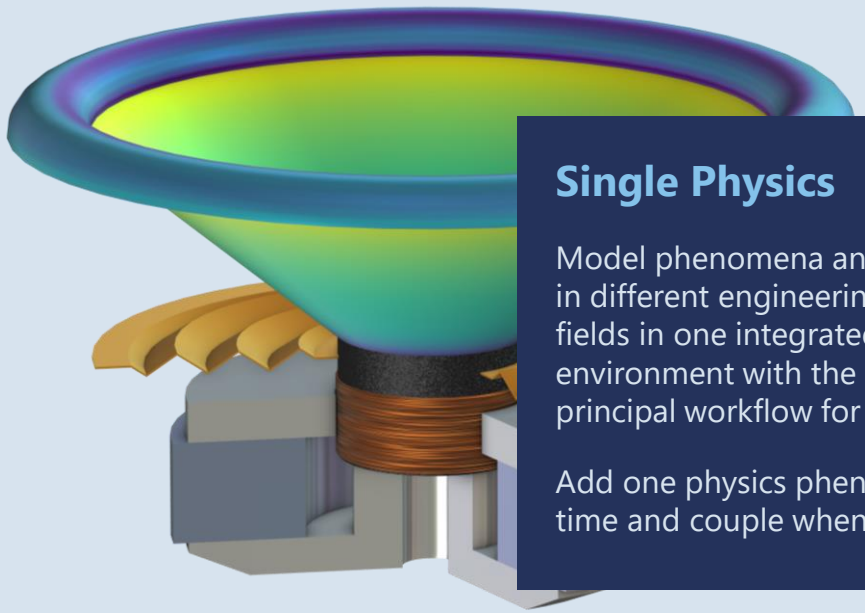
Ross Hubble, COMSOL

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

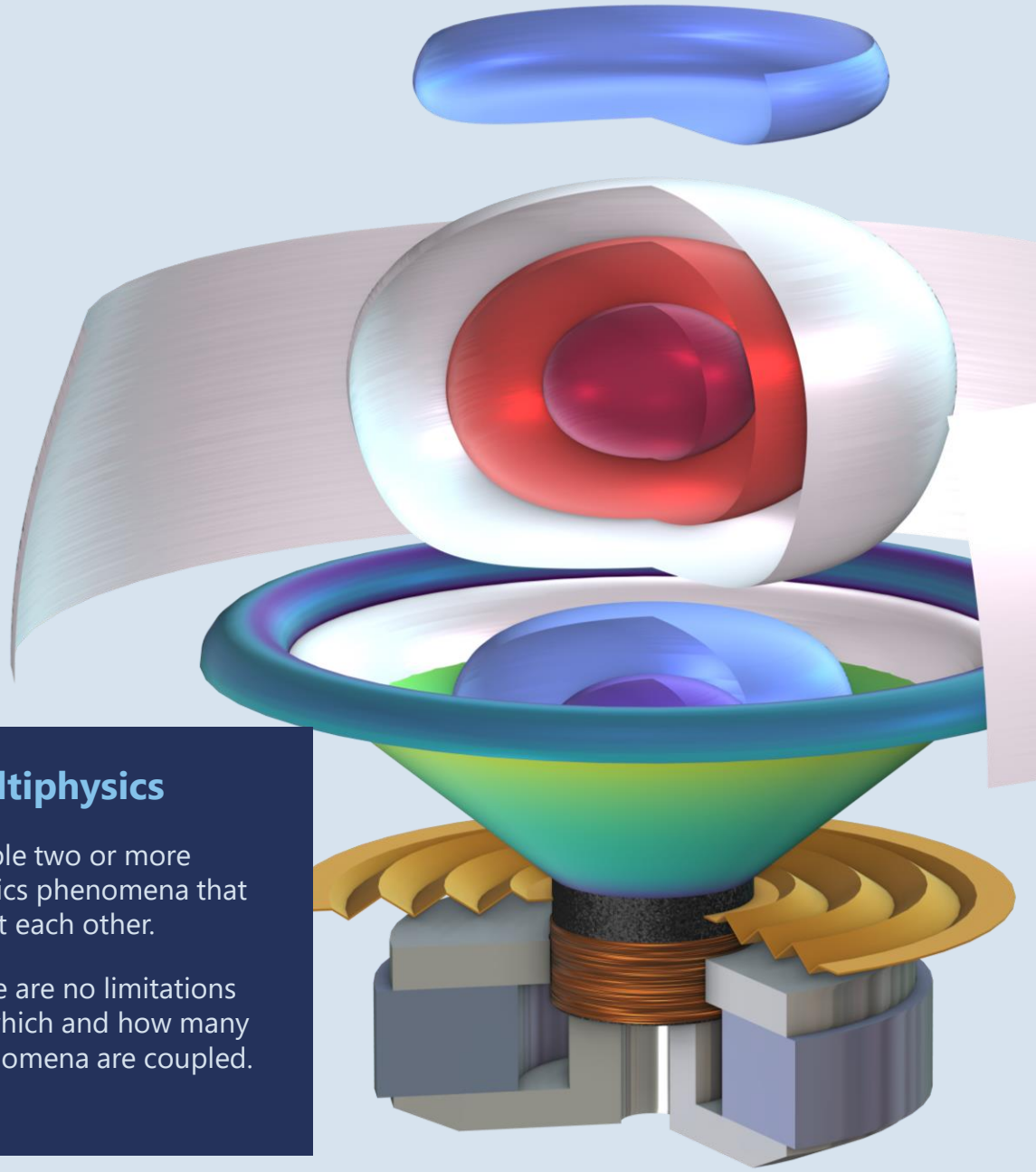
Model phenomena and processes in different engineering and physics fields in one integrated environment with the same principal workflow for all areas.

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.

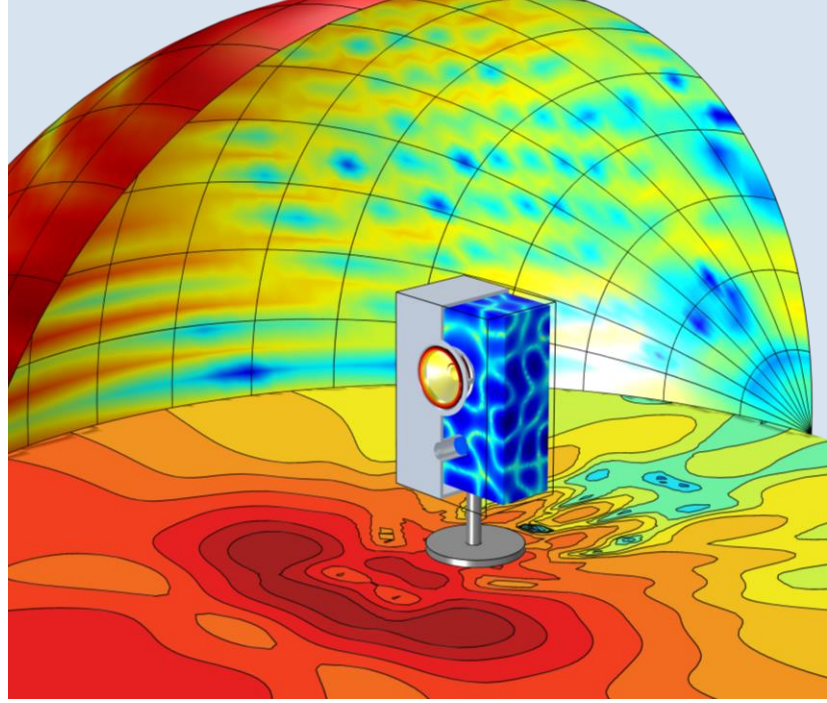
- 35 add-on modules with dedicated user interfaces and tools for modeling and simulation in electromagnetics, fluid flow, heat transfer, structural mechanics, acoustics, and chemical engineering
- 14 interfacing products to connect simulations with spreadsheet, technical computing, CAD, and ECAD
- Based 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

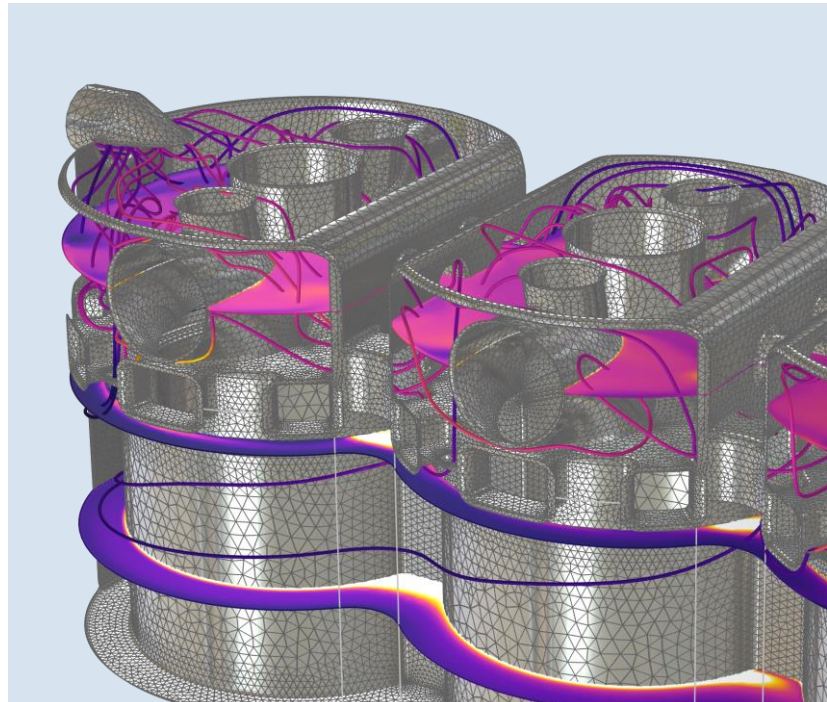
APPLICATIONS

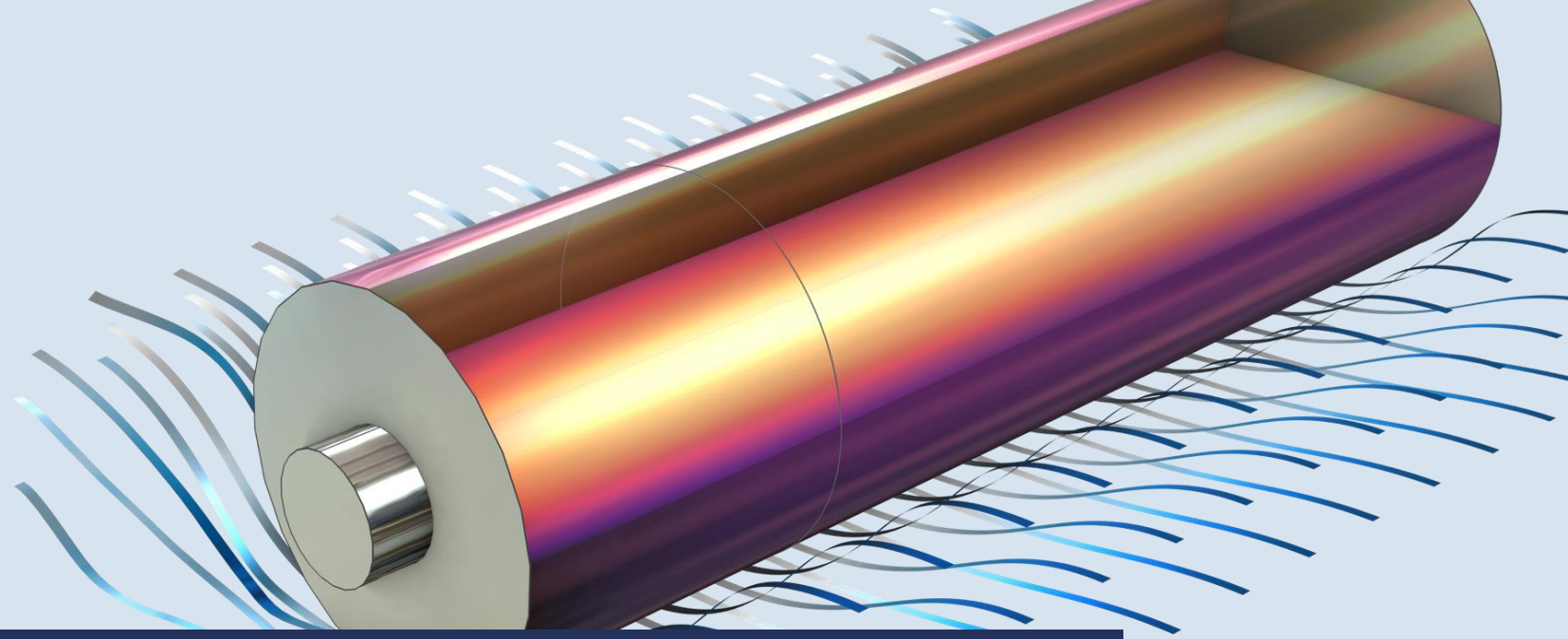
Build apps with the Application Builder. Compile apps into standalone executable files with COMSOL Compiler™. Host and administer apps with COMSOL Server™.

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

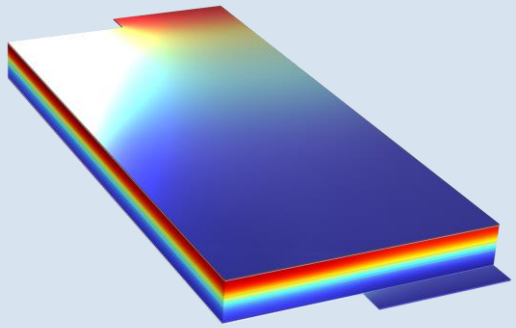
Thermal Management

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

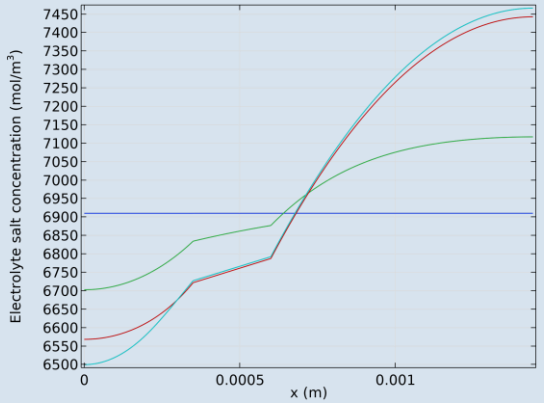
Study Types

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

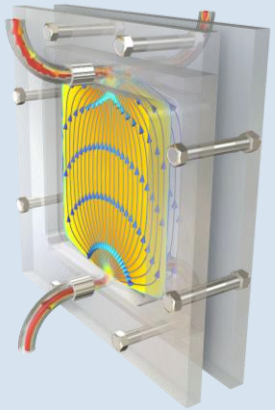
The Battery Design Module: Chemistries



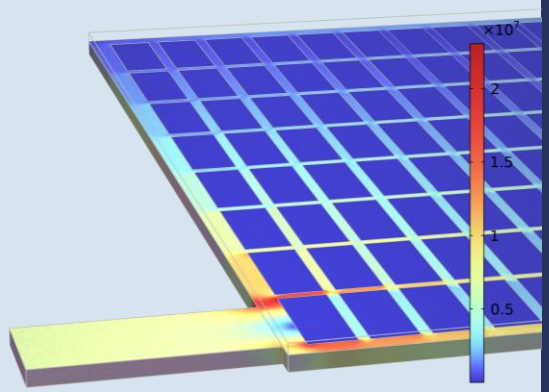
Lithium-ion (Li-ion) battery: 3D Newman model of a pouch cell.



1D nickel metal hydride (NiMH) battery: electrolyte salt concentration.



Vanadium redox flow battery: flow field in free and porous media.

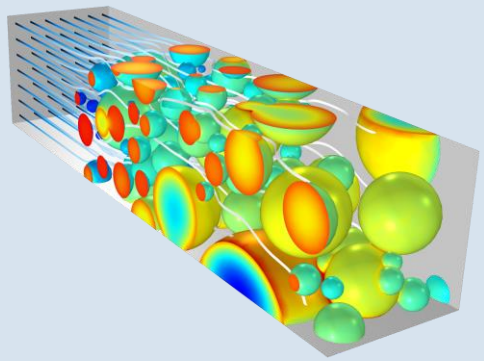


Lead–acid battery: collector current density.

- 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

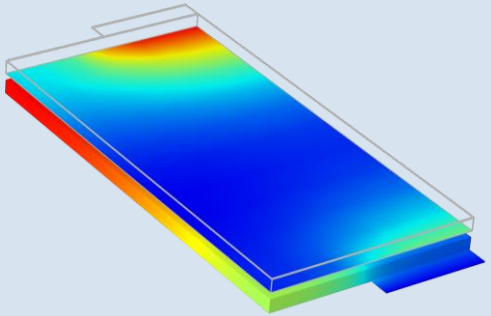
*EIS = electrochemical impedance spectroscopy

Battery Model Types in the Battery Design Module



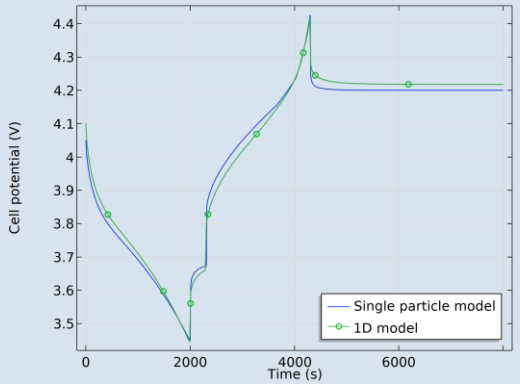
Heterogeneous Models

- 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



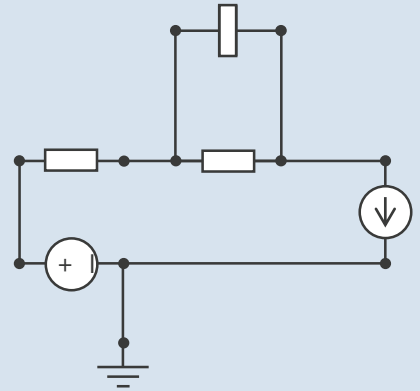
Homogeneous Models

- 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

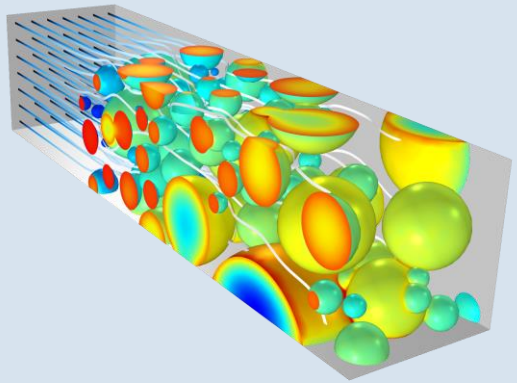
- 0D, plus 1D particle
- Lumped cell parameters
- Computes the SOC* to determine the OCV*
- For battery packs and systems
- Real-time parameter estimation

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

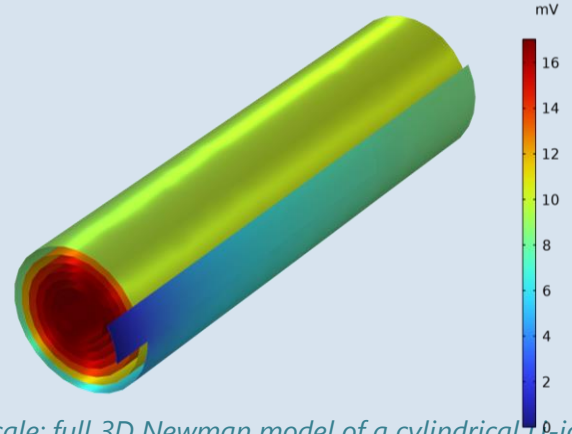
Accurate
Wide range of validity
Expensive to compute

Fast
Limited range of validity

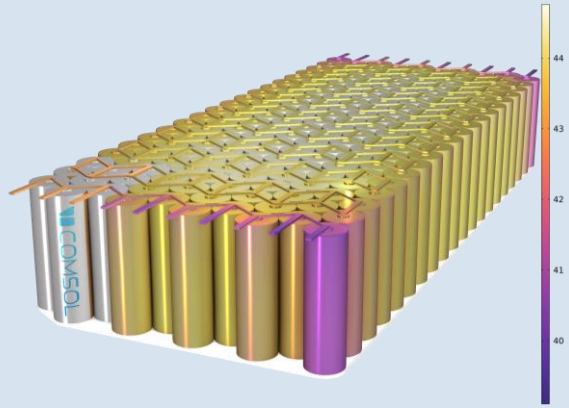
The Battery Design Module: Scales



Microscale: heterogeneous 3D model of a Li-ion electrode.



Cell scale: full 3D Newman model of a cylindrical Li-ion cell.



Pack scale: distributed lumped cell model for each Li-ion cell with 3D heat transfer.

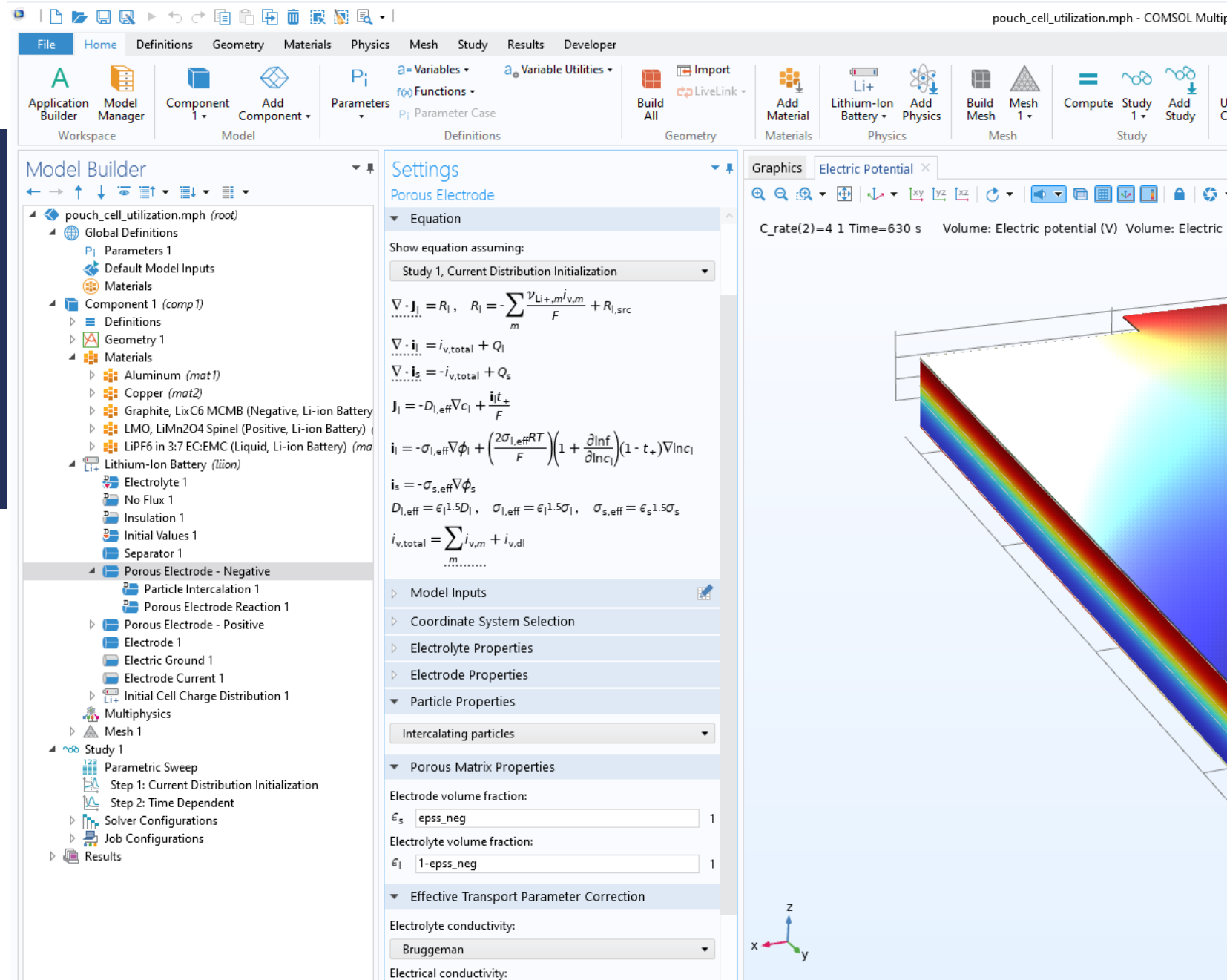
- Modeling from microscale to pack scale
- Full electrochemistry in all scales in 1D, 2D, and 3D
- 1D detailed electrochemistry or 0D lumped cell models for modeling many cells at the pack scale, e.g., for thermal management models
- Time-dependent studies, including transient effects, charge–discharge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



Battery Chemistries

Other examples

Lead Acid

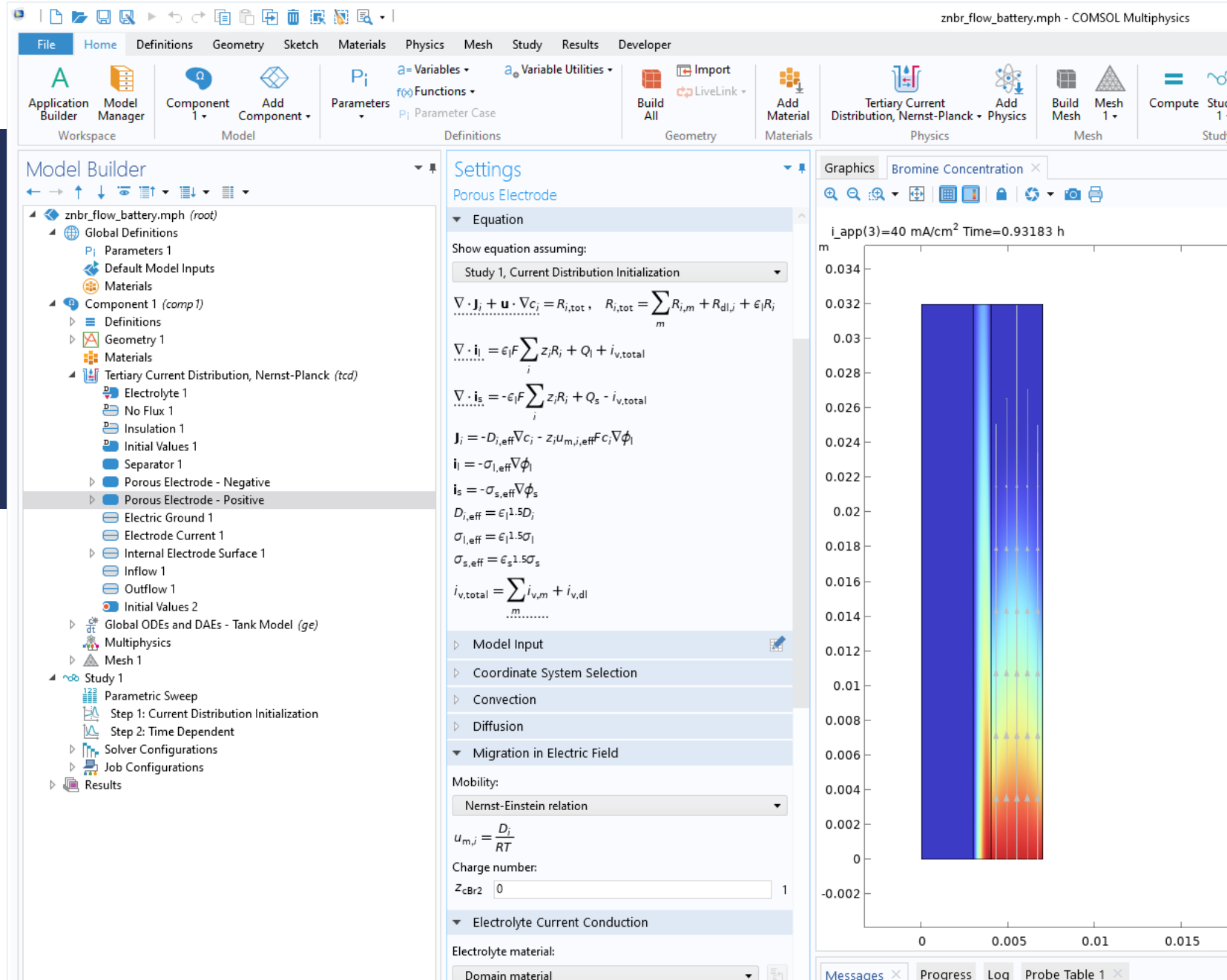
Nickel Metal Hydride

Lithium-Sulfur, Li-S

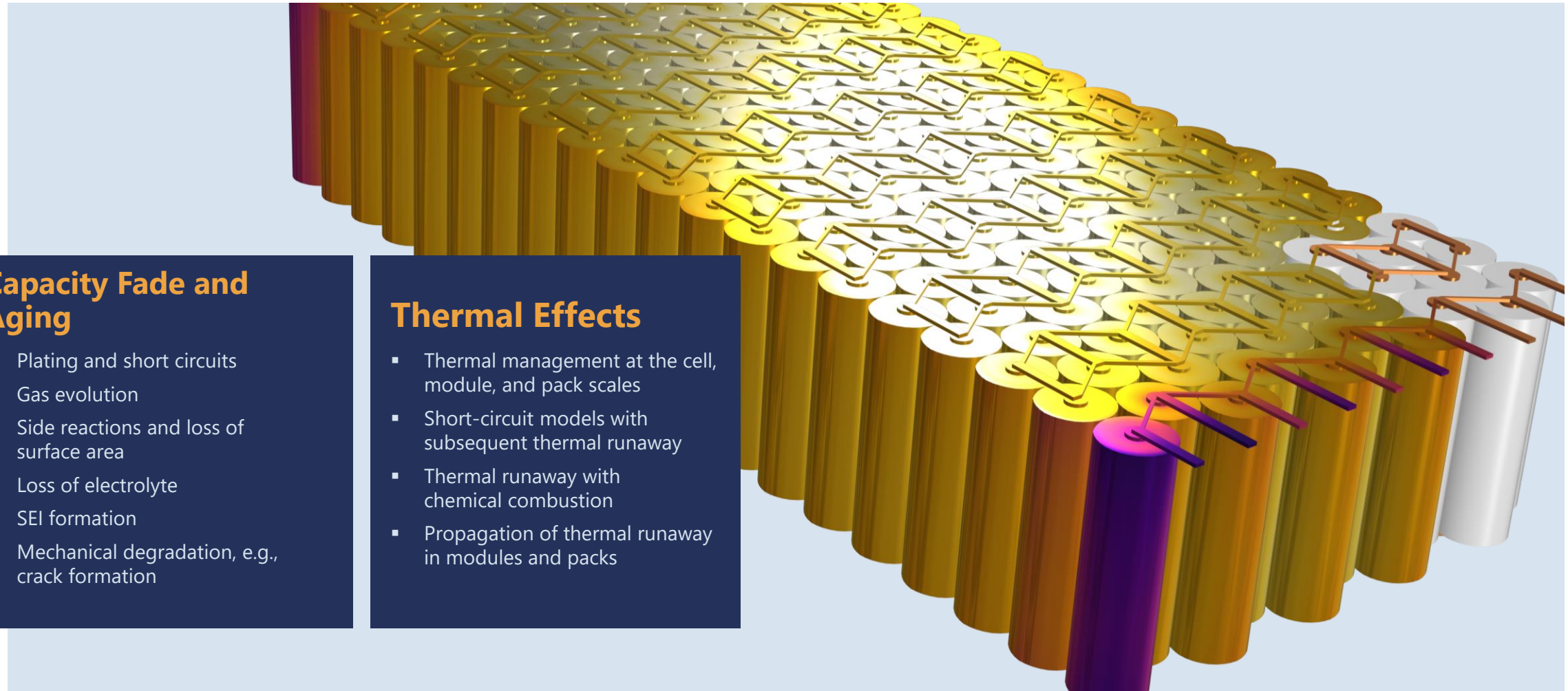
Nickel-Cadmium, NiCd

Zink-Silver Oxide, Zn-AgO

Zink-Bromine, Zn-Br



Aging and Thermal Management

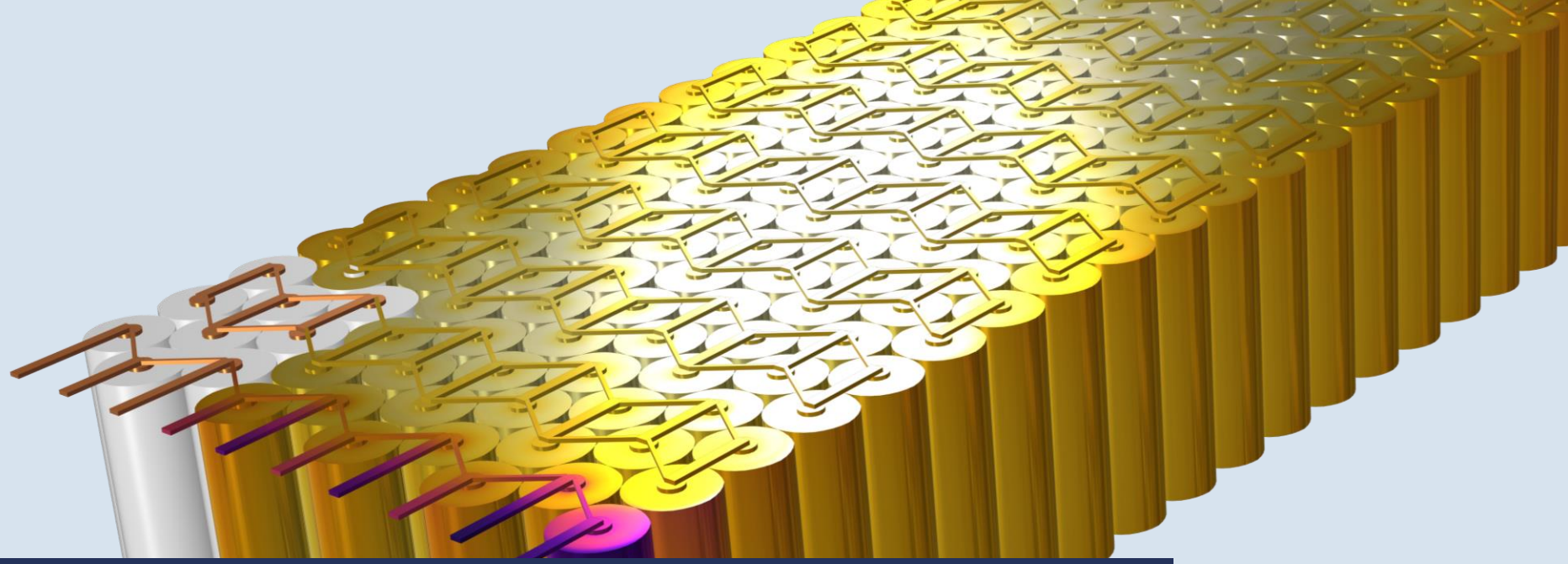


Capacity Fade and Aging

- 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

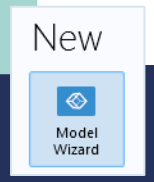
Worst Case

- Find maximum temperature during misuse
- Avoid thermal runaway

Demonstration

COMSOL

1



2

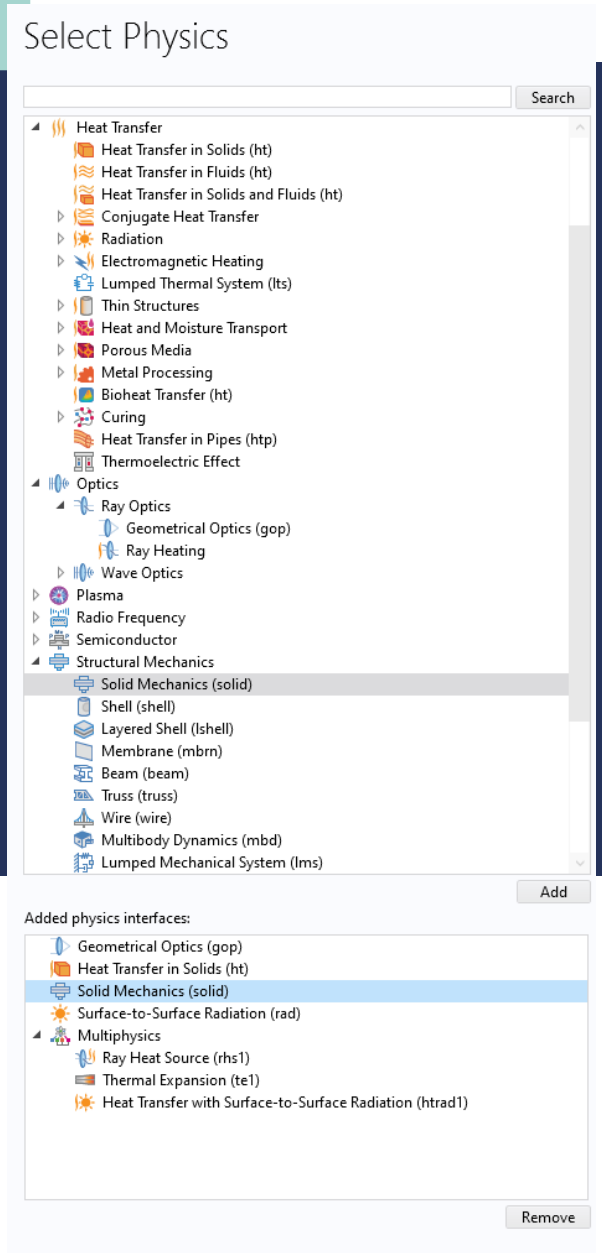
THE FIRST STEP

The Model Wizard

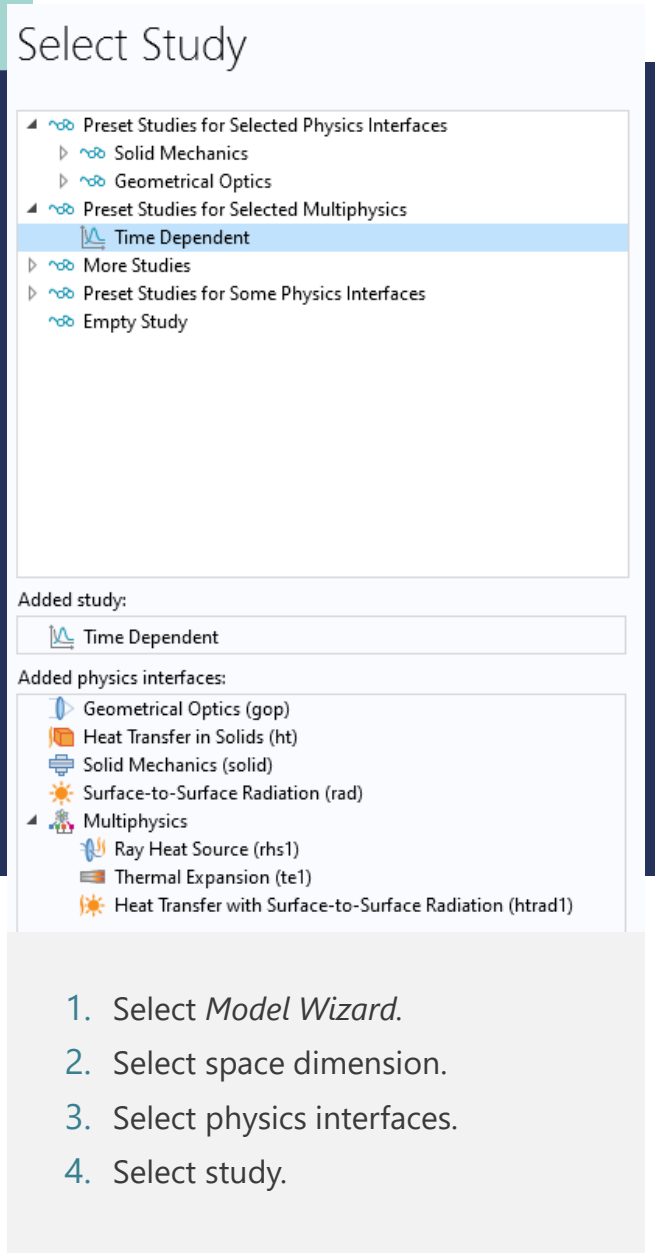
When creating a new model, the Model Wizard assists with selecting:

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

3



4



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

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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

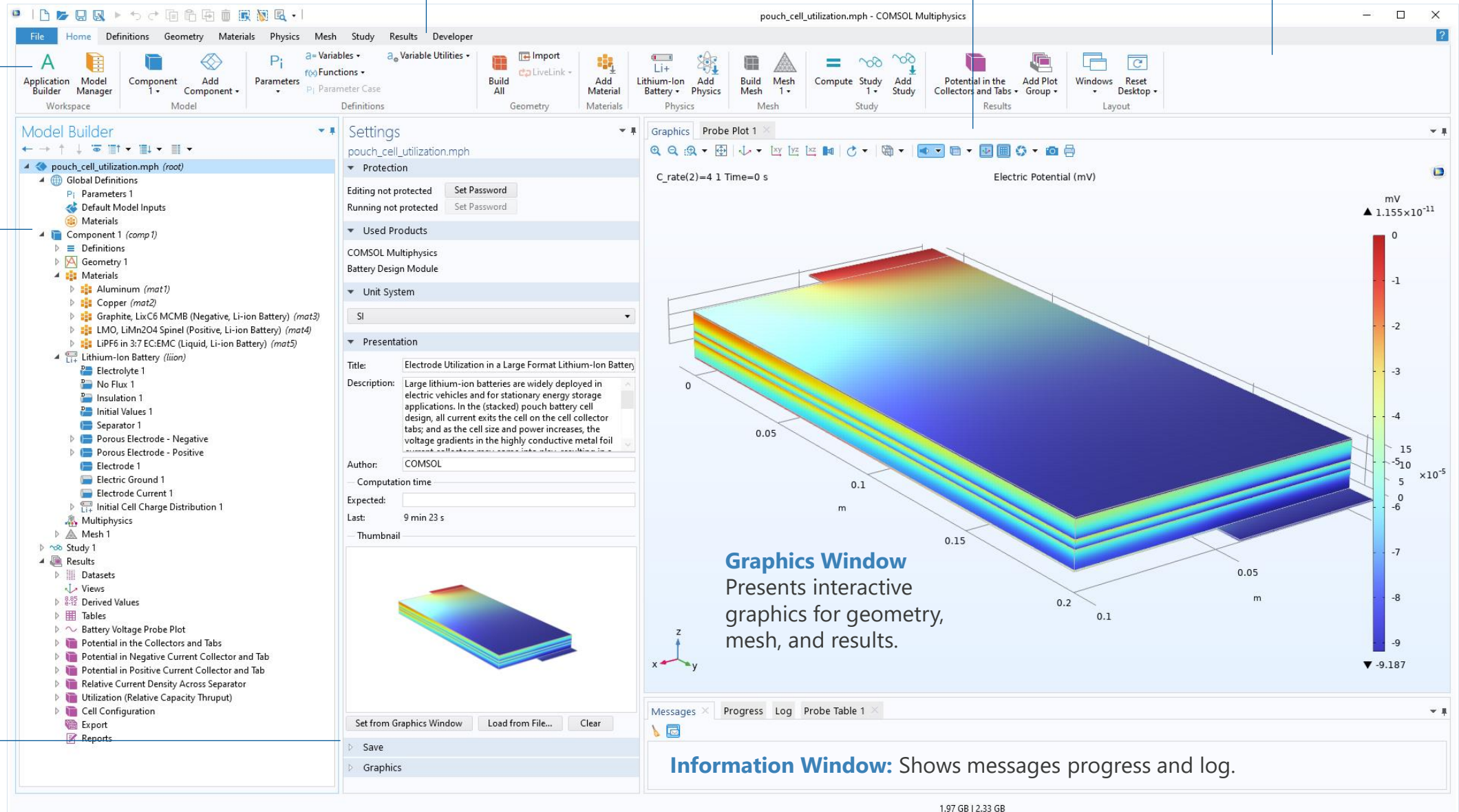
Shows the settings for the node that is selected in the model tree.

Ribbon

Controls for all steps of the modeling process.

Graphics Window Toolbar

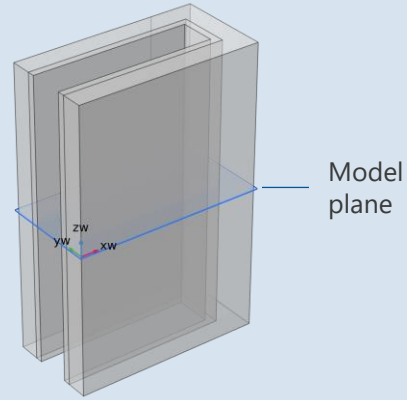
COMSOL Desktop® Model Builder



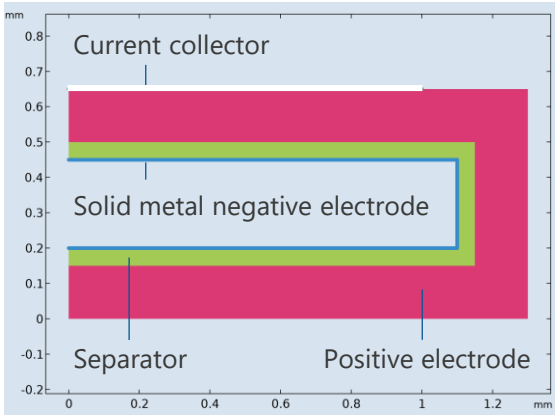
Graphics Window
Presents interactive graphics for geometry, mesh, and results.

Information Window: Shows messages progress and log.

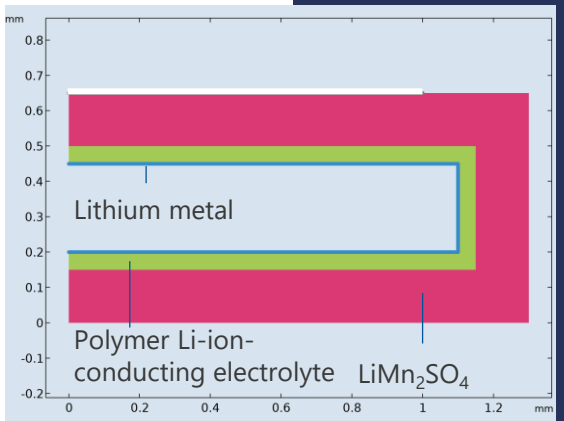
Model Definition



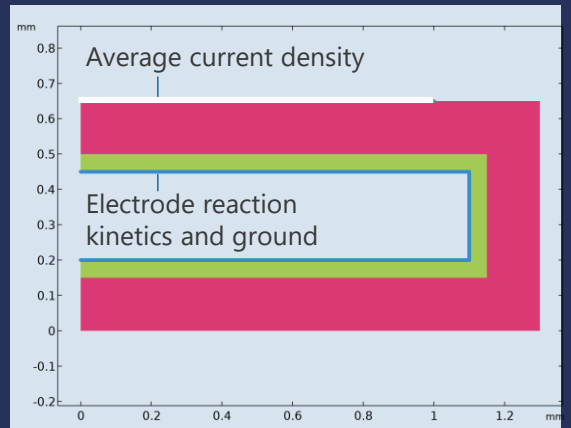
2D cross section of a 3D geometry.



Cell configuration.



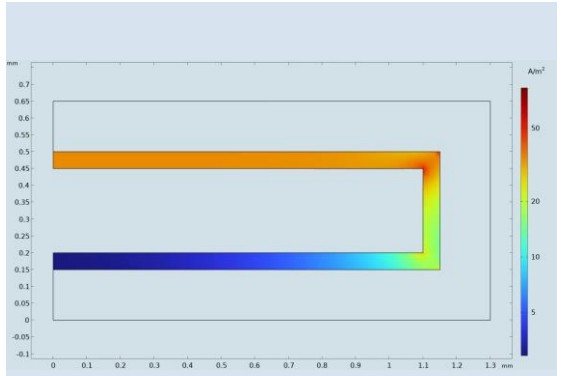
Materials.



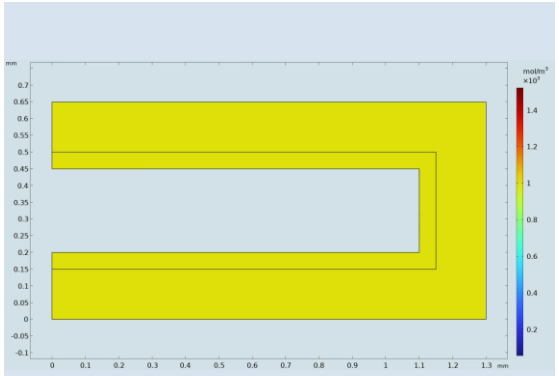
Boundary condition.

- 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

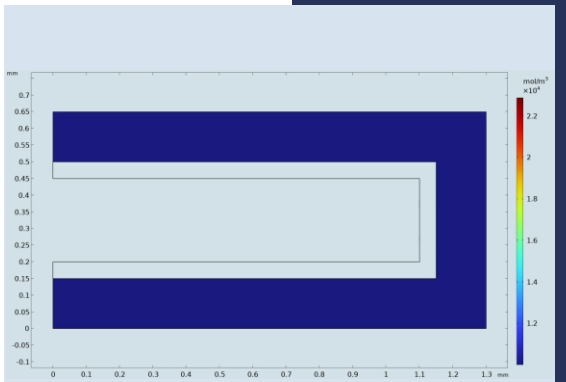
Model Results



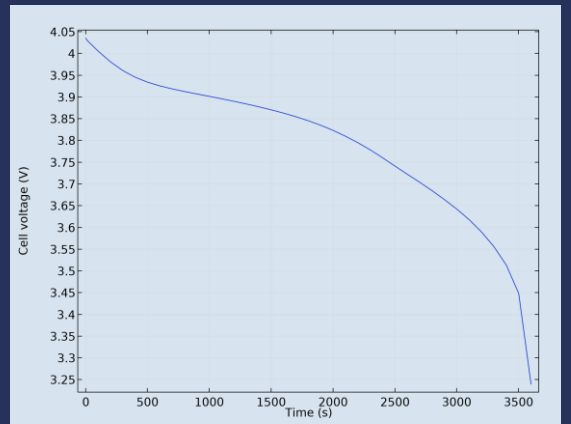
Animation of the current density in the electrolyte.



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



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



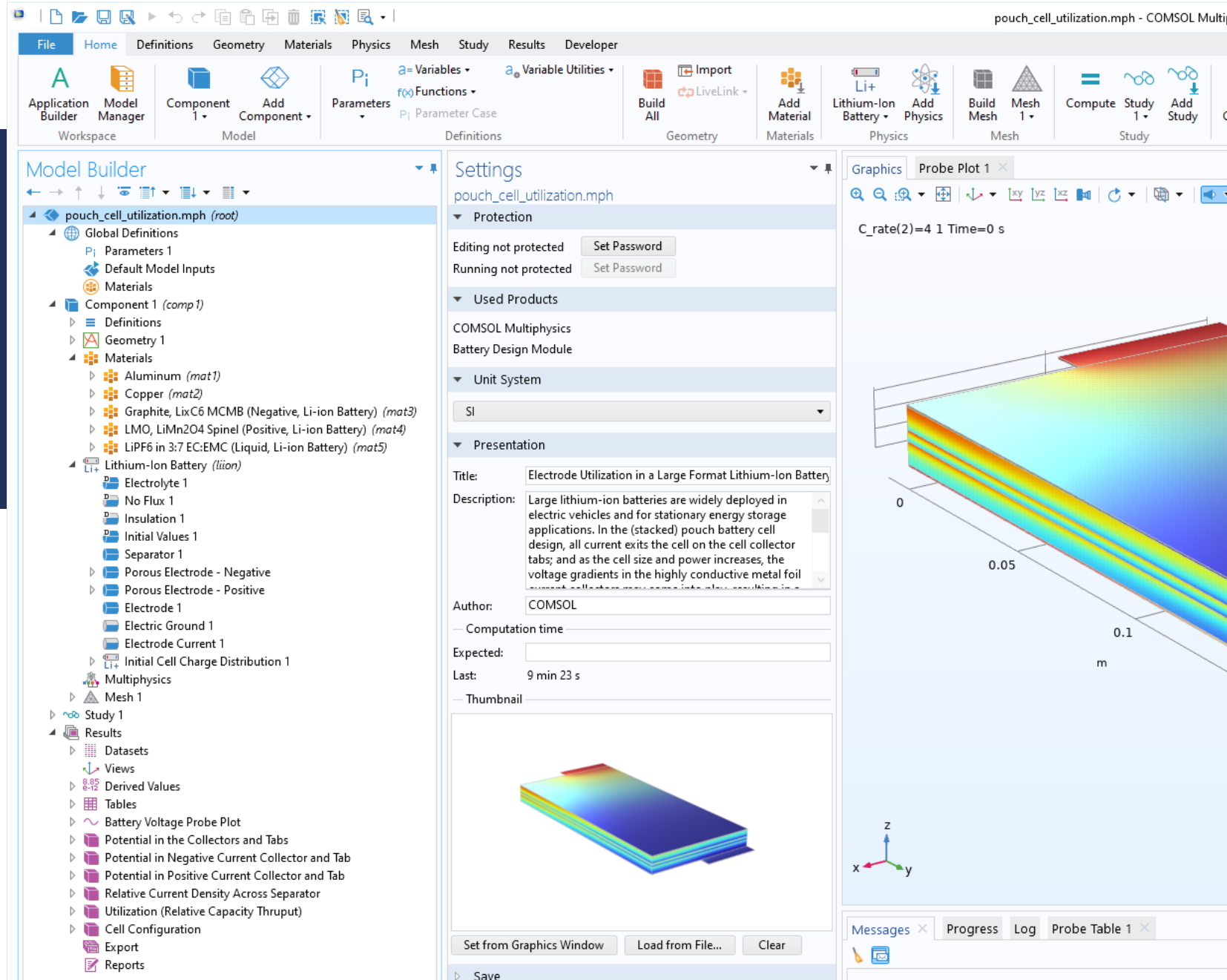
Cell voltage vs. time.

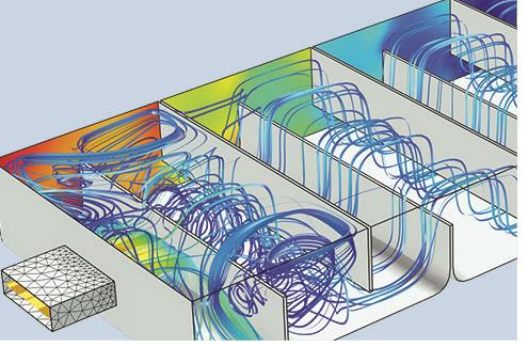
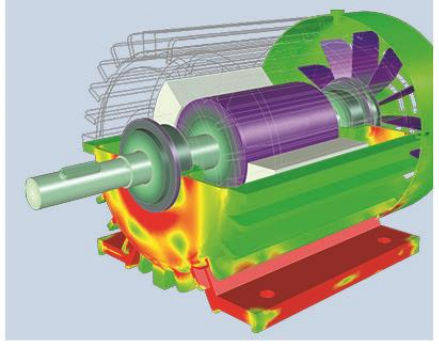
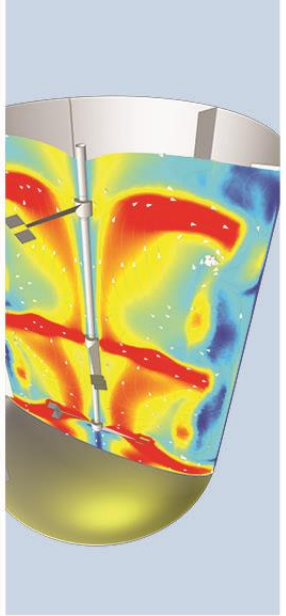
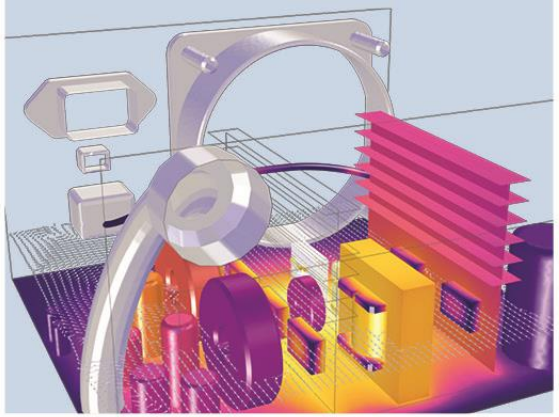
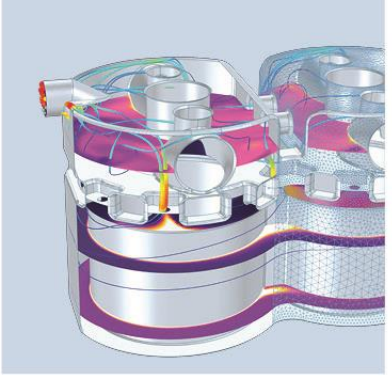
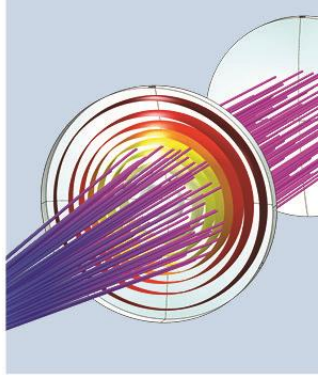
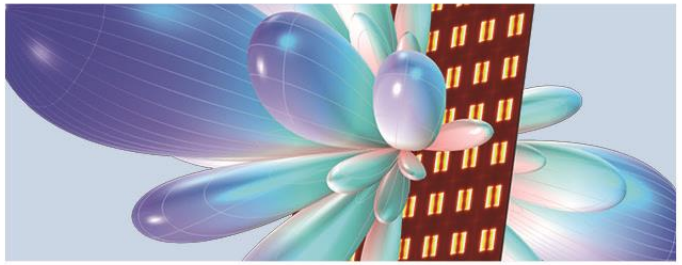
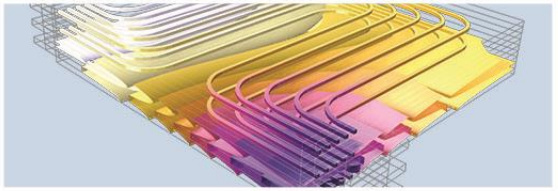
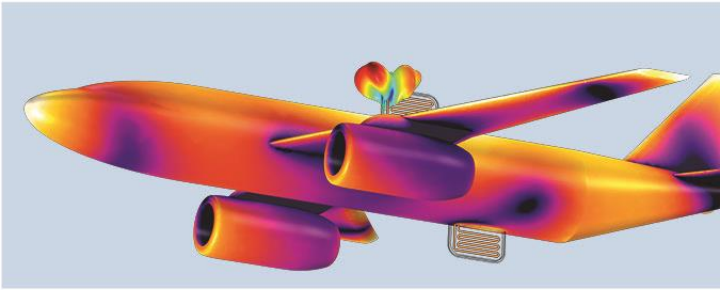
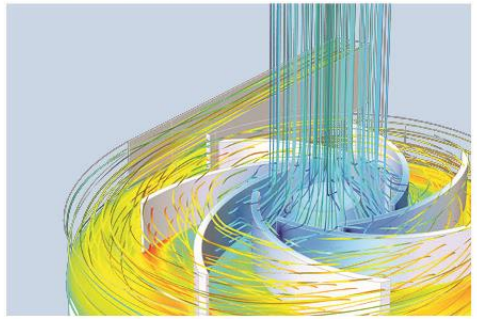
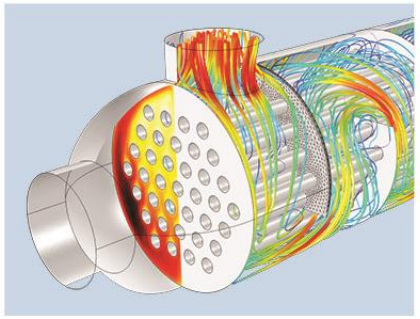
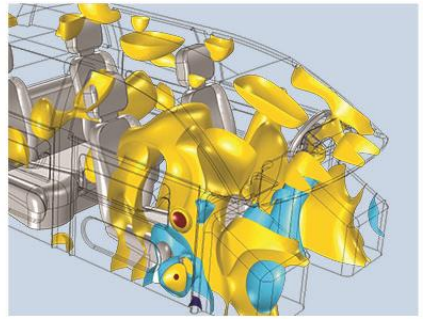
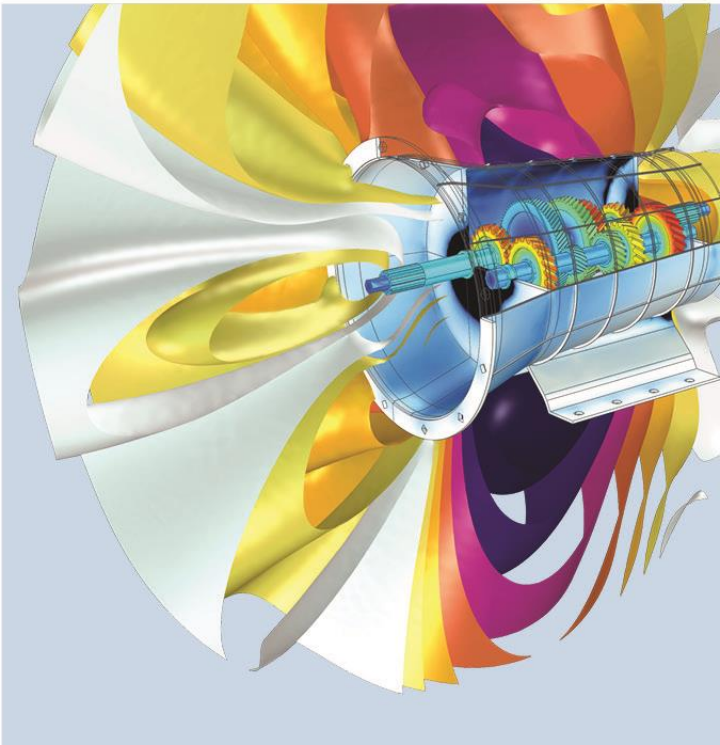
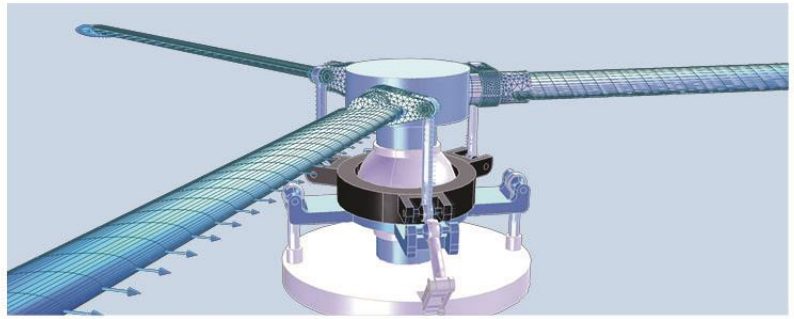
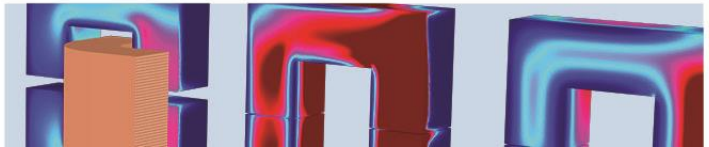
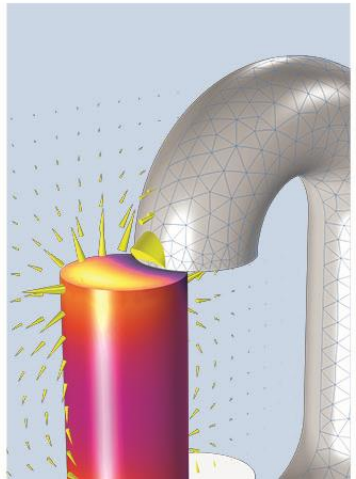
- The positive electrode initially discharges in the regions close to the current collector, *i.e.* the upper rectangular part
- As the lithium concentration is depleted, the regions further away from the current collector are discharged
- In this case, the position of the current collector requires 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



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