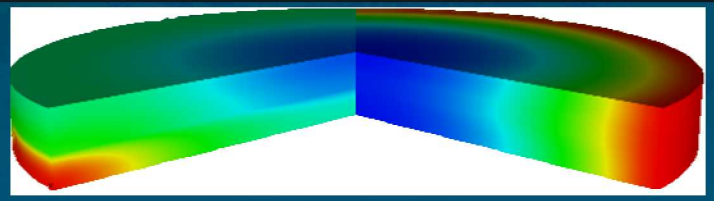
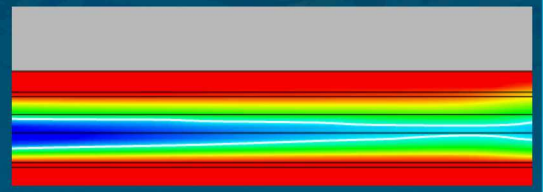
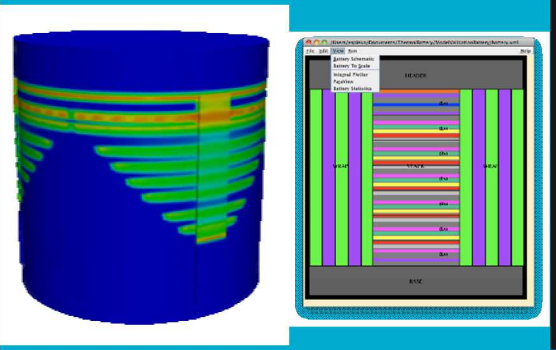
SAND2018-6114C

TABS: A Thermal Battery Desktop Design Tool







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PRESENTED BY

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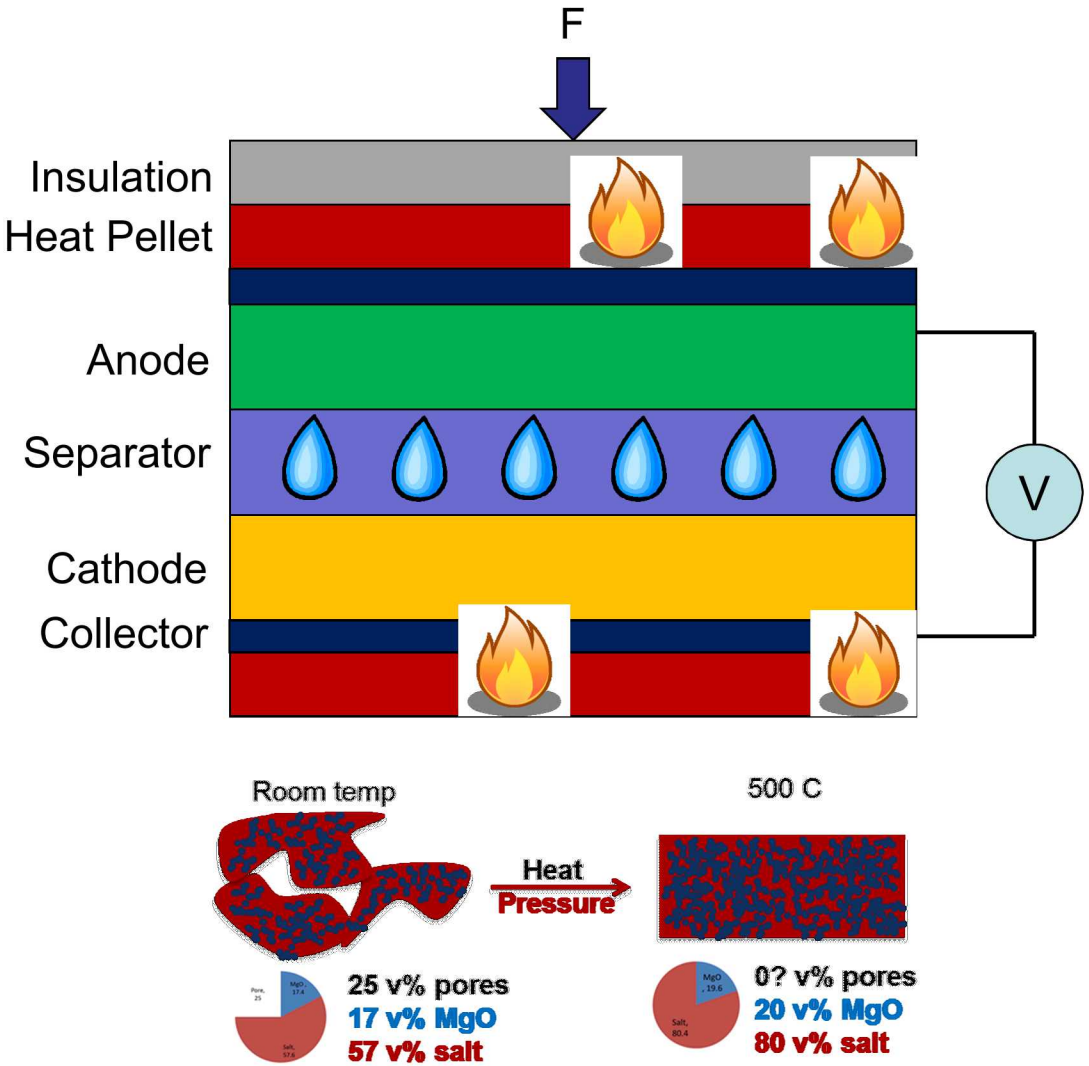
Physical mechanisms in thermal batteries

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 of thermal batteries?

- Predict activation times
- Predict electrochemical performance
- Optimize volume, insulation, manufacturing
- Understand system-level effects

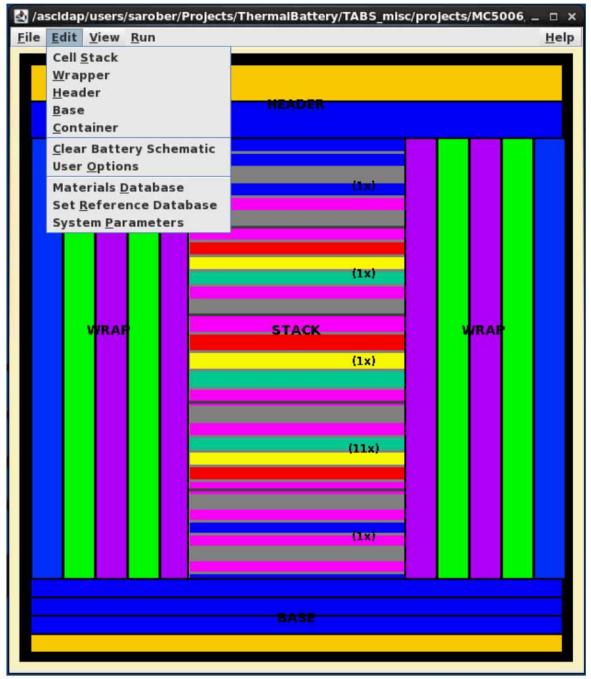


Thermal battery activation is a true multi-physics process!

TABS: The Thermally Activated Battery Simulator

TABS design principles

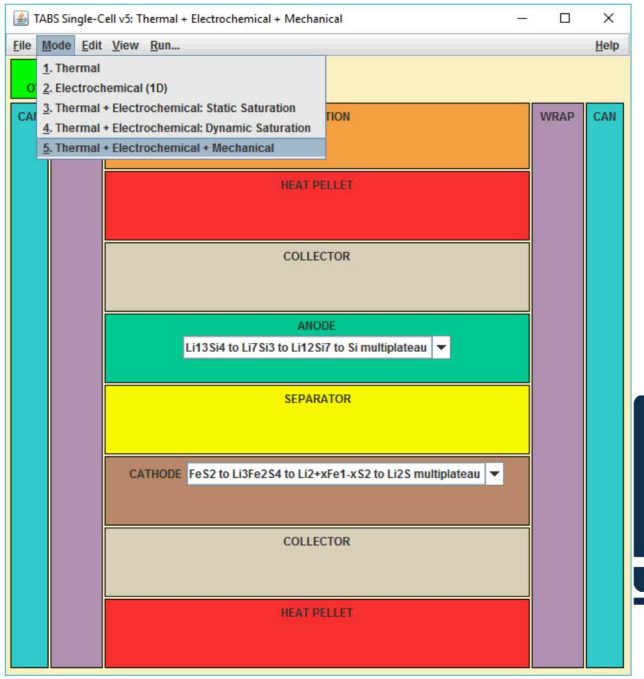
- Create a user interface **intuitive to battery designers**, not just for computational scientists
- Be **computationally efficient**, so many design iterations can be explored in a single work day
- Present the user with the most **relevant quantities of interest**, yet enable them to explore more deeply
- Have **demonstrated credibility**, such that the user knows when and how much to trust the solutions



TABS-FB: Full Battery

- Thermal

TABS FULL BATTERY



TABS-SC: Single Cell

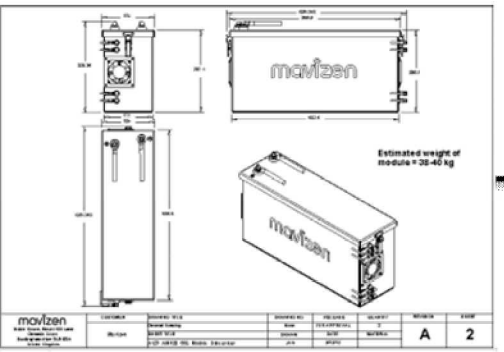
- Thermal
- Mechanical
- Flow
- Electrochemical

TABS SINGLE CELL

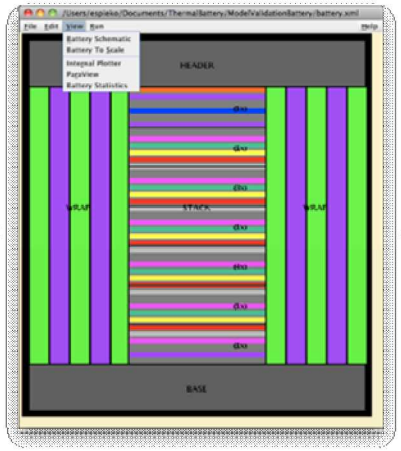
Two powerful performance/design models with an easy-to-use interface

Typical TABS workflow

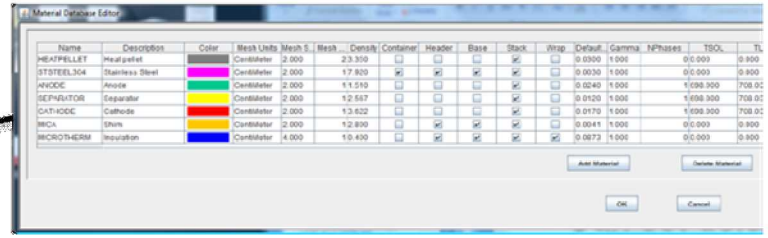
Battery definition (drawings)



Build battery



Define/use materials



Input decks

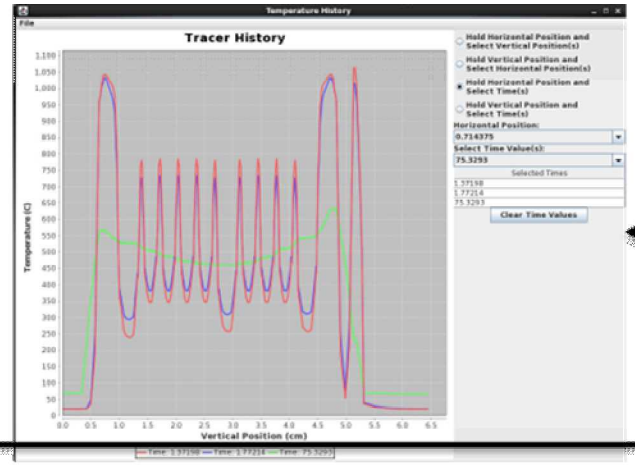
DAKOTA WRAPPER

Perform simulation (Sierra/Aria)

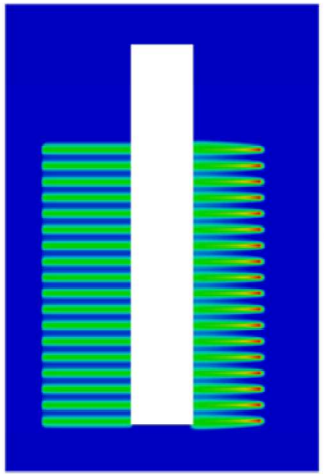
COMPSIM THERMAL FLUIDS

Post-process results

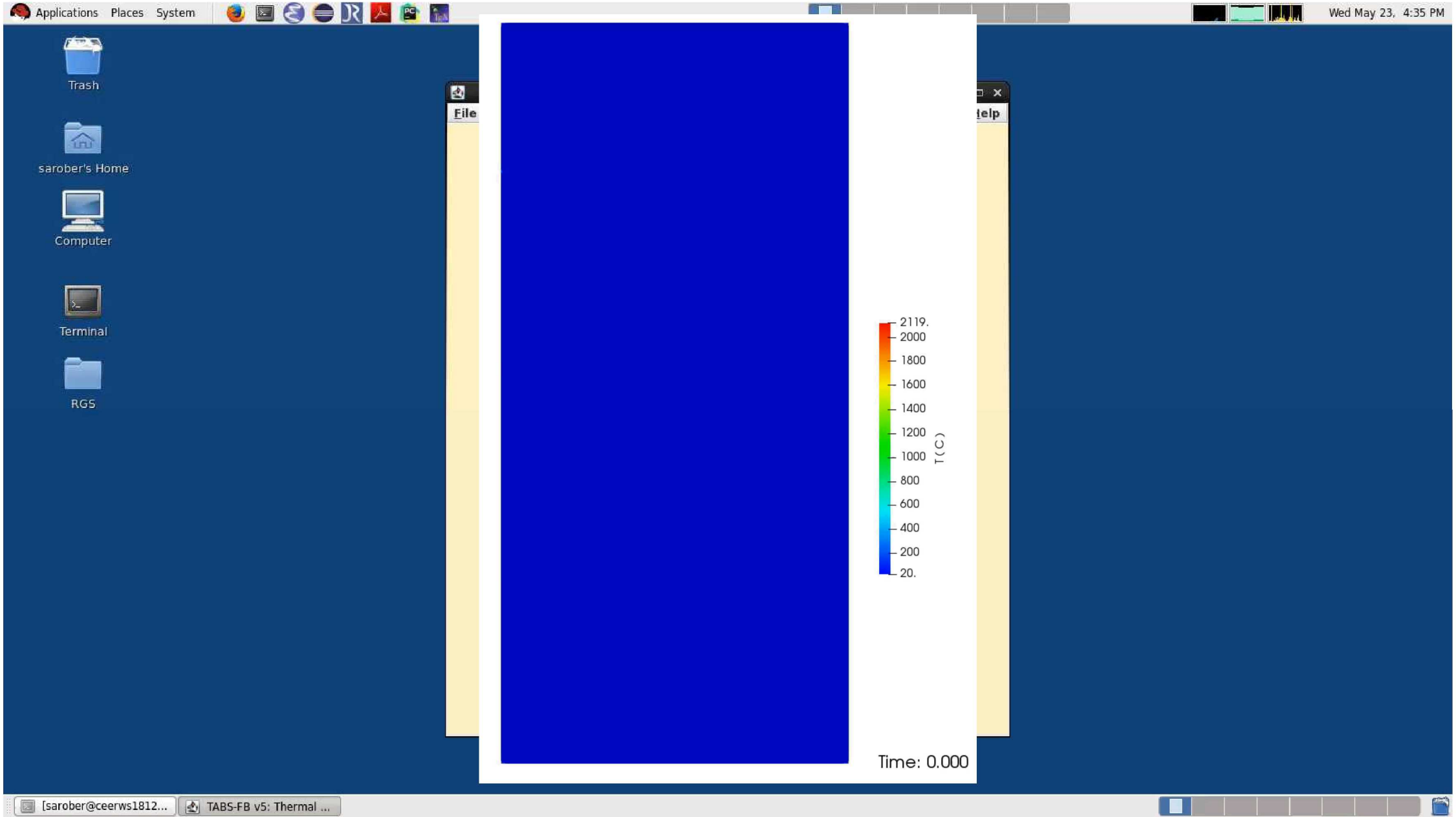
Internal plotter (line plots)



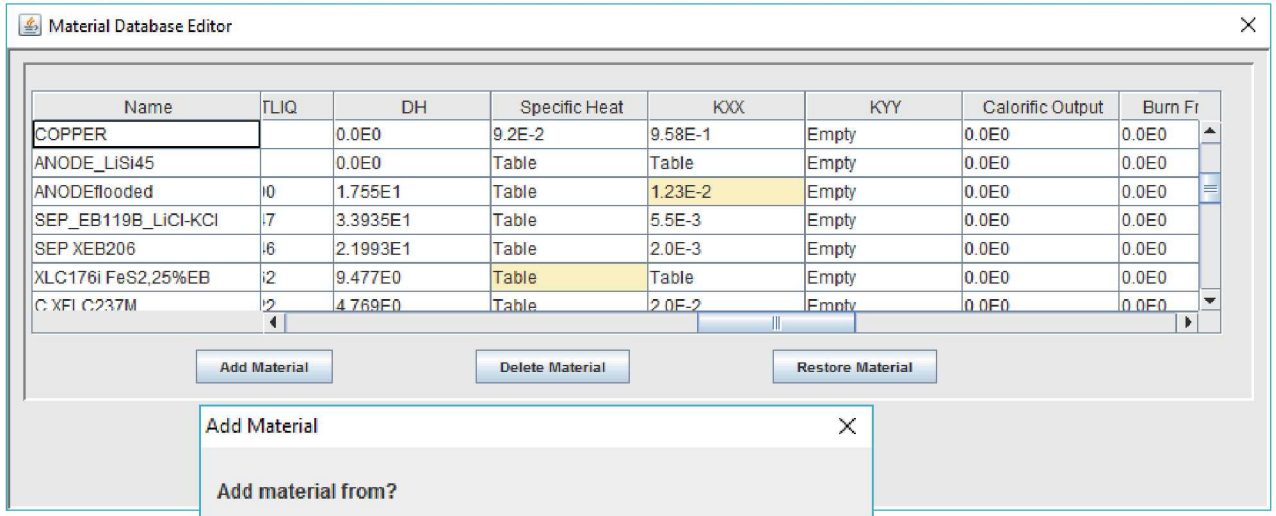
Paraview (visualize)



Setting up and running a TABS full battery thermal simulation

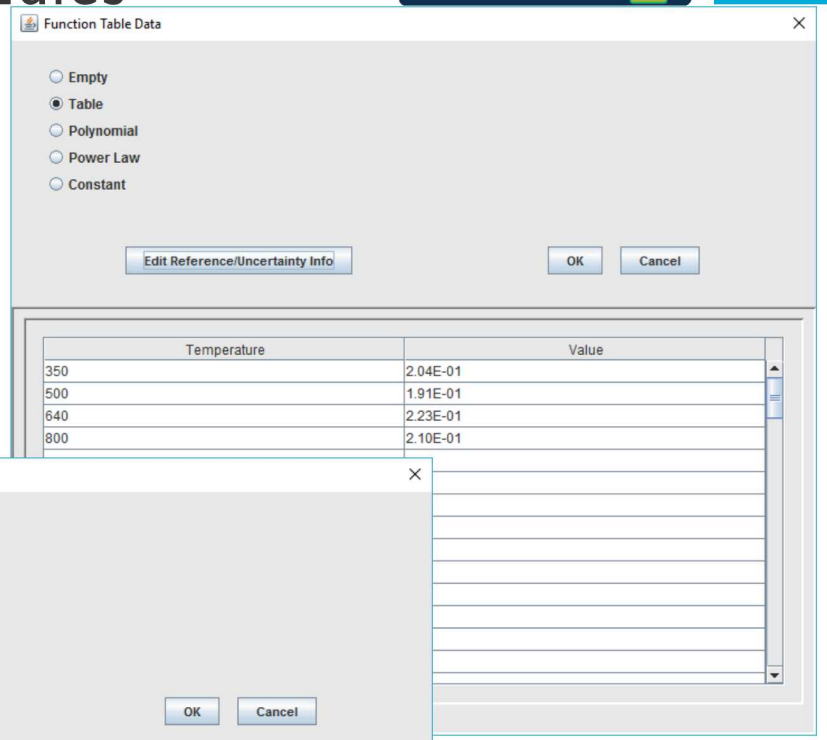


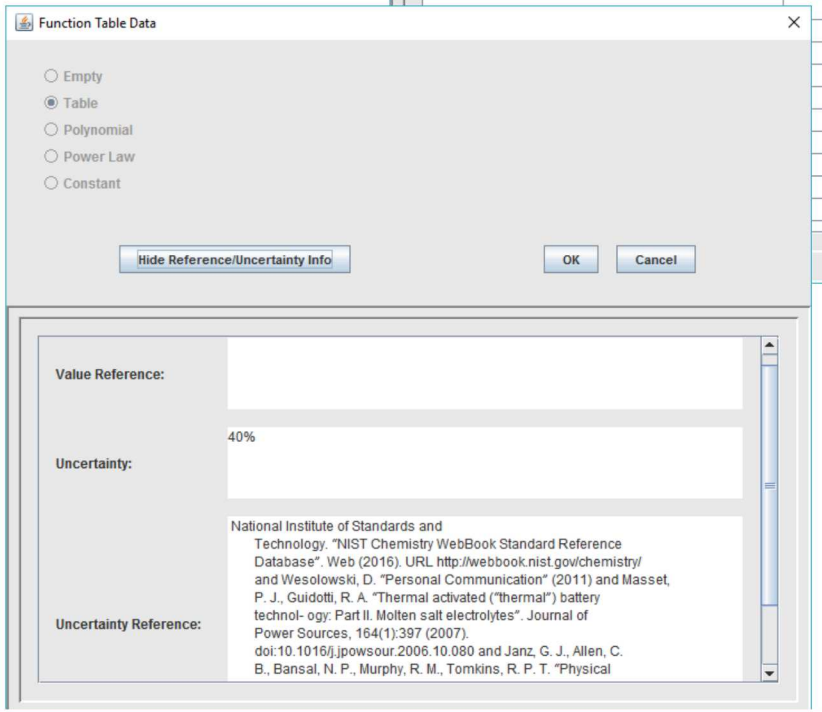
Materials database editor – common across TABS modules



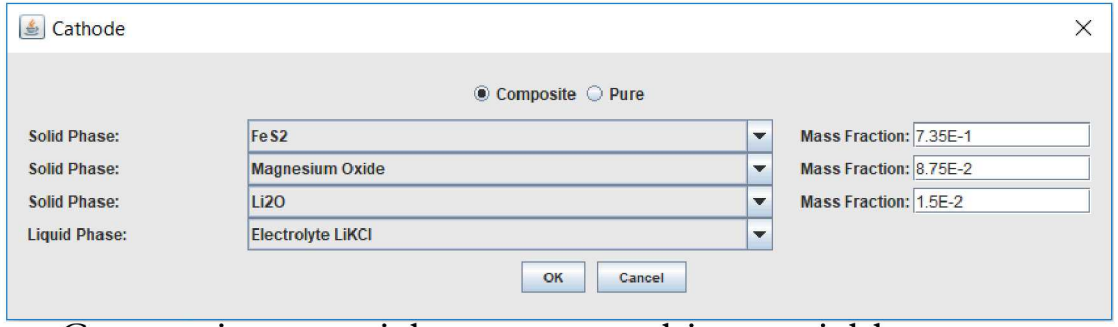
MDb editor allows for easy creation/modification of new materials; highlights deviations from reference database

All properties now edited in separate pop-up window





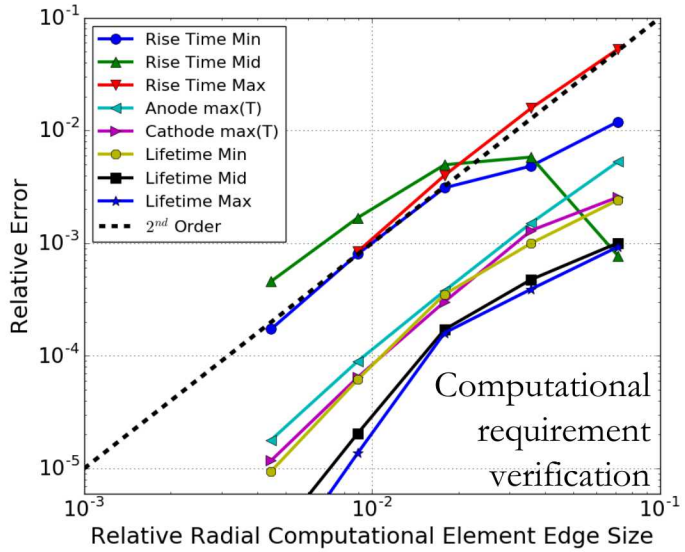
Credibility, reference, and uncertainty info now available

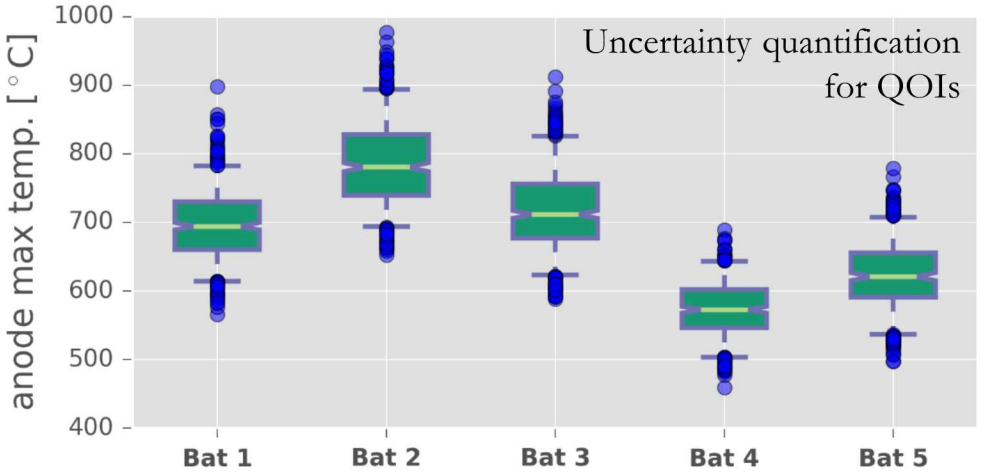


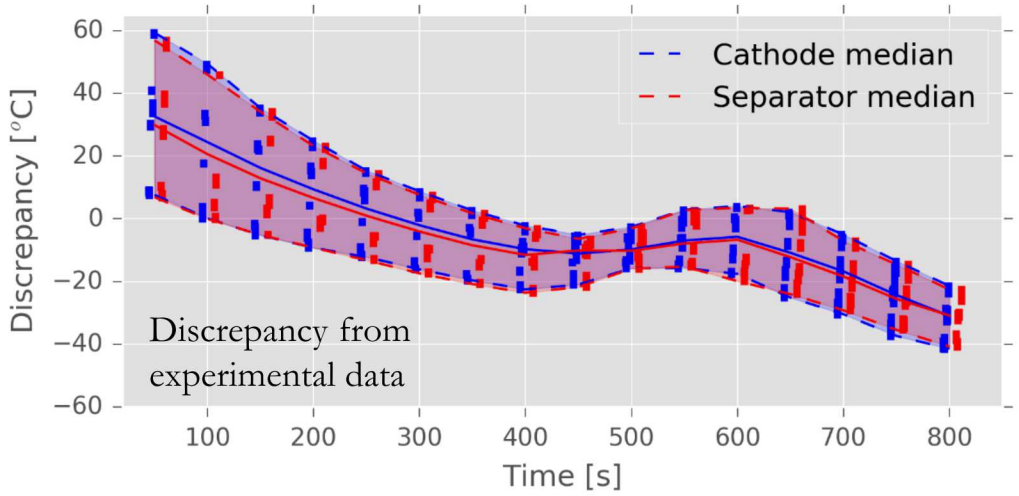
Composite materials capture multi-material layers to enable evolving phase-averaged properties

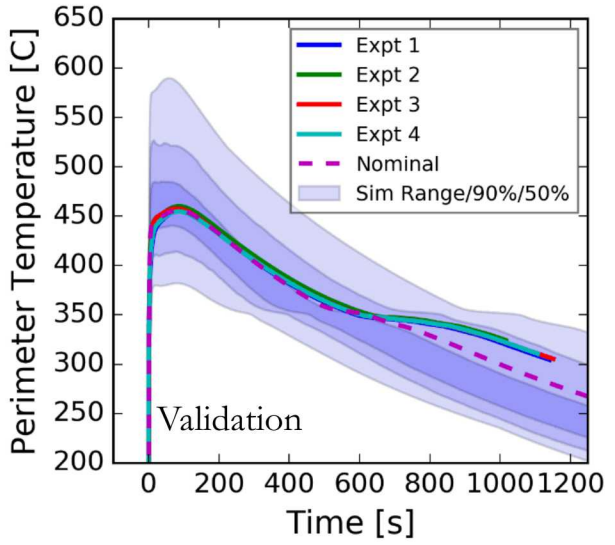
Database pre-populated with credible properties for common materials, yet easily extensible

TABS-FB credibility assessment









Verification, validation, and uncertainty quantification (V&V/UQ) establish model credibility

Setting up an electrochemical simulation in TABS-SC

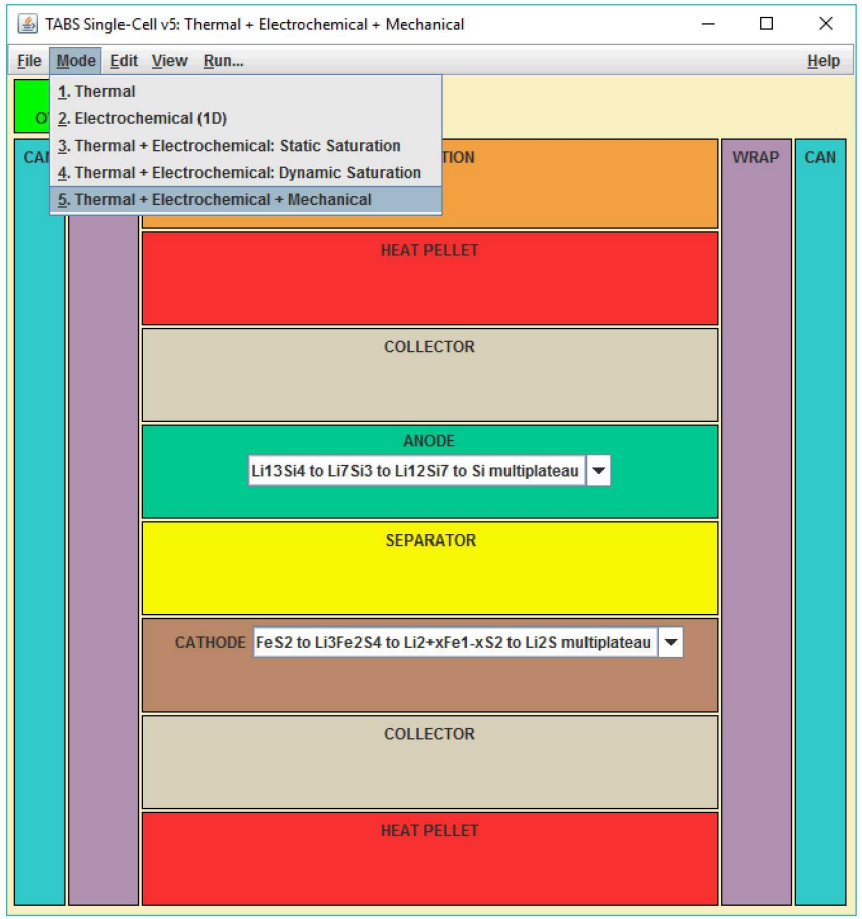
TABS-SC brings electrochemical (current/voltage) predictions

- Thermal: Heat generation (burning, Joule) and transport
- Fluid: Two-phase porous flow in anode/separator/cathode
- Mechanical: Separator deformation, insulation rebound, stack force
- Electrochemistry: Species diffusion, electrical transport, sub-grid multi-plateau electrochemical reactions

Multiple fidelity modes (details in next talk, Voskuilen):

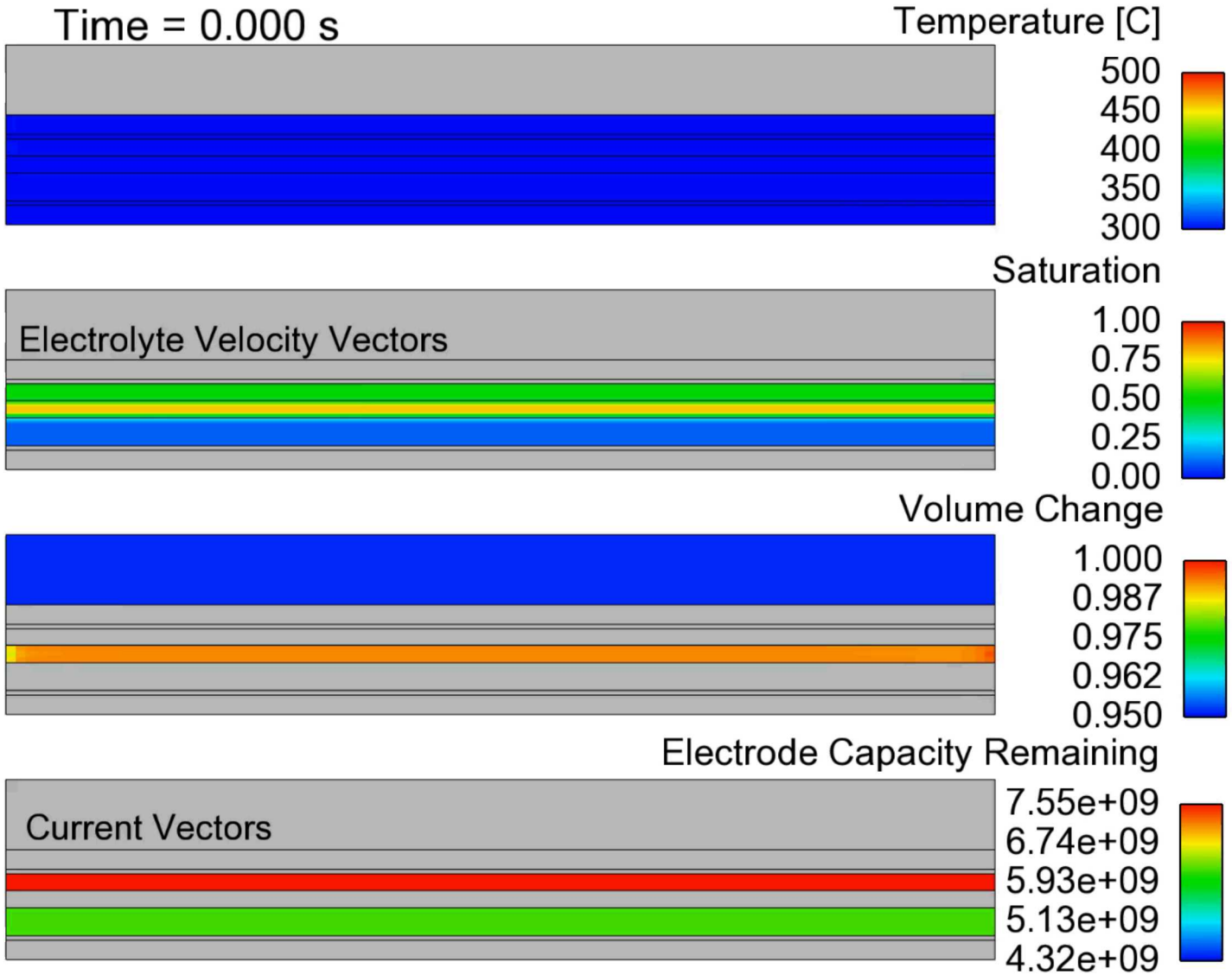
- 1: Thermal
- 2: Electrochemical (1D)
- 3: Static partially saturated fluid + thermal + electrochemical
- 4: Fluid + thermal + electrochemical
- 5: Fluid + thermal + electrochemical + mechanical

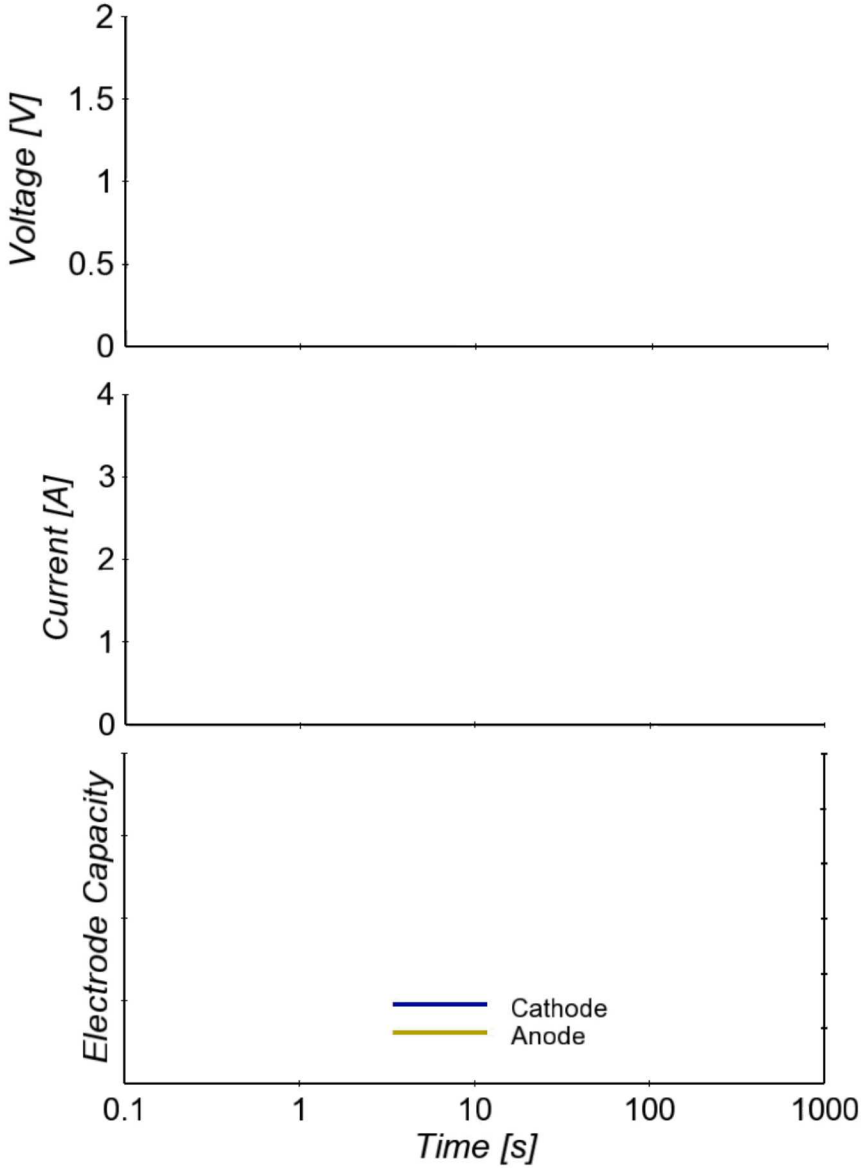
Same easy setup at TABS-FB!



TABS-SC is multi-physics solver for current and voltage at the single-cell scale

TABS-SC multi-physics visualization demonstration

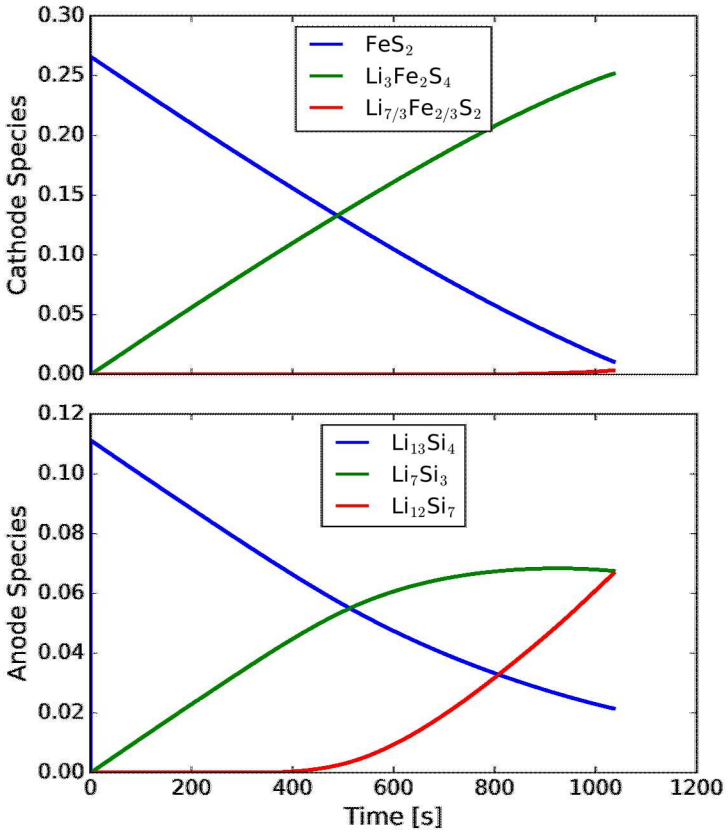




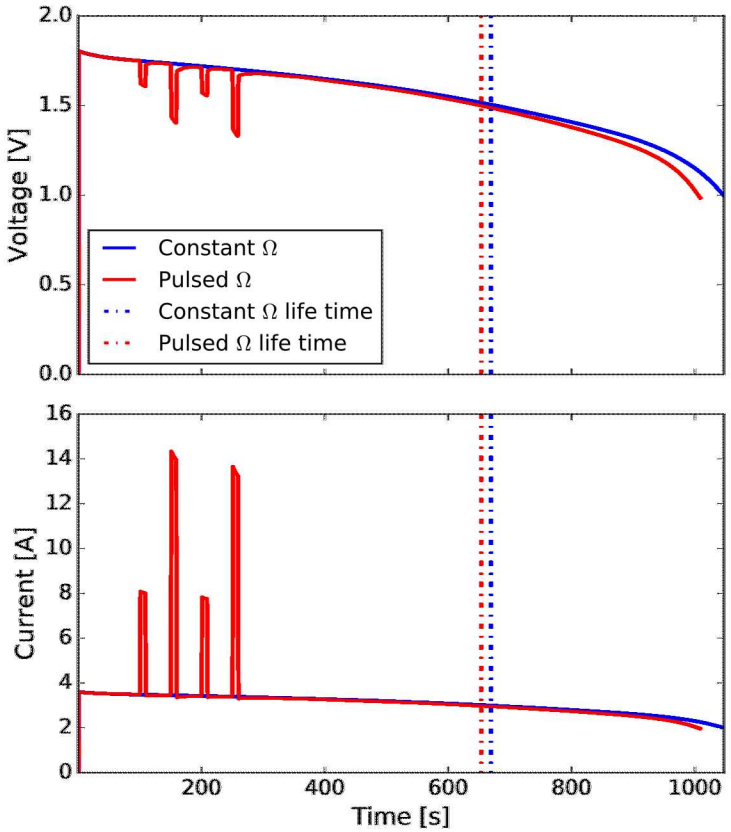
Additional quantities of interest from TABS-SC

QOI	Value
Rise time (@1.5V)	0.425 s
Lifetime (@1.5V)	691 s
Max Anode T	507 C
Max Cathode T	483 C
Max Voltage	1.80 V
Max Current	3.59 A
Separator Strain	16.3%

Scalar QOIs represent quick look at first-order design parameters. Predictions all in expected ranges



Reactions in cathode are fast, while anode access multiple simultaneous reaction plateaus



Pulses accelerate reactions and reduce life time

Valuable design insight post-processed from simulation results, immediately available in Excel file

Obtaining and using TABS

Obtaining TABS

- Export controlled under EAR99
- Licensing under a no-fee Government Use Notice (GUN) for direct support of government contracts/work
- Small separate contract required for installation, training, and support
- Contact Scott Roberts (sarober@sandia.gov) for more information

Computational requirements

- Runs natively under Linux and Mac OS, supporting Windows via virtual machine
- Can run efficiently on a multi-core desktop workstation
  - TABS-FB: 1-5 minutes
  - TABS-SC: 15-60 minutes, depending on physics fidelity mode

A peek into the future of TABS

TABS GUI and models under development for past 17 years

- 2001: TABS v1 – Full battery thermal (DIFUZN)
- 2011: TABS v2 – Transition to Sierra, user interface improvements
- 2013: TABS v3 – Burn-front model, 1D electrochemistry
- 2017: TABS v4 – 2D single-cell electrochemistry, thermal credibility assessment
- 2018: TABS v5 – Single-cell multi-physics model

What's next for TABS?

- 2019: TABS v5.1 – Improved calibration/parameters, advanced post-processing, credibility assessments
- 2020: TABS v6 – Initial electrochemical (voltage/current) capability at the full battery scale
- 2023: TABS v7 – Full multi-physics (electrochemical+fluid+mechanical) capability at the full battery scale

Thank you for your attention!

Questions?

TABS
THERMALLY ACTIVATED BATTERY SIMULATOR

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