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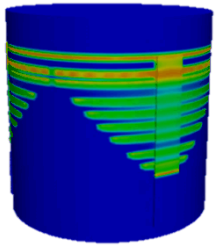

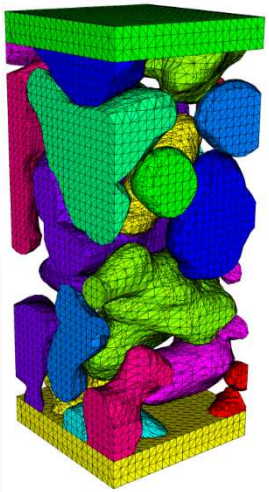

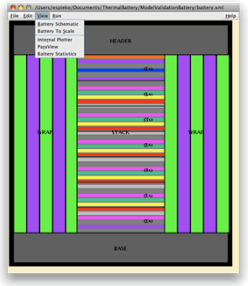

Multiphysics modeling of thermal batteries

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Thermal/Fluid Component Sciences Department
Sandia National Laboratories, Albuquerque, NM

The Future of Munitions Batteries Workshop
Army Research Laboratory, Adelphi, MD
December 7, 2016

Sandia National Laboratories

Exceptional service in the national interest

Not yet reviewed for public release

U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

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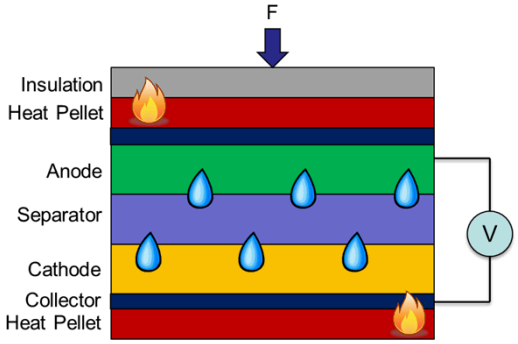
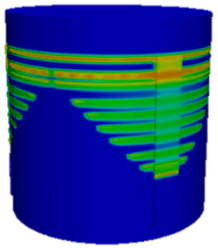
Unclassified

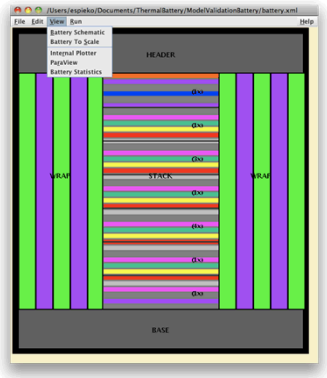
Outline

- Motivation for modeling thermal batteries

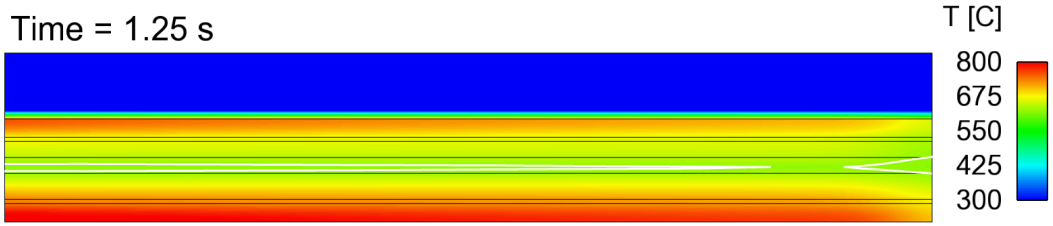


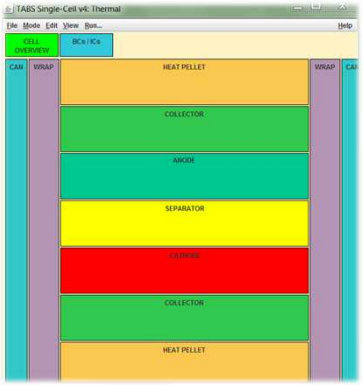
- Full-battery thermal models and the TABS-FB GUI





- Multiphysics models of a single cell and the TABS-SC GUI

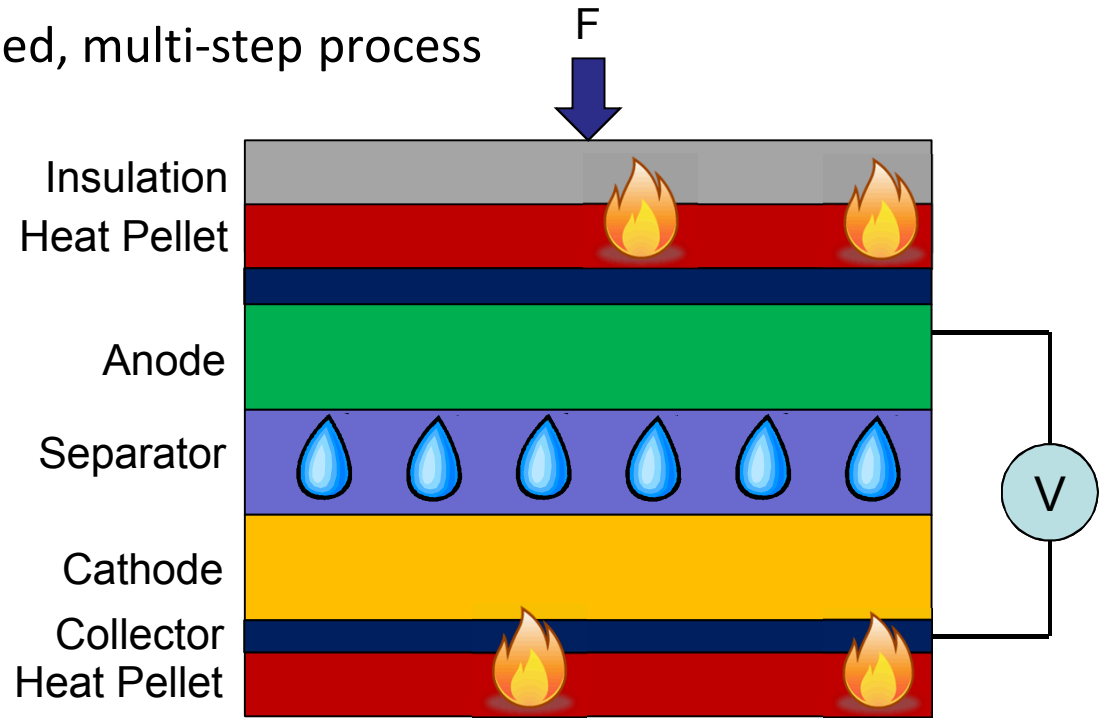




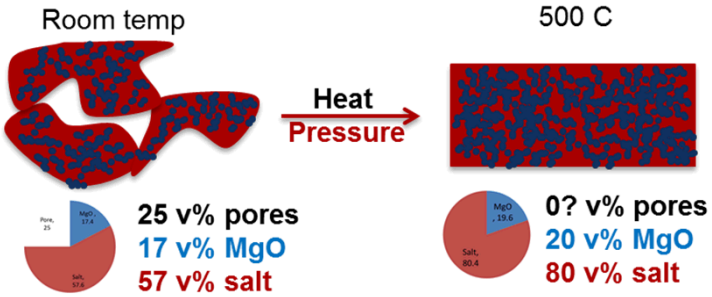
- Summary and future directions

Physical mechanisms in molten salt battery activation

- Battery activation is a complicated, multi-step process
  - Heat pellet burning
  - Thermal diffusion
  - Melting of the electrolyte
  - Deformation of the separator
  - Rebound of the insulation
  - Flow of the electrolyte
  - Activation



- Why performance models?
  - Predict activation times
  - Predict electrochemical performance
  - Understand effect of complex load profiles
  - Optimize volume, insulation, manufacturing

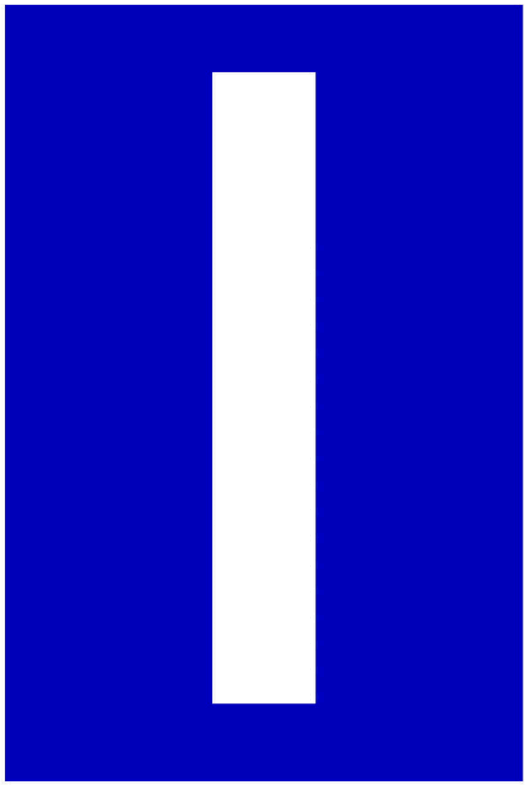


A true multi-physics problem!

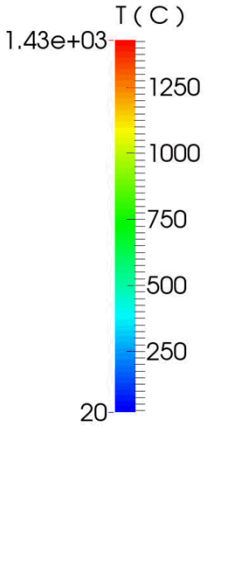
Full-battery thermal models

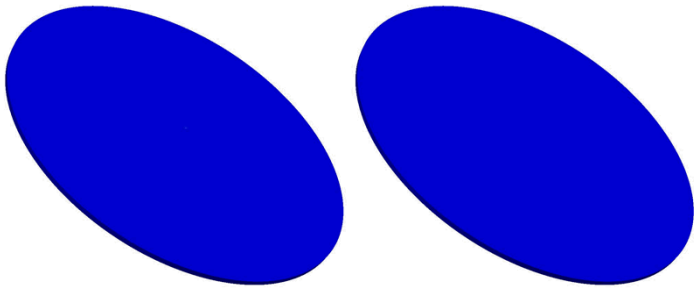
- Based on standard heat conduction model

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T + Q$$

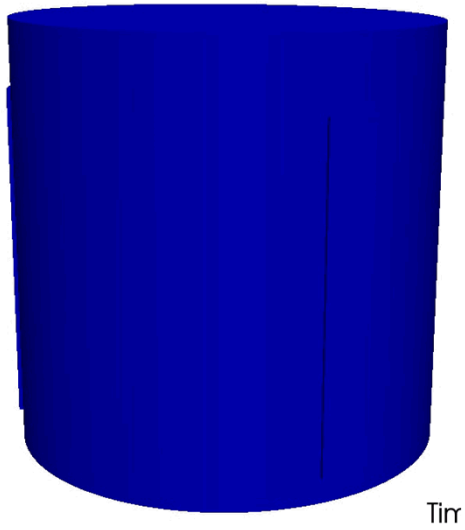


Center-fired configuration





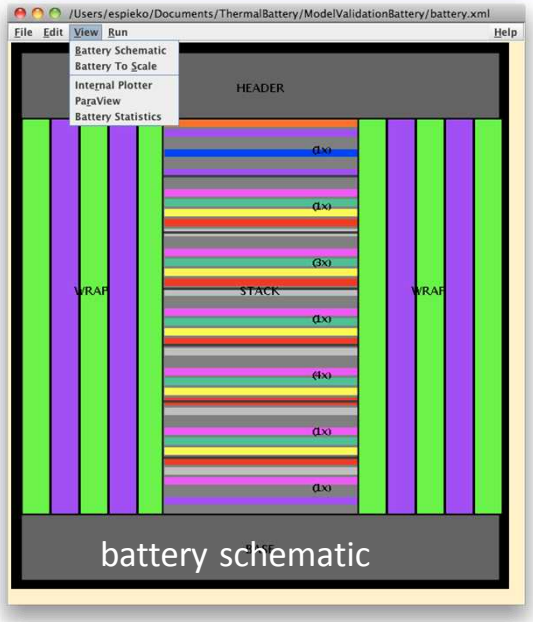
Burn front Volume source

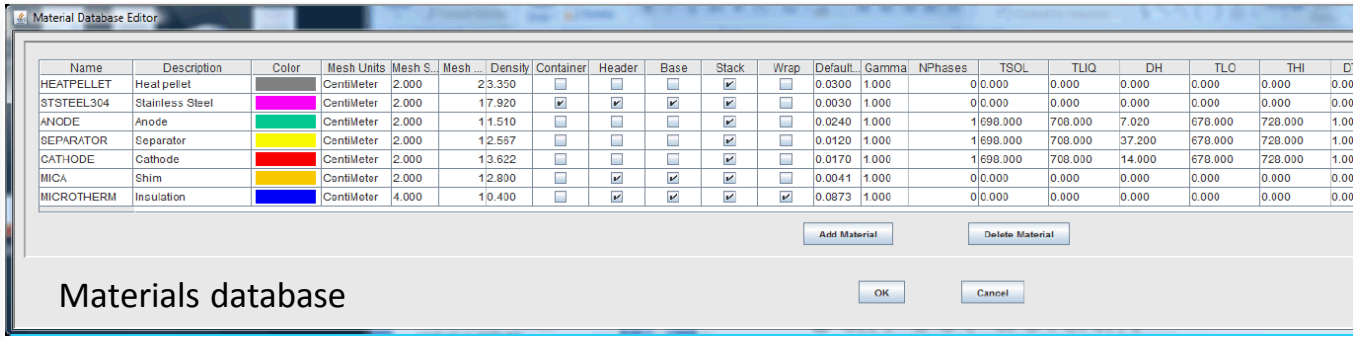


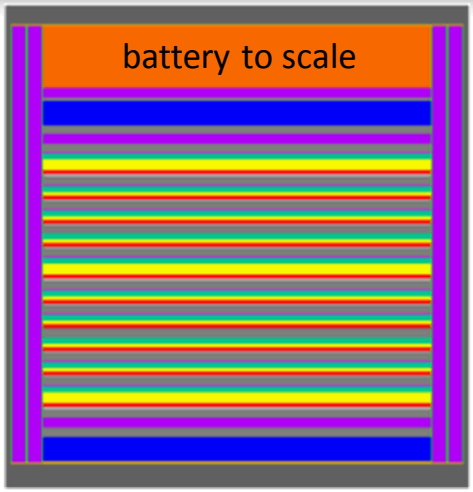
Side-fired configuration

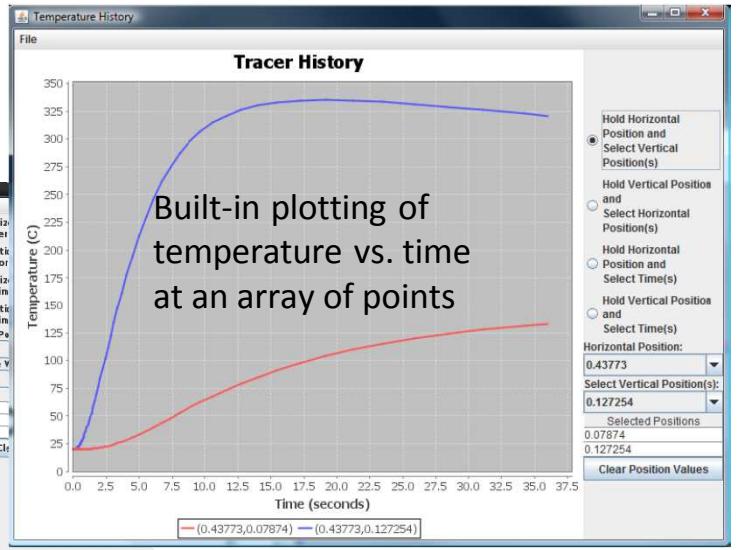
Prediction of QOIs (run time, life time) and thermal runaway assessments

TABS-FB (Thermally Activated Battery Simulator - Full Battery)







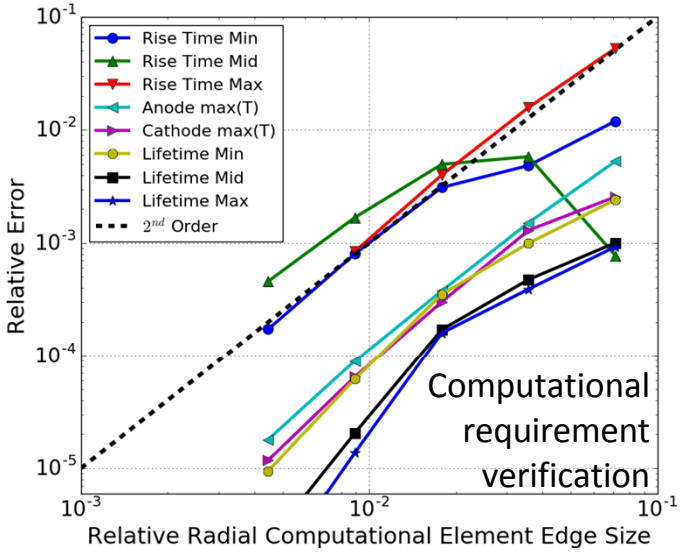


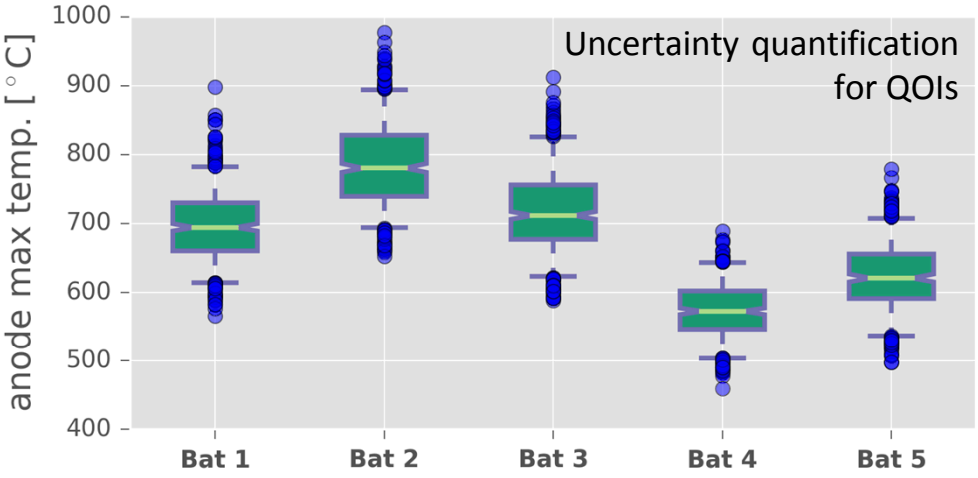
Temperature through stack at times

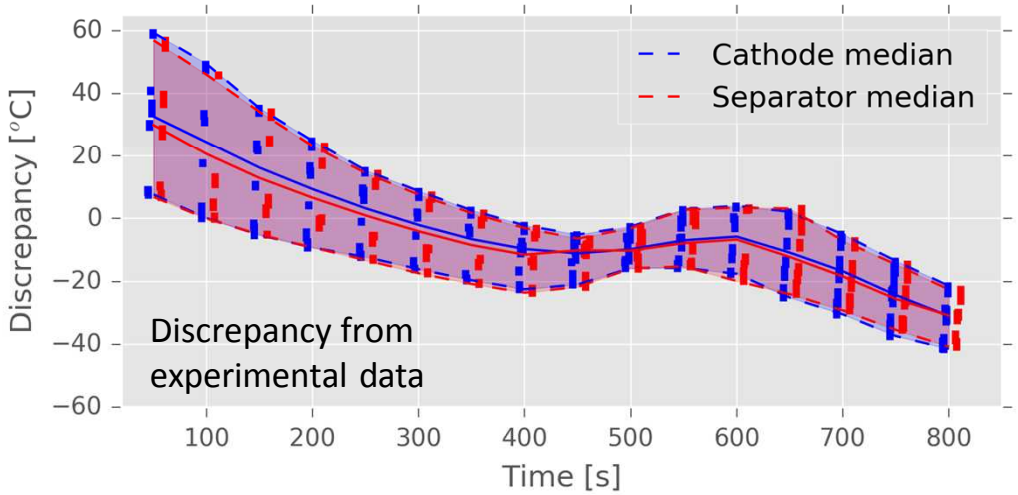
COMPSIM THERMAL FLUIDS

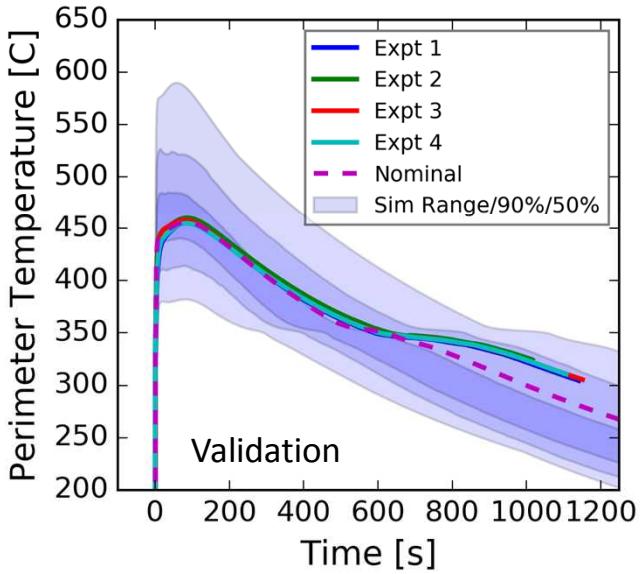
Design tool for high-fidelity modeling (Sierra/Aria) with a user-friendly interface

Thermal model credibility



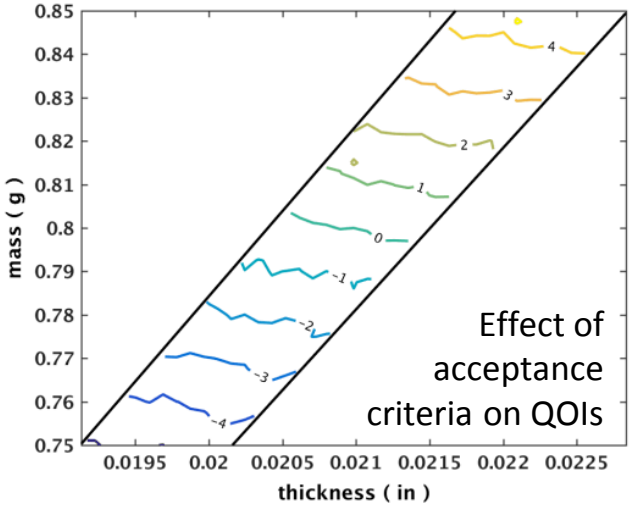


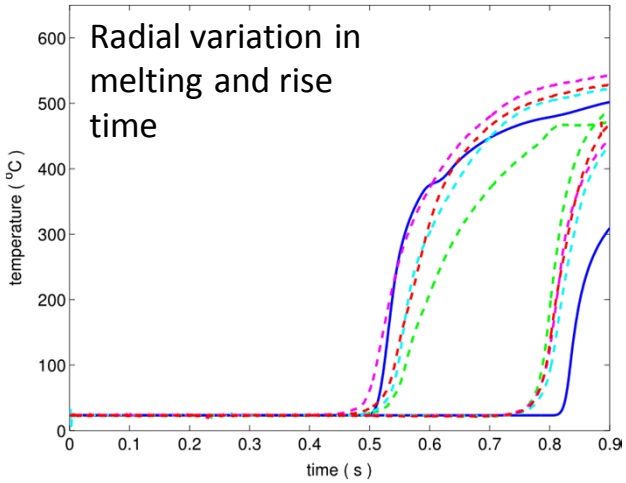


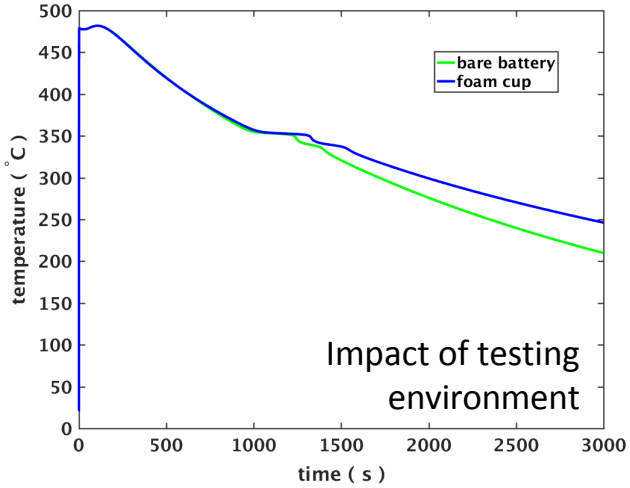


Verification, validation, & uncertainty quantification establish model credibility

Impact of thermal modeling using TABS-FB





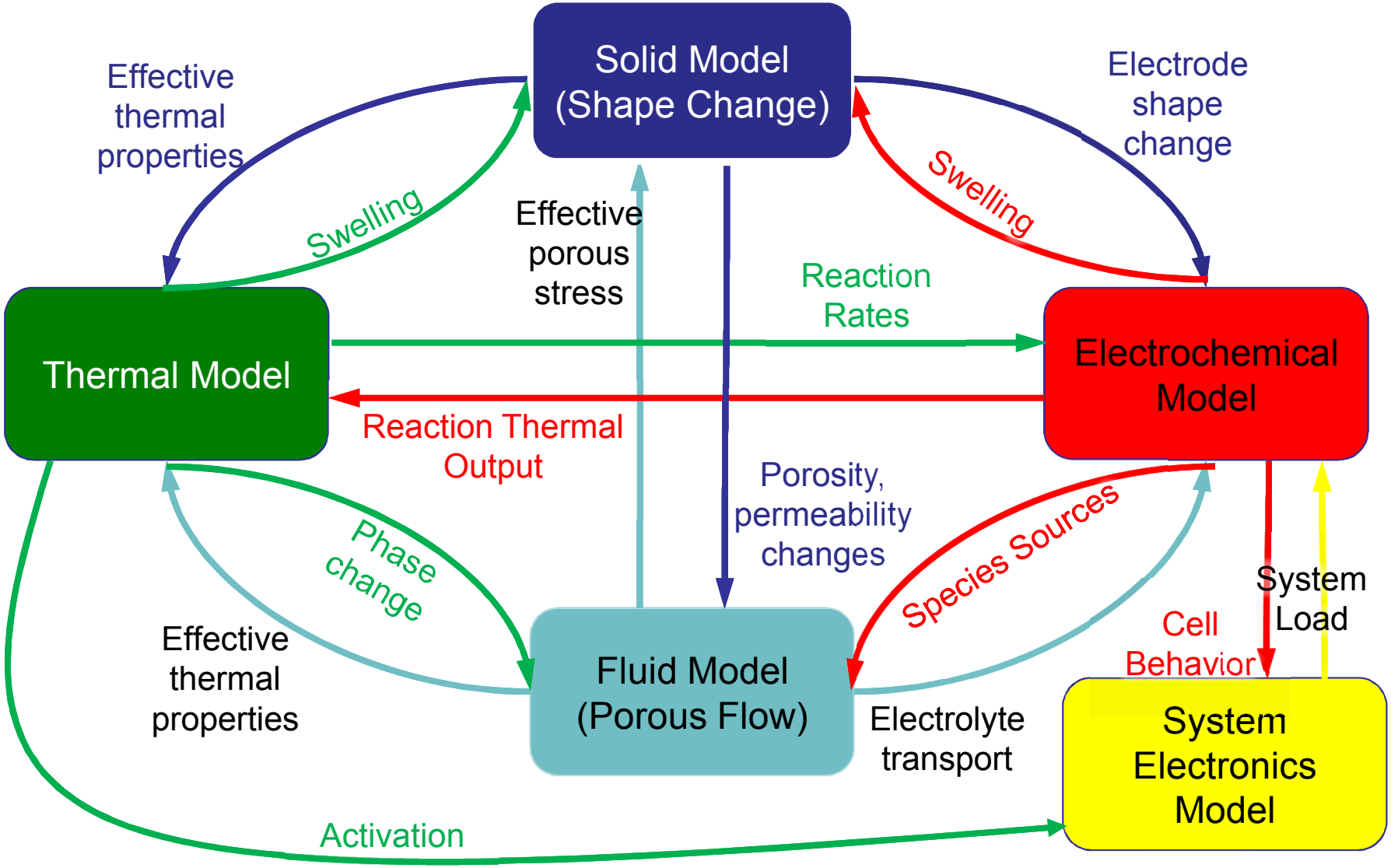


Other examples include:

- Reduction of development battery build cycles
- Thermal impact on next assembly
- Accelerated cycles of learning
- Assessment of abnormal environments
- Assessment of abnormal operation (misfire)
- … and many, many more …

Many demonstrated impacts to Sandia battery development programs

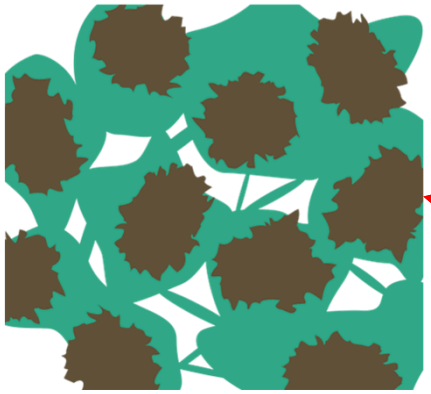
Physical models and couplings

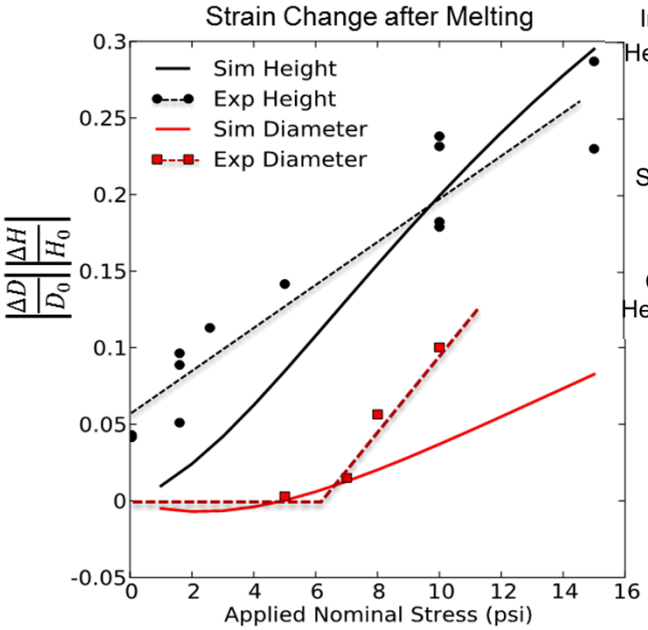


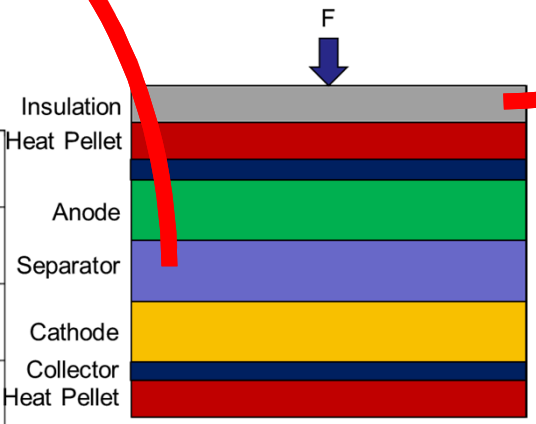
There's a lot going on in a thermal battery!

Models: Mechanical deformation

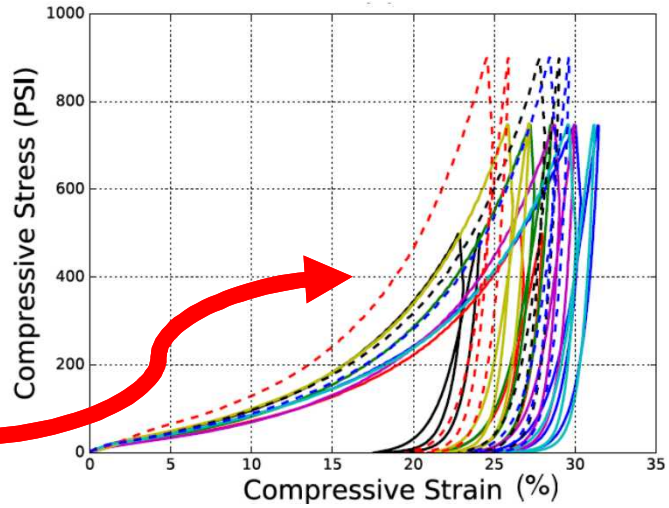
Separator deformation

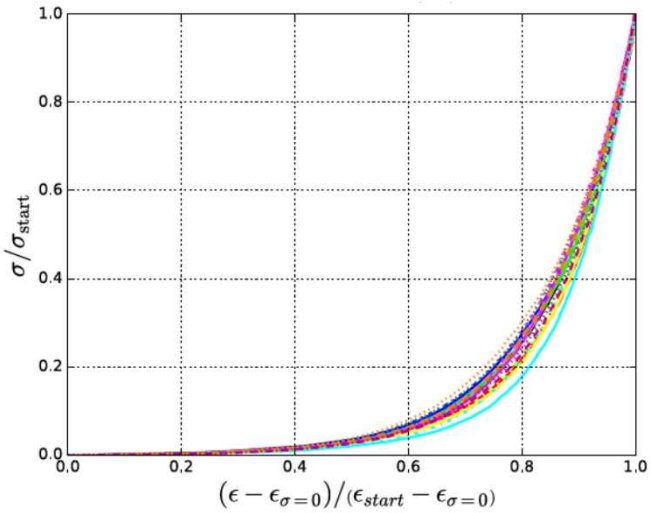






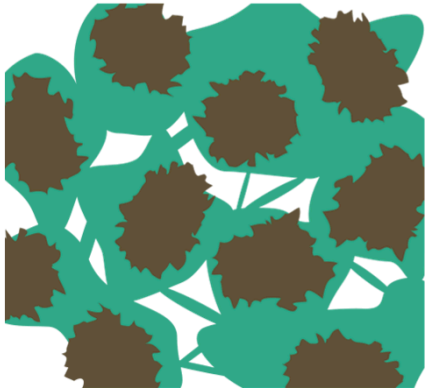
Insulation deformation and rebound



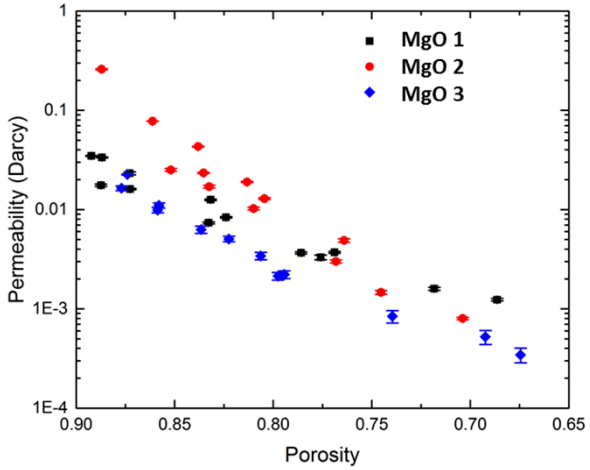


Mechanical deformation and forces hold the stack together

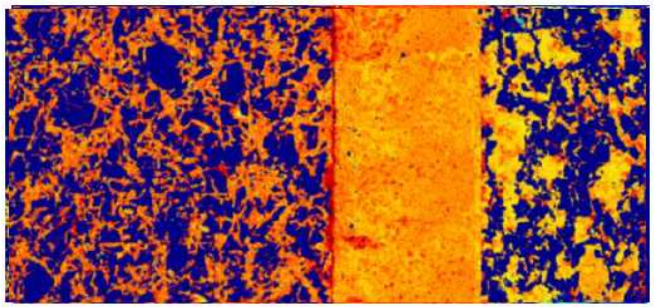
Models: Two-phase porous flow and species transport

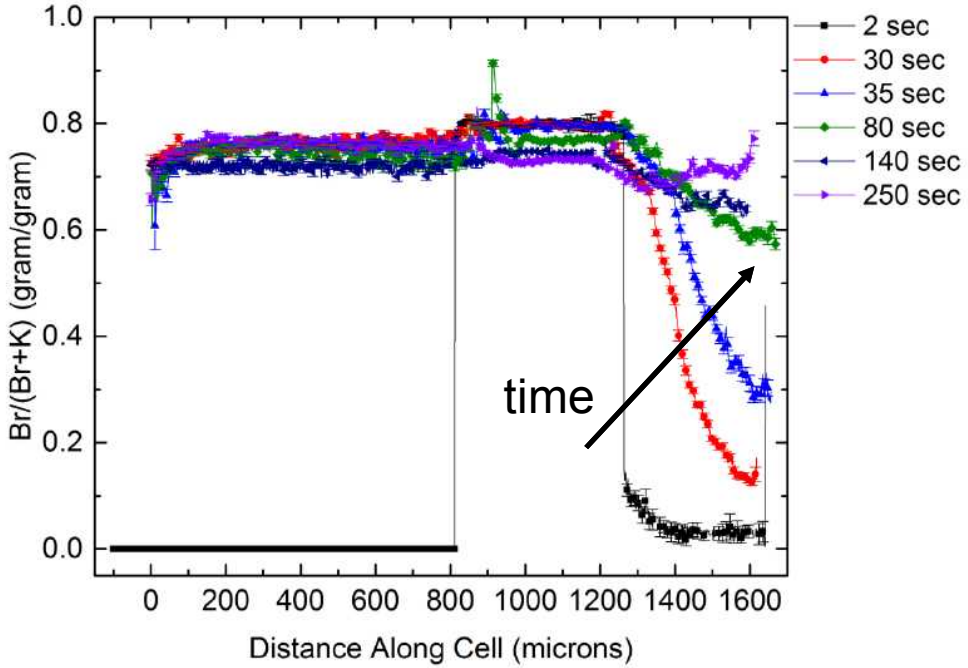


Three-phase separator
(MgO, E-lyte, void)



Flow resistance depends on porosity





Data shows electrolyte wicks quickly into anode and diffuses slowly into cathode

Electrolyte (and constituent species) governs ionic transport

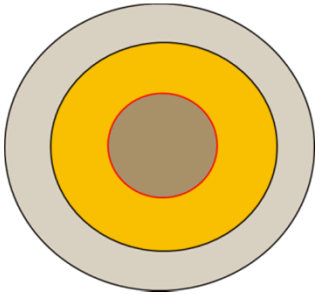
Models: Electrochemistry

- Reactions, especially for the cathode, are stoichiometrically complicated

$$\text{Cathode}: \mathrm{FeS_2} \rightleftarrows \mathrm{Li_3Fe_2S_4} \rightleftarrows \mathrm{Li_{2+x}Fe_{1+x}S_2} + \mathrm{Fe_{1-y}S} \rightleftarrows \mathrm{Li_2FeS_2} \rightleftarrows \mathrm{Li_2S} + \mathrm{Fe}$$

$$\text{Anode}: \mathrm{Li_{13}Si_4} \rightleftarrows \mathrm{Li_7Si_4} \rightleftarrows 4\mathrm{Si}$$

- Cantera's "Electrode Object" deploys multiple sub-grid models
  - Infinite capacity
  - Finite capacity
  - Newman reaction extent
  - Multi-plateau



Shrinking Core Model

- Multiple plateaus can react simultaneously
- Diffusional losses with transport

- Primary electrochemical coupling is the temperature

$$\frac{\partial C_{\mathrm{Li^+}}}{\partial t} + \underline{\nabla} \cdot \underline{J}_{\mathrm{Li^+}} = 0$$

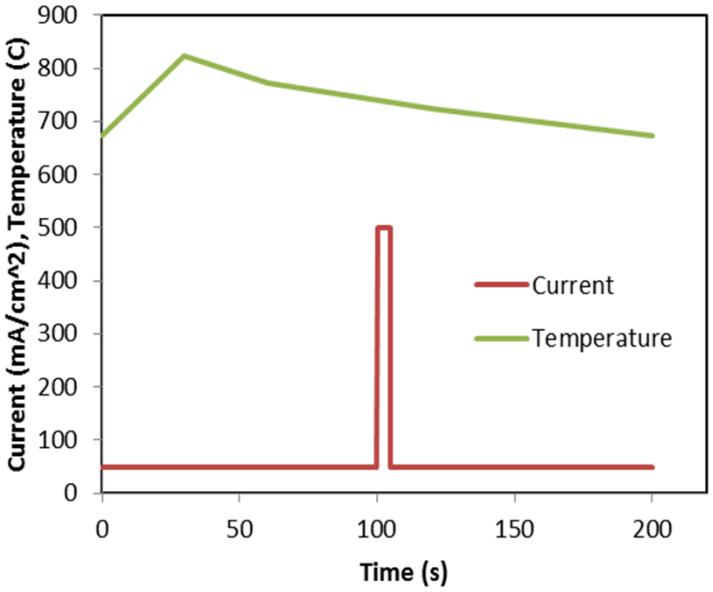
- Sierra solves species and current transport

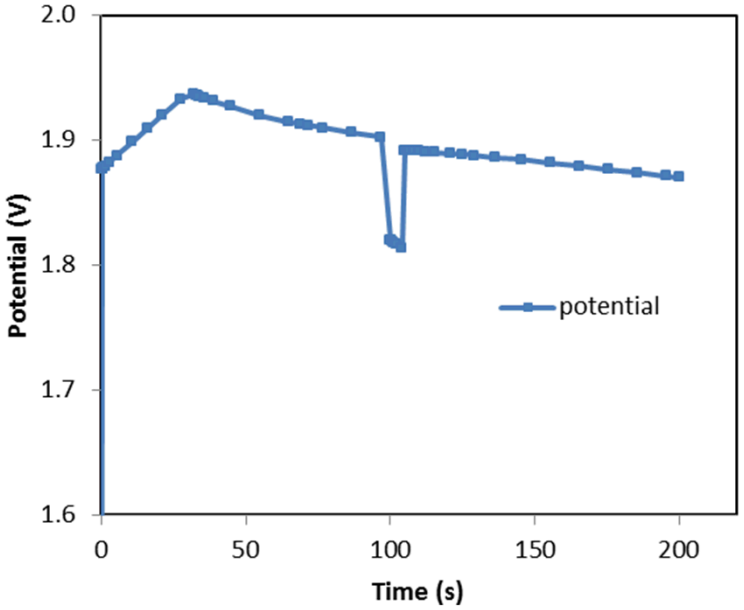
$$\underline{\nabla} \cdot (\sigma \underline{\nabla} \phi_{\mathrm{s}}) = 0$$

Electrochemical reactions are the primary output of a battery

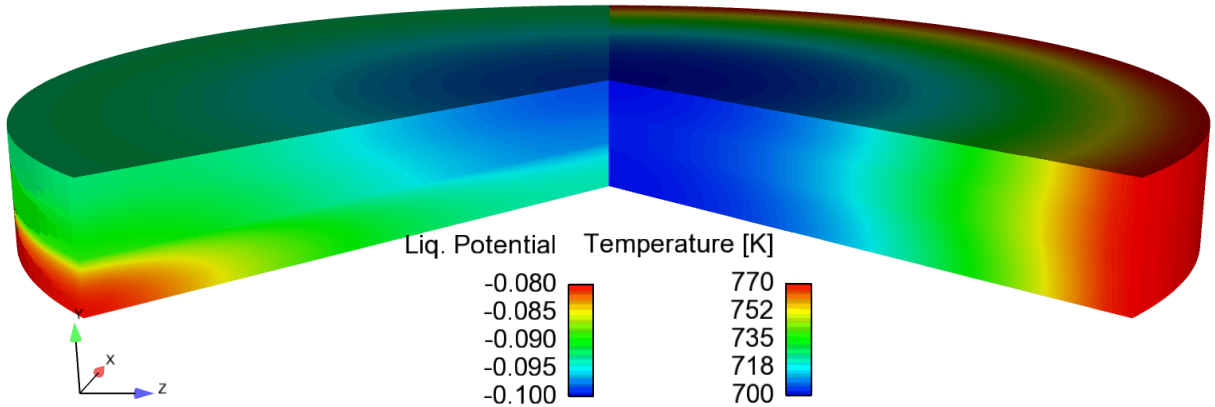
Thermo-electrochemical coupling

- Voltage responds to temperature and current



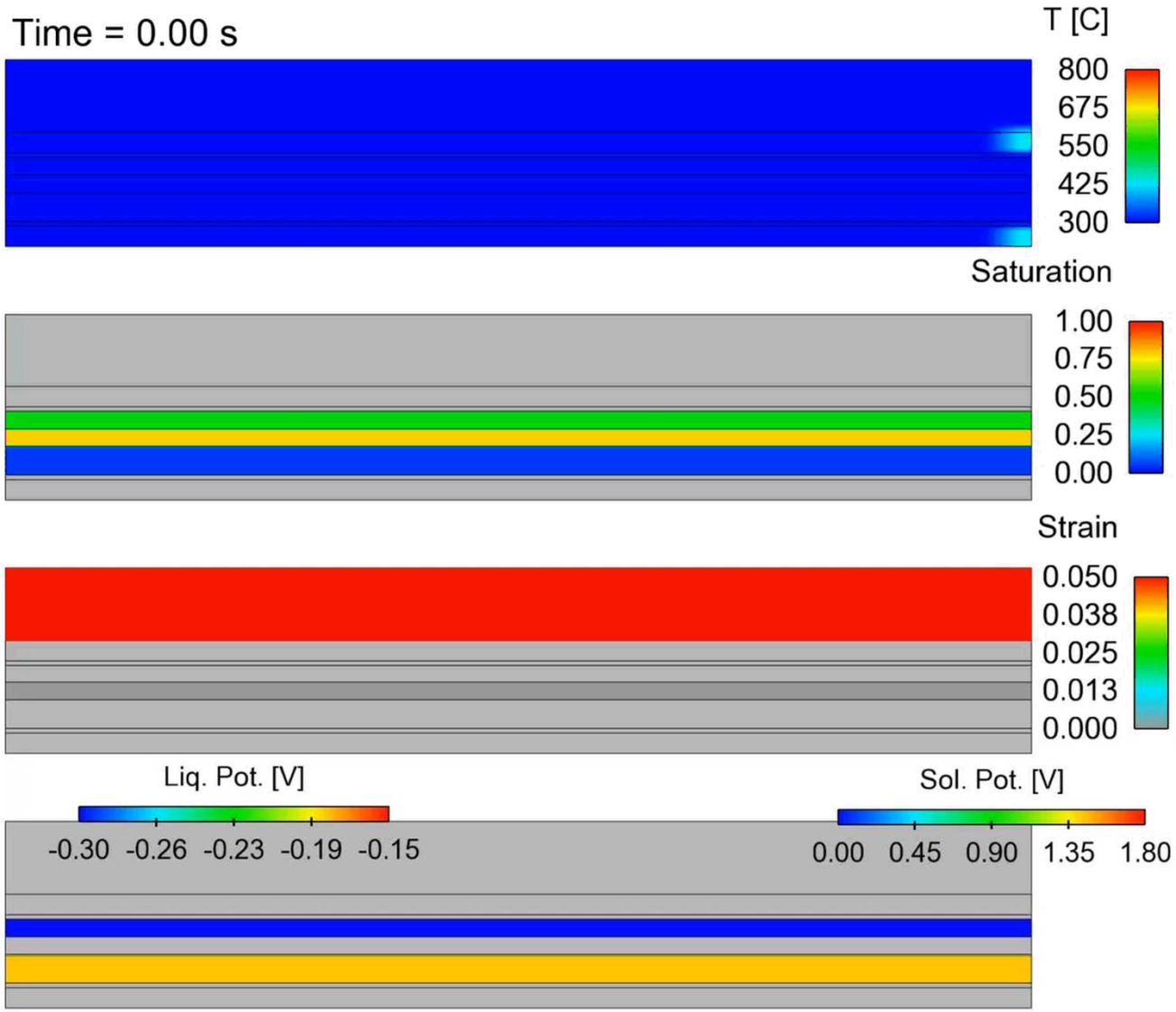


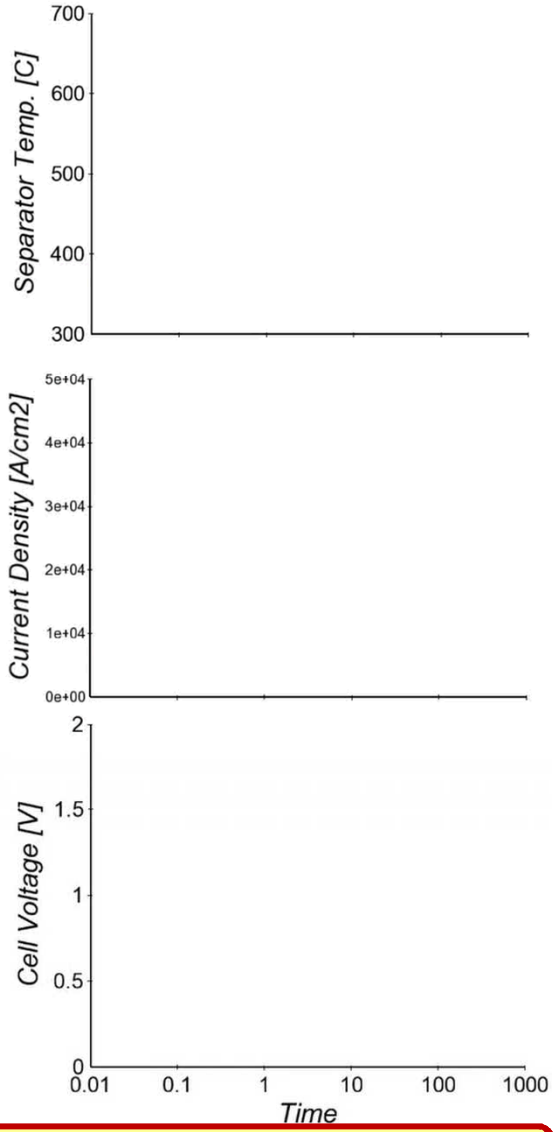
- Spatial temperature variations affect local potentials



Spatial and temperature dependence is critical

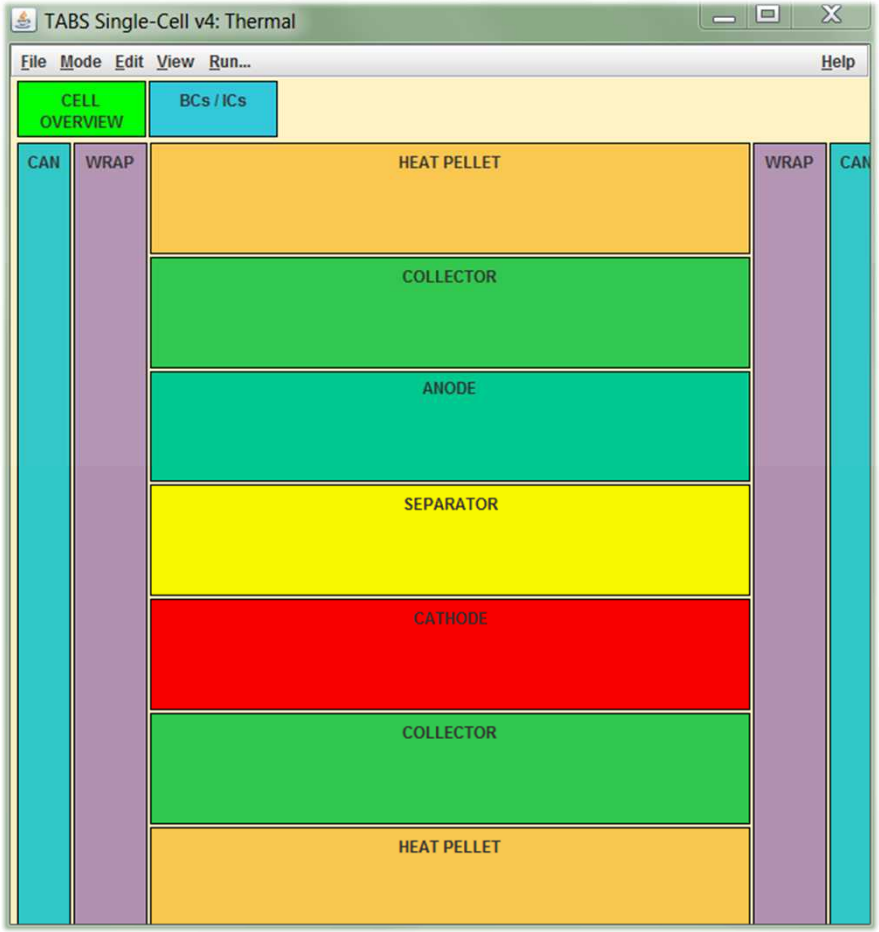
Full multi-physics single-cell simulation



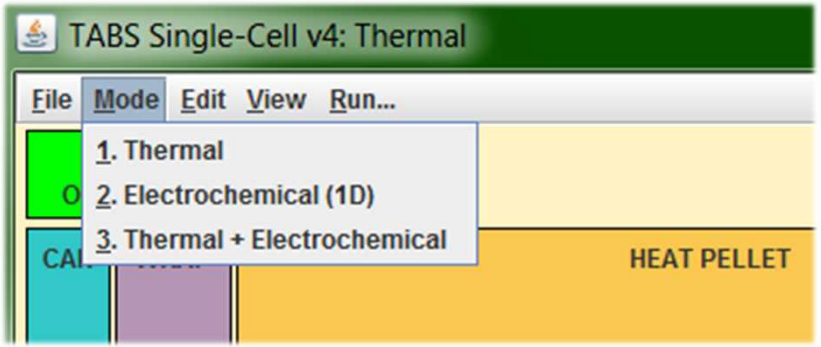


Detailed transient simulations give insight into battery performance during activation

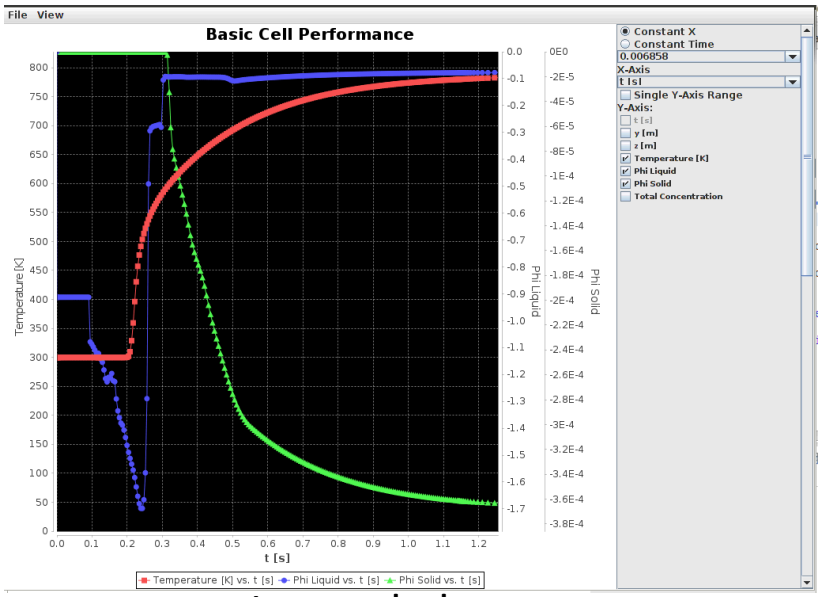
Sandia TABS-SC (Single Cell) v4



Main window shows single-cell schematic



3 mode selections available



Internal plotter

Design tool for multi-physics electrochemical simulation of a single cell

What's next for Sandia thermal battery modeling?

- This year:
  - Deployment of TABS v4, with improved FB model and new SC capabilities
  - Finalized technical reports on FB credibility, SC model documentation
  - Credibility assessment on SC models with accompanying report
  - TABS v5 with additional SC capabilities and improvements

- Future years:
  - Full-battery electrochemical models
  - 3D modeling workflow
  - Thin film battery materials
  - Workflow and properties for battery ageing

So how can I use Sandia TABS?

Sandia National Laboratories

- TABS available under a U.S. Government Use Notice – No cost
  - Available to U.S. Government and Industry supporting government contract
  - Export controlled software – EAR99
- Support contract for installation, training, and support
  - Some JMP/TCG-V support for government entities
  - MIPR available more detailed government support
  - SPP agreements available for industry support
  - Minimal initial investment required
- Hardware requirements
  - Typical desktop/workstation computer is sufficient
  - OS: Linux (preferred), Mac, Windows (through Linux virtual machine)

Sandia National Laboratories

Sandia thermal battery modeling and TABS POC:

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Phone:	(505) 844-7957	(505) 284-0172 [STE]

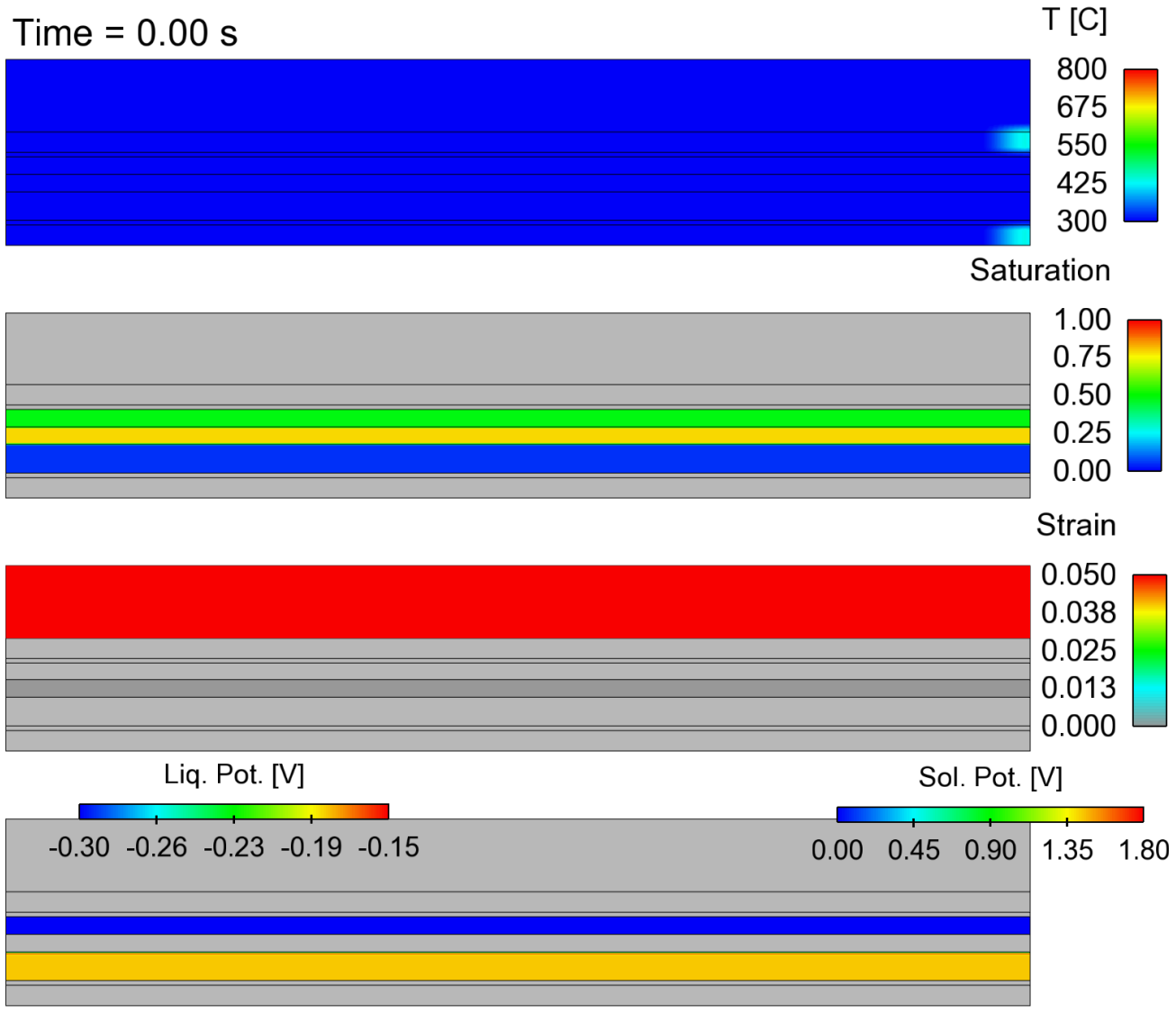
Thank you!

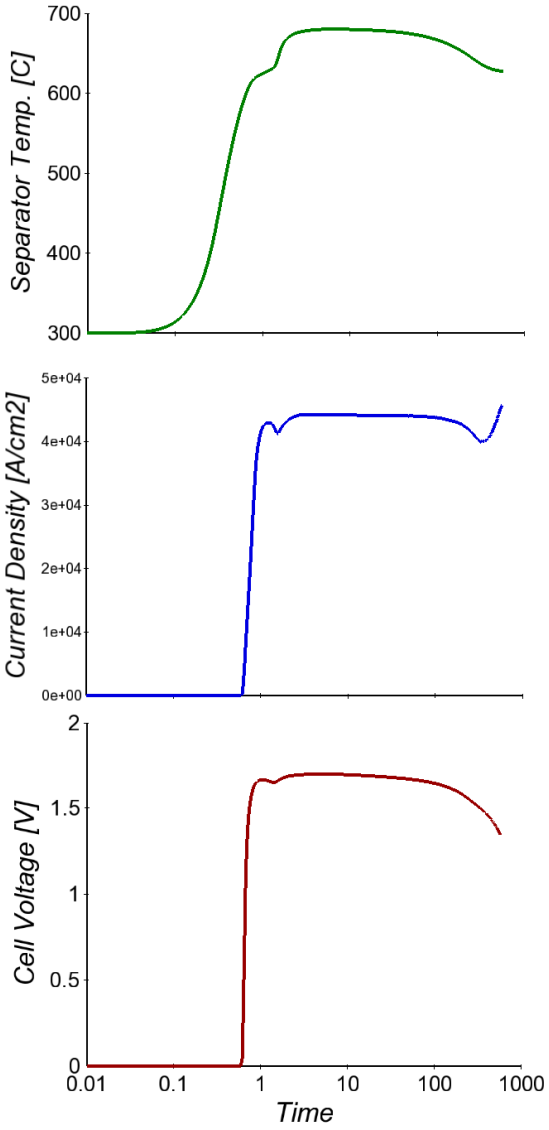
QUESTIONS / DISCUSSION

Sandia National Laboratories

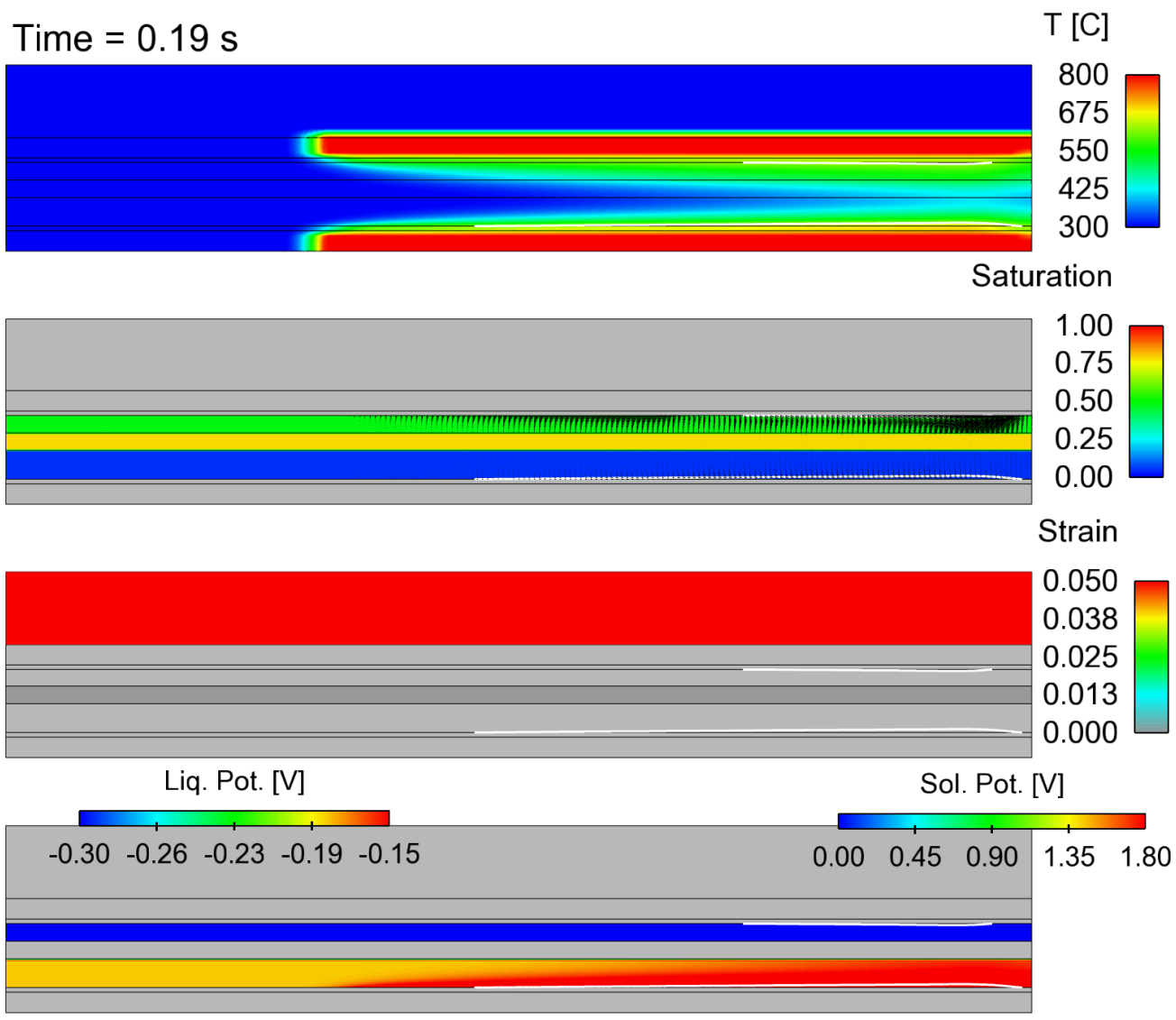
BACKUP SLIDES (MOVIE STILLS)

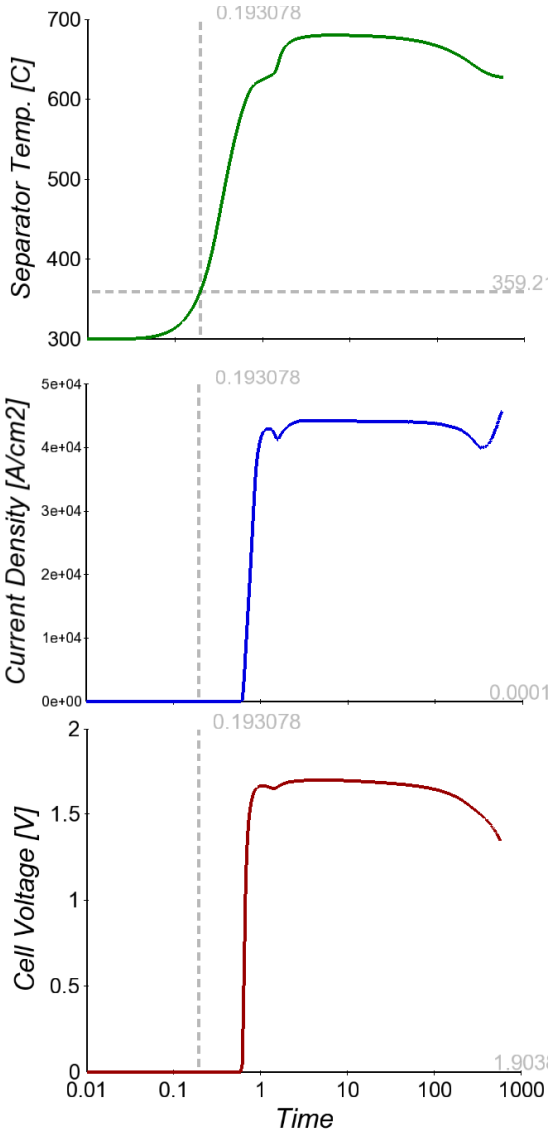
Full multi-physics single-cell simulation



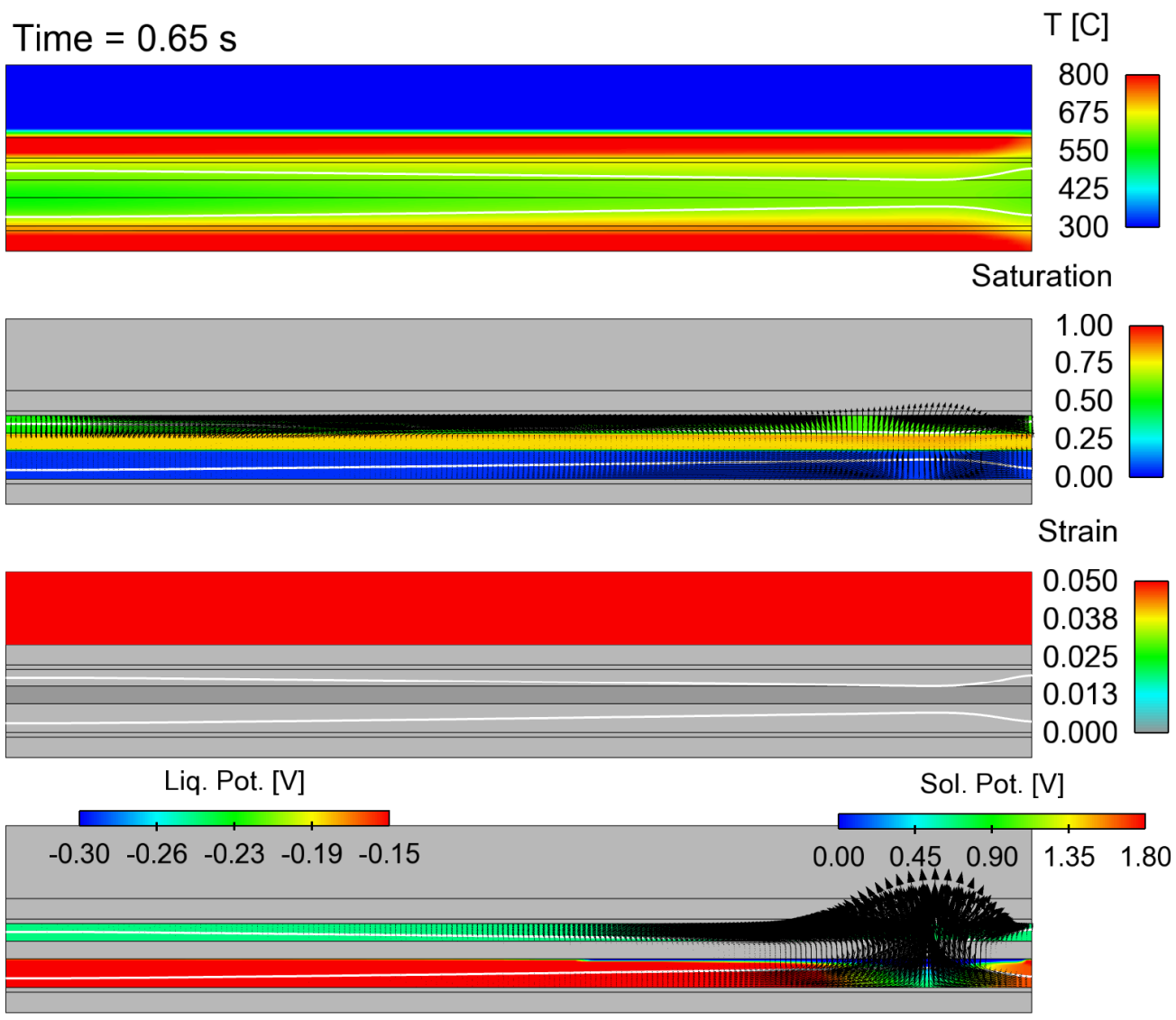


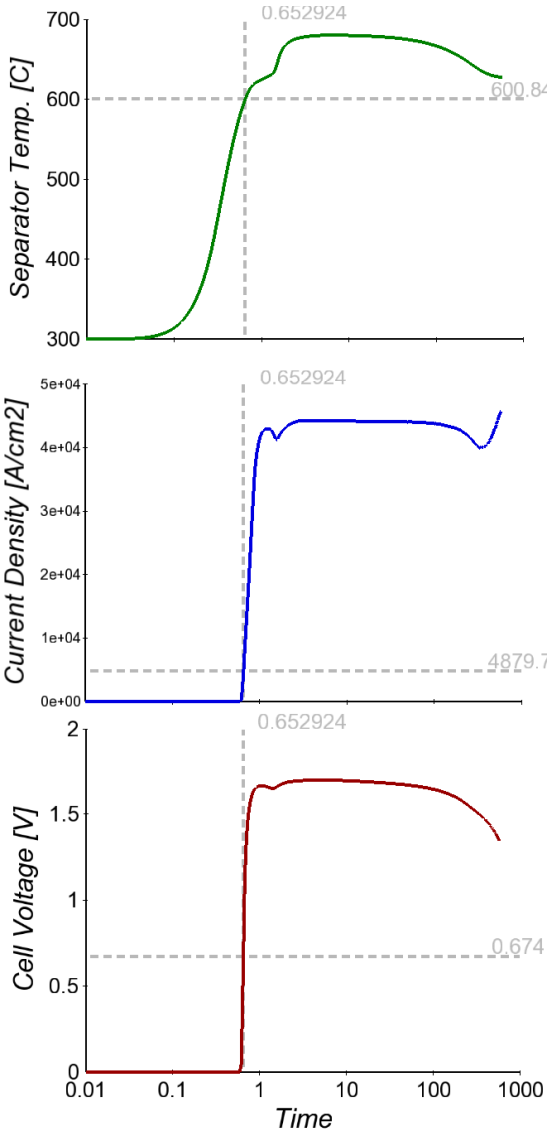
Full multi-physics single-cell simulation



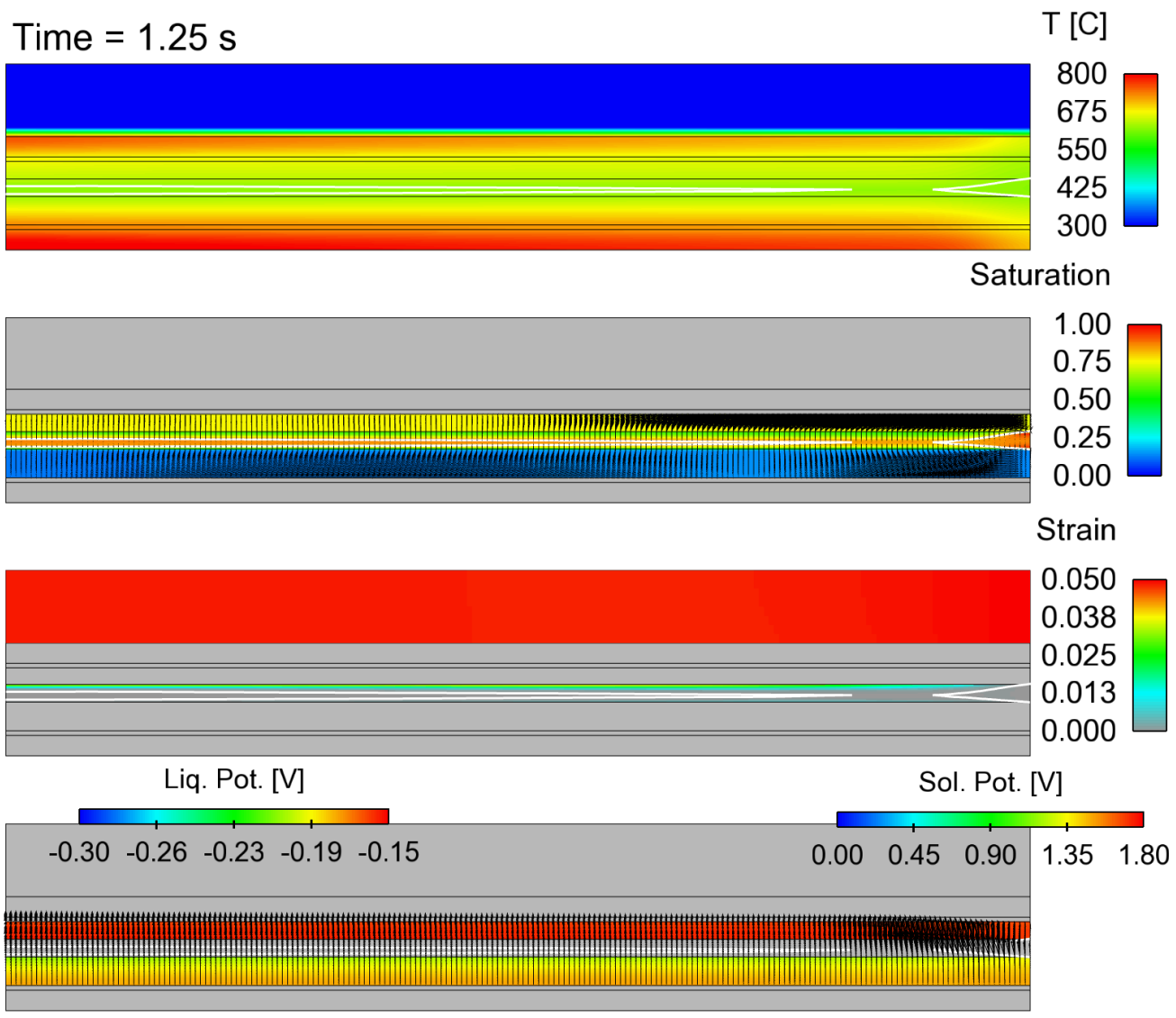


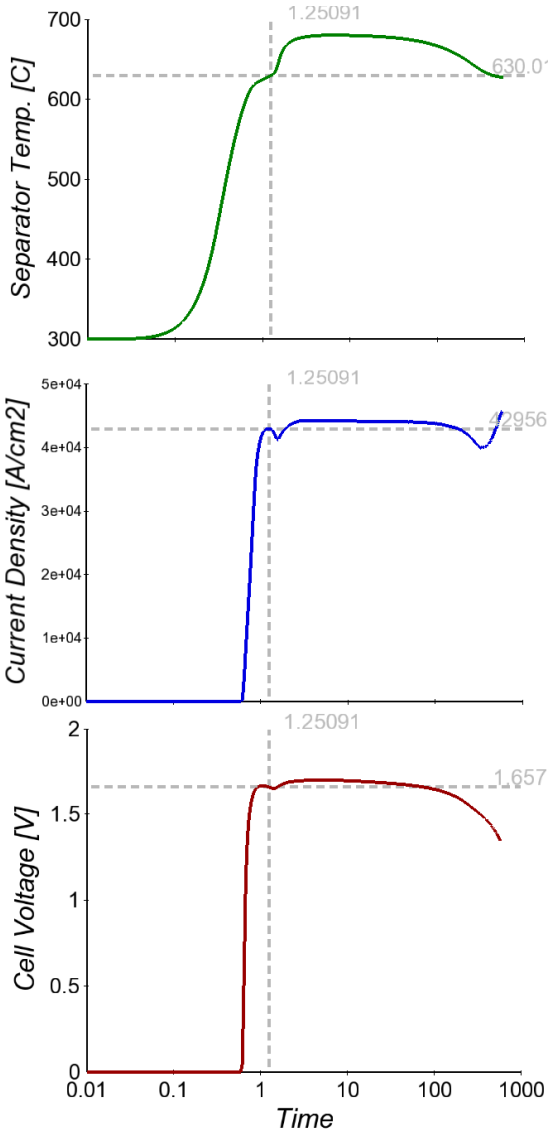
Full multi-physics single-cell simulation



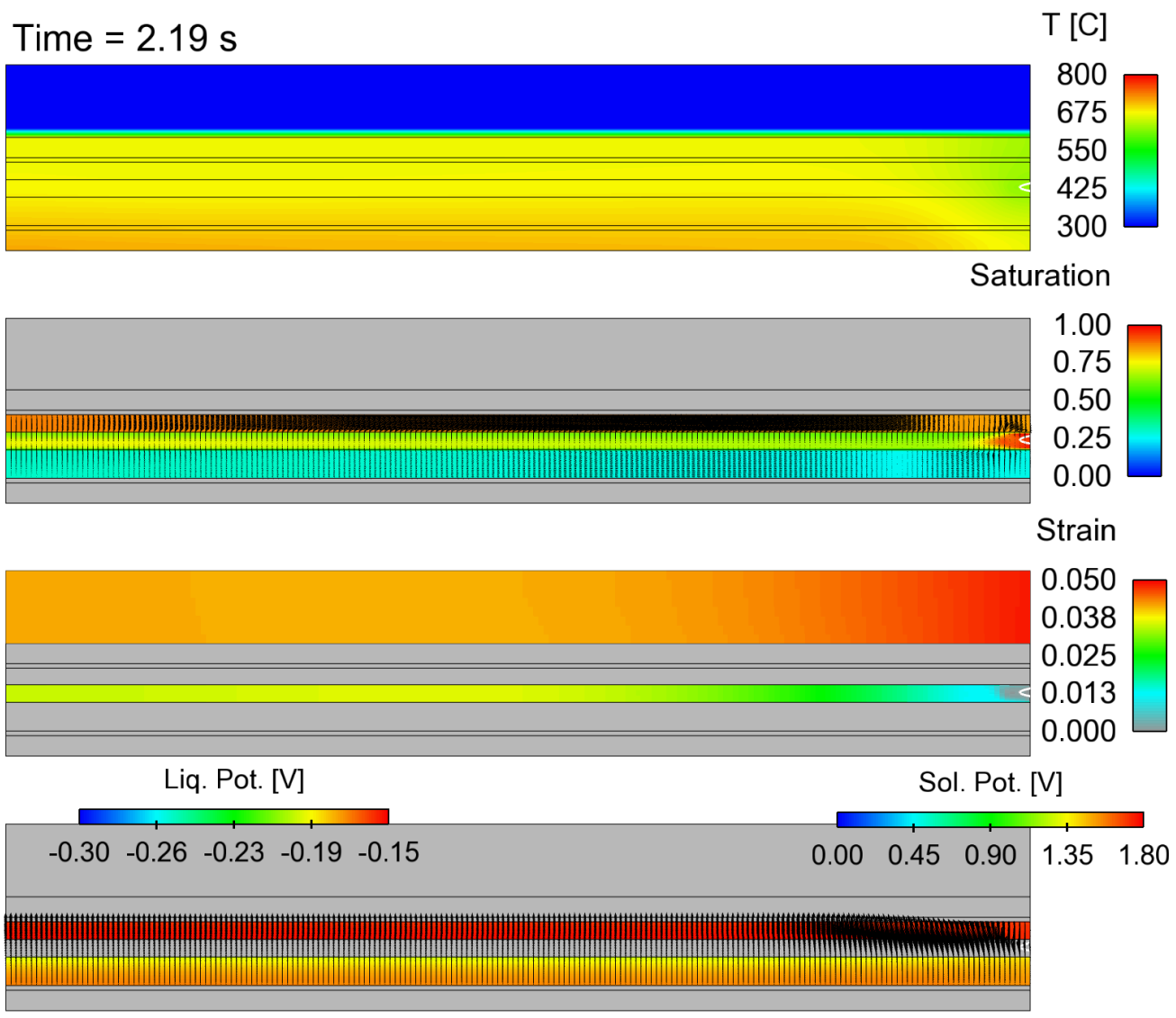


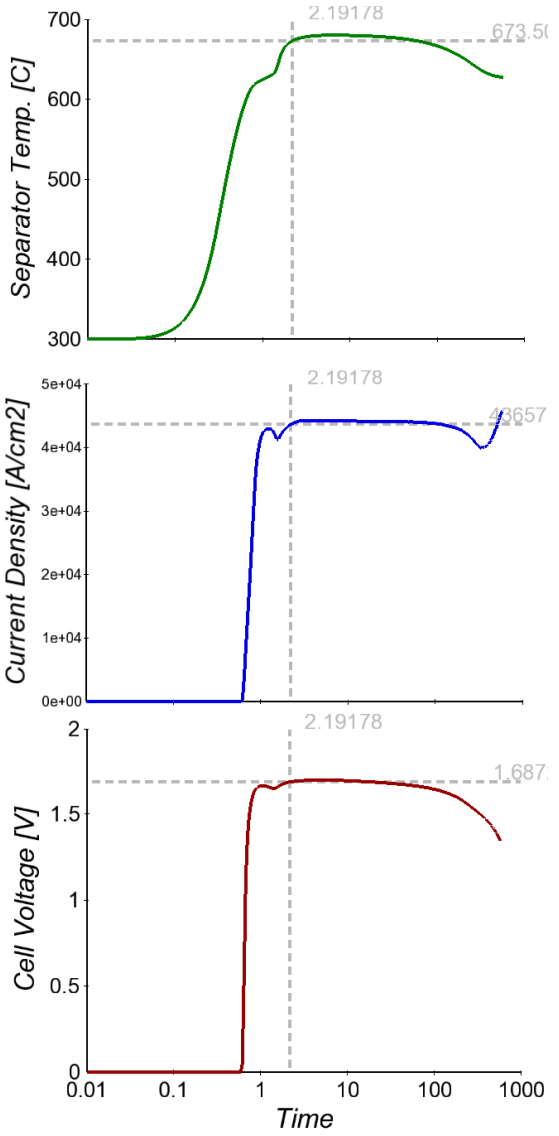
Full multi-physics single-cell simulation





Full multi-physics single-cell simulation





Full multi-physics single-cell simulation