



Exceptional service in the national interest

Development of a Cloud-Based Tool for Predicting Thermal Battery Performance: TABS v6

Scott A. Roberts, Ph.D.

June 28, 2023

49th Power Sources Conference

Co-authors: Adam V. Baca, Sylvain R. Bernard, Wesley A. Brooks, Ashley C. Fate, Emily Heintzelman, Edward S. Piekos, Tyler G. Voskuilen



TABS: The Thermally Activated Battery Simulator

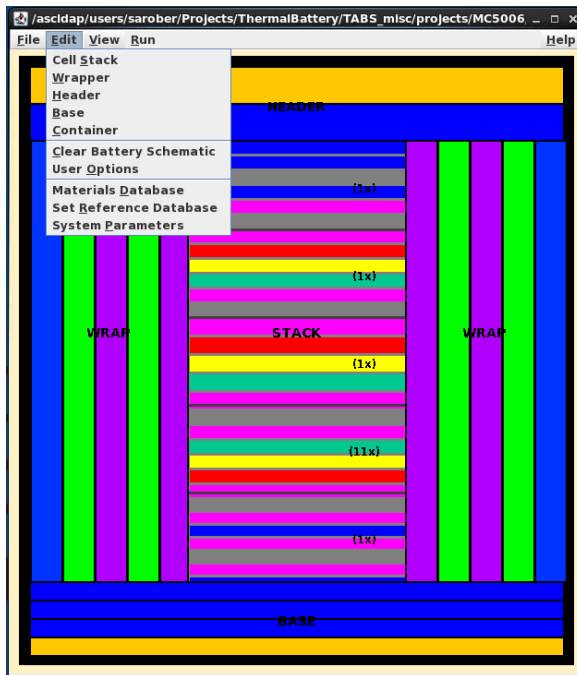
TABS design principles

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

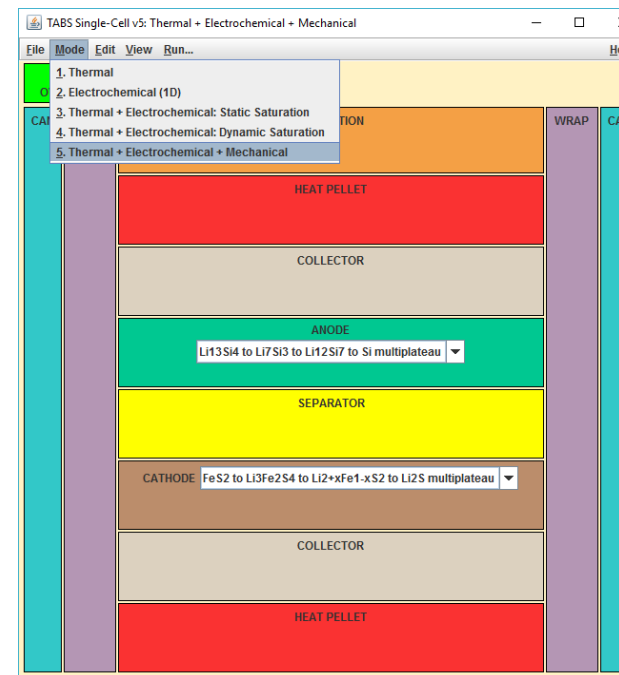
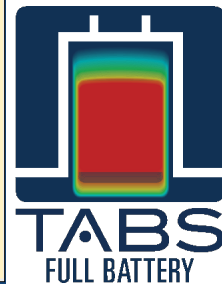
Present the user with the most **relevant quantities of interest**, yet enable them to explore more deeply

Have **demonstrated credibility**, such that the user knows when and how much to trust the solutions



TABS-FB: Full Battery

- Thermal



TABS-SC: Single Cell

- Thermal
- Mechanical
- Flow
- Electrochemical



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

Recent model development has focused coupled thermal-electrochemical response of full batteries

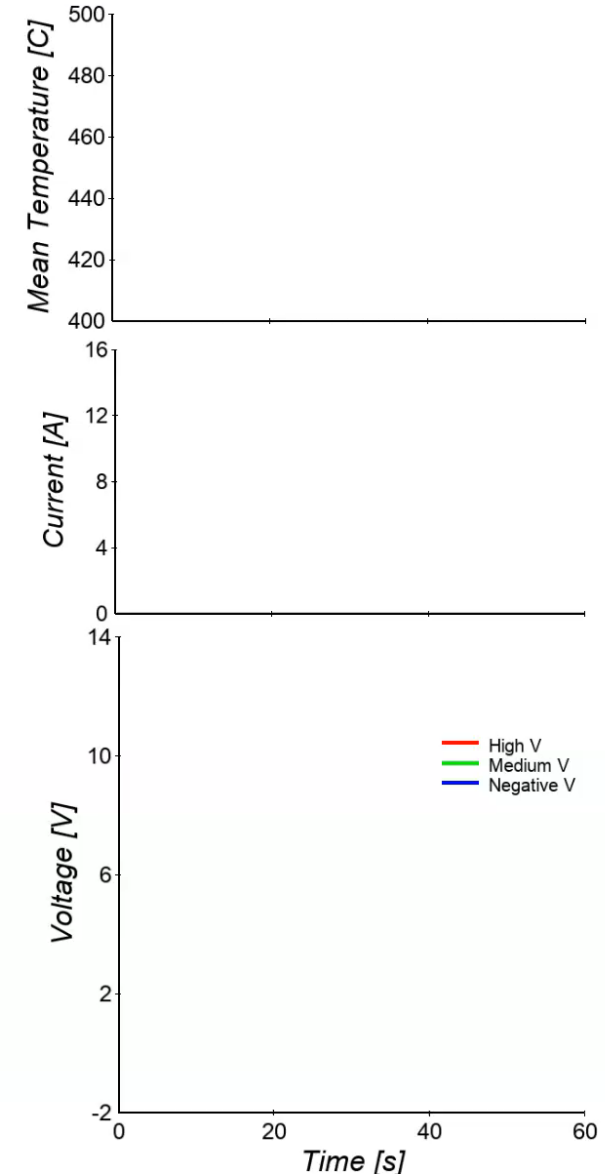
Time = 0.00 s

Current Density [A/m²]
0.0e+00 5.0e+04 1.0e+05



0 150 300 450 600
Temperature [C]

-2 2 6 10 14
0 4 8 12
Voltage [V]





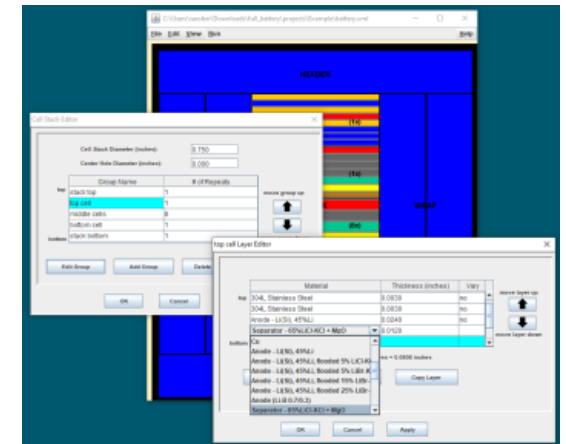
So what's wrong with TABS?



≠



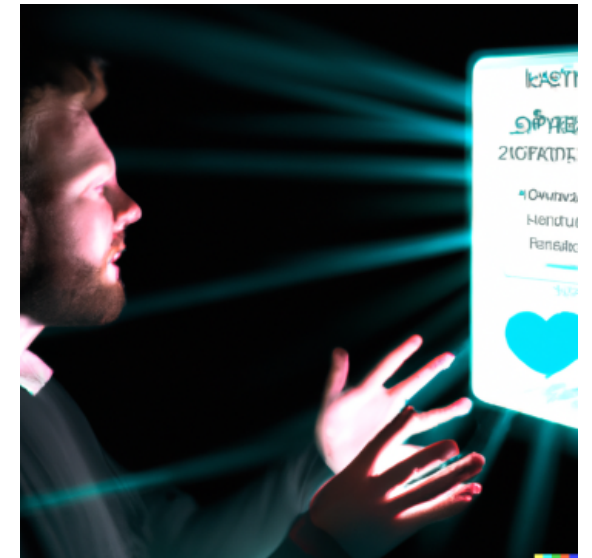
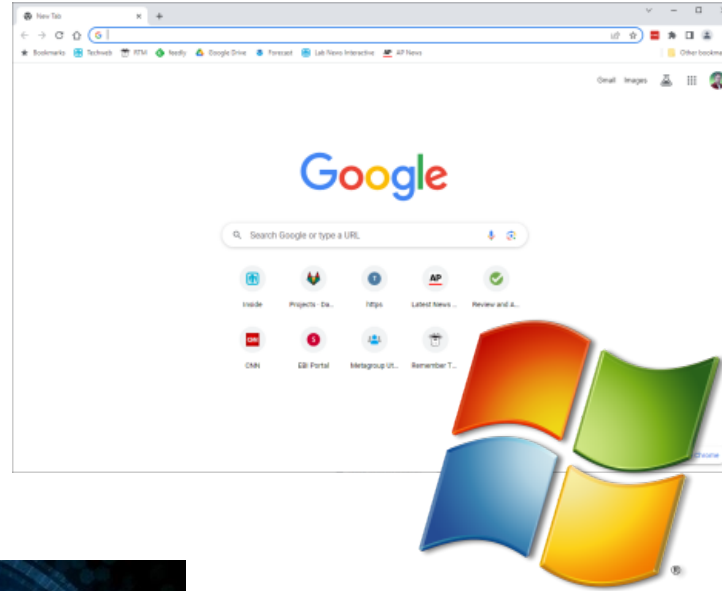
≠



Legacy TABS is powerful and impactful, but not prepared to maximize potential

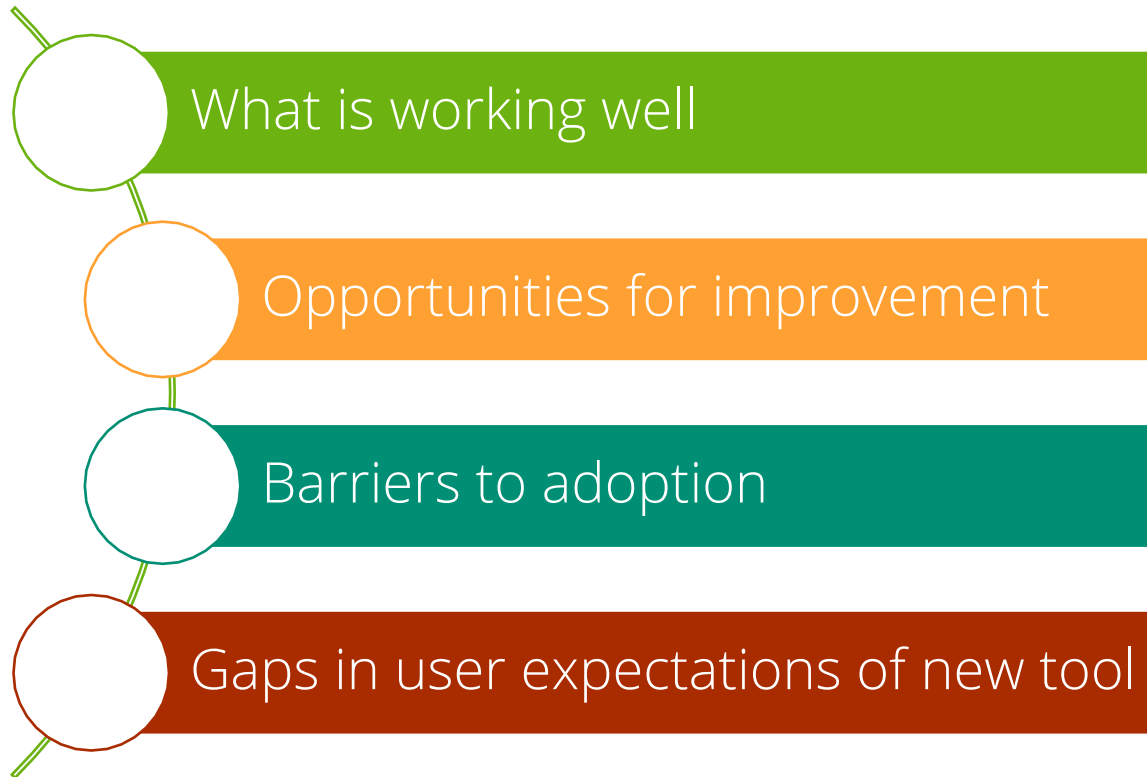


TABS v6 designed from scratch to address prior deficiencies and provide an experience that delights our users

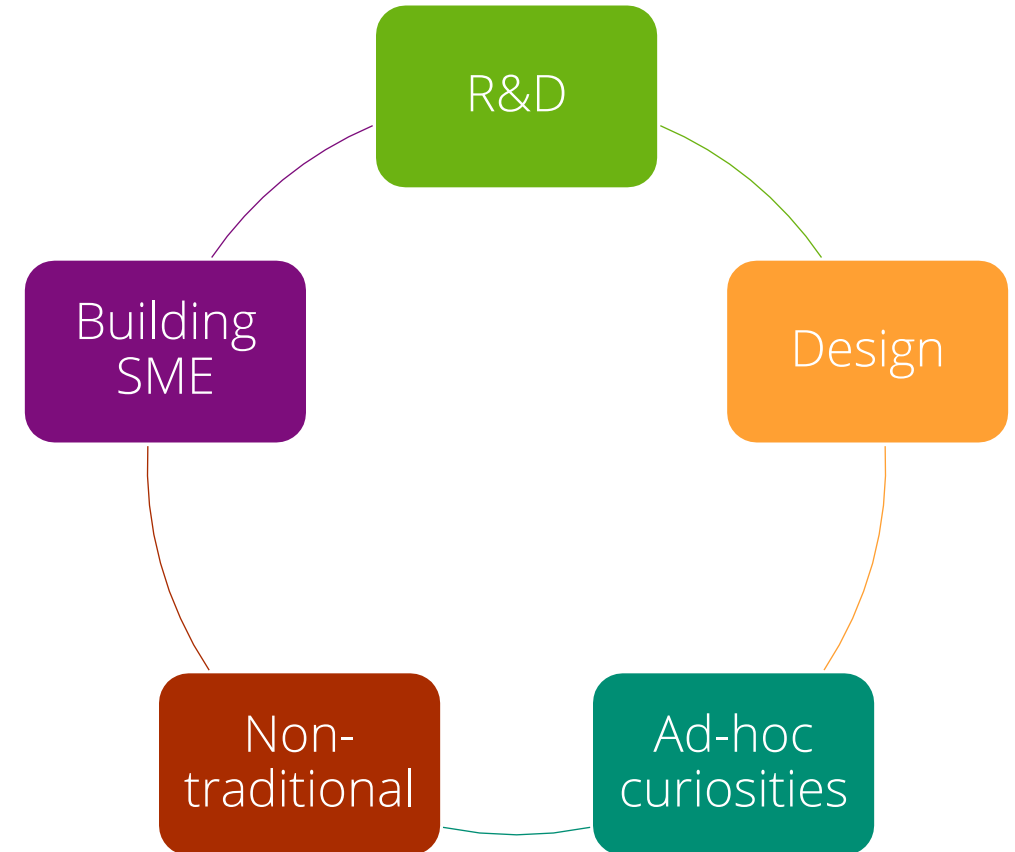


Embarked in foundational user experience research to design a tool that exceeds user's needs and desires

Interviewed current and prospective users (within Sandia, DOD, and AWE) to identify:



Identified 6 use cases:





User interface design evolves from low-fidelity mockups to implemented code, with user testing throughout development

The image illustrates the progression of user interface design for the TABS (Thermal Analysis Battery Simulation) software. It features three overlapping visual elements:

- Low-fidelity Mockup (Left):** A wireframe sketch of the software's layout, showing a sidebar with navigation options like 'Project Details', 'Design & Material Specifications', 'Environment', 'Electrochemical Boundary Condition', 'Summary', 'Simulate', 'View Results', and 'Simulation Log'. It also includes a 'Material Database' section and a 'Summary Tree'.
- Implemented Code (Center):** A screenshot of the actual web application. The interface is clean and professional, with a top navigation bar containing 'My Projects', 'Documentation', and 'System Preferences'. The main content area is titled 'Electrochemical Boundary Conditions' and includes a 'Battery Workflow' sidebar with options like 'Project Details', 'Battery Design', 'Environment', 'Thermal Boundary Conditions', 'Electrochemical Boundary Conditions', 'Summary/Preflight Check', 'Simulation Parameters', and 'View Results'. The 'Utilities' section includes 'Materials Database', 'Export Project Options', and 'Version History'.
- Configuration Page (Right):** A detailed view of the 'Electrochemical Boundary Conditions' configuration page. It shows a 'Collector' section with 'Top insulation' and 'Cells' (Cell 1, Cell 2, Cell 3, Cell 4) each having a color-coded bar representing a boundary condition. The 'Assign Boundary Conditions (Electrochemical)' section allows users to specify 'Tap Name' (e.g., 'tap_neg6V'), 'Collector' (e.g., '2: ST_STEEL_304'), 'Load Type' (Current, Voltage, Resistance), 'Value Type' (Constant, Table, Polynomial), 'Value' (e.g., '6'), and 'Units' (Volts). A 'DELETE TAP' button is also visible.



TABS v6 highlights: Landing page with templates, recent projects

TABS

MY MATERIALS DATABASE MY PROJECTS DOCUMENTATION SYSTEM PREFERENCES

Help Mode S

Welcome to TABS

Thermally Activated Battery Simulation Tool

Create a new battery, or modify a battery template.

Blank Project
Start from scratch – assign materials, boundary conditions and voltage taps

Import
Import legacy batteries or projects from others

User Material Database
View your own local material database. Make edits, add new materials.

Battery Templates

Search

FULL BATTERY
Created from a template of

FULL BATTERY
Created from a template of

FULL BATTERY
Created from a template of

FULL BATTERY
Created from a template of

FULL BATTERY
Created from a template of

FULL BATTERY
Created from a template of

FULL BATTERY
Created from a template of

FULL BATTERY
Created from a template of

FULL BATTERY
Created from a template of

FULL BATTERY
Created from a template of

RECENT

FAVORITES SHARED WITH ME

Search

Name

Scott's Generic Battery
Owner
A thermal battery made up by Scott Roberts.
Modified Date: 6/22/2023, 12:50:57 PM
Create Date: 6/22/2023, 12:17:15 PM
ACTIONS

Items per page: 10 1-1 of 1

TABS v6 highlights: Materials database hierarchy to maintain high-pedigree reference materials while exploring

The screenshot displays the TABS v6 Materials Database interface. A green notification banner at the top states: "Material created successfully" with a "CLOSE" button. Below this, a teal banner reads: "HEATPELLET86-14 - b has been added". A central modal window provides details for the newly added material:

HEATPELLET86-14 - b has been added to the Battery Scott's Generic Battery Project Materials
You can make this material accessible to all your projects by using the "manage" button.

The modal includes a "Manage Material" button with a double-headed arrow icon. Below this, a "My Materials" section shows a hierarchy: "You are here" (blue button) pointing to "Battery Project Materials" (green button).

The main interface shows a sidebar with "Materials Database" selected. The "Filters" section includes "My Favorites", "Reference Materials", and "New Materials". The "Material Location" section has checkboxes for "Header/Base", "Stack", "Wrap", and "Container". The "Material Function" section has checkboxes for "Separator", "Anode", "Cathode", "Heat Sources", "Collector", "Insulation", and "Electrolyte". The "Composition" section has checkboxes for "Pure" and "Composite".

The main content area displays a list of materials. The selected material, HEATPELLET86-14 - b, is highlighted. A table below the material entry shows various properties:

Property	Value
IdealCapacity	6
CellVoltage	7
CaloriesPerGram	8
BurnFrontSpeed	9
MoleFractionLi	1010

On the right side of the interface, a "Value Reference" section shows "None". An "Uncertainty" section shows "15%". An "Uncertainty Reference" section provides a citation: "Love, C. M., Etter, D. E., Glaub, J. E. 'Thermal Conductivity of Iron/Potassium Perchlorate Heat Powder'. MLM-3173, Monsanto Research Corp: Mound, Miamisburg, OH (2984) and National Institute of Standards and Technology. 'NIST Chemistry WebBook Standard Reference Database'. Web (2016). URL http://webbook.nist.gov/chemistry/".



TABS v6 highlights: Building a battery from scratch in < 5 minutes

The screenshot displays the TABS v6 web application interface. The browser address bar shows the URL: `tabs-dev.sandia.gov/specifications?battery=6494902b0e9dc2d9a9009acd`. The application has a dark theme with a green accent color.

Navigation Bar: Includes a hamburger menu, the TABS logo, and links to **MY MATERIALS DATABASE**, **MY PROJECTS**, **DOCUMENTATION**, and **SYSTEM PREFERENCES**. On the right, there is a **Help Mode** toggle and a user profile icon labeled 'S'.

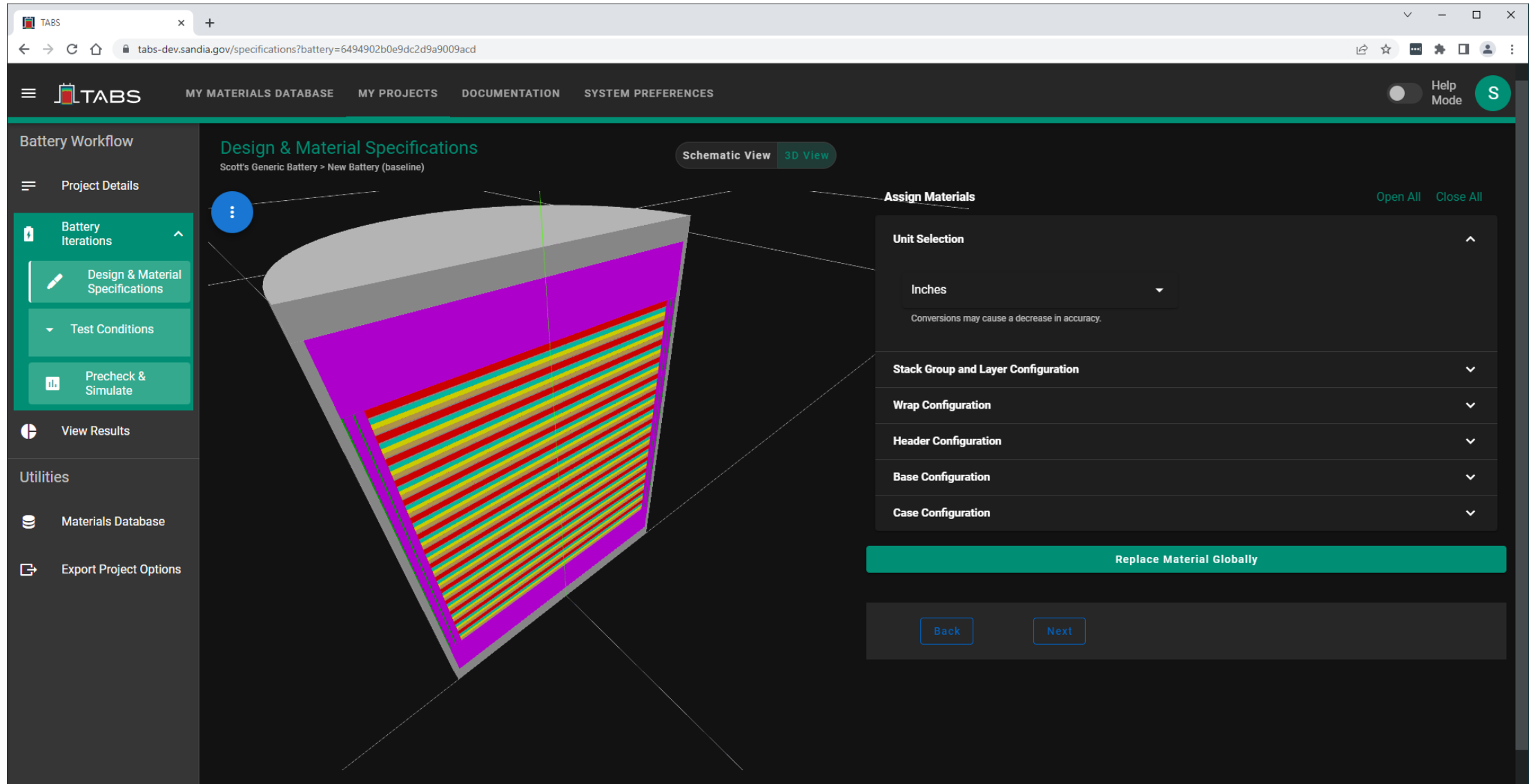
Battery Workflow: A sidebar on the left contains the following options: **Project Details**, **Battery Iterations** (with a sub-menu for **Design & Material Specifications**, **Test Conditions**, and **Precheck & Simulate**), **View Results**, and **Utilities** (including **Materials Database** and **Export Project Options**).

Main Content Area: The title is **Design & Material Specifications** for **Scott's Generic Battery > New Battery (baseline)**. It features two tabs: **Schematic View** (active) and **3D View**. The schematic view shows a battery layout with a central **Stack** (highlighted in green) flanked by **Wrap** sections, all within a **Case** boundary. The layout is divided into **Header**, **Base**, and **Case** regions.

Assign Materials Panel: Located on the right, it includes a **Unit Selection** dropdown set to **Inches** with a note: "Conversions may cause a decrease in accuracy." Below this is a list of configuration sections, each with a red exclamation mark icon: **Stack Group and Layer Configuration**, **Wrap Configuration**, **Header Configuration**, **Base Configuration**, and **Case Configuration**. At the bottom of this panel is a green button labeled **Replace Material Globally** and navigation buttons for **Back** and **Next**.



TABS v6 highlights: Building a battery from scratch in < 5 minutes



TABS v6 highlights: Specifying boundary conditions and electrochemical loads in multiple formats

The screenshot displays the TABS v6 web application interface. The browser address bar shows the URL: `tabs-dev.sandia.gov/electrochemical?battery=6494902b0e9dc2d9a9009acd`. The application header includes the TABS logo and navigation links: MY MATERIALS DATABASE, MY PROJECTS, DOCUMENTATION, and SYSTEM PREFERENCES. A 'Help Mode' toggle and a user profile icon are also present.

The left sidebar contains a 'Battery Workflow' section with the following options: Project Details, Battery Iterations (expanded), Design & Material Specifications, Test Conditions (expanded), Thermal Boundary Conditions, Electrochemical Boundary Conditions (selected), Analysis Parameters, Precheck & Simulate, View Results, Utilities, Materials Database, and Export Project Options.

The main content area is titled 'Electrochemical Boundary Conditions' and shows the configuration for 'Scott's Generic Battery > New Battery (baseline) > Default Test Condition'. The 'Collector' is set to '1: ST_STEEL_304'.

The 'Assign Boundary Conditions (Electrochemical)' panel is open, showing the configuration for 'High - Collector 1'. The 'Tap Name' is 'High' and the 'Collector' is '1: ST_STEEL_304'. The 'Load Type' is set to 'Current' (radio button selected). The 'Value Type' is set to 'Table' (radio button selected). The 'Value' is defined by a table with 'Time (ms)' and 'Value' columns. The 'Units' are set to 'Amps'.

Time (ms)	Value
0	0
1000	0.5
1500	1
2000	0.5
50000	0.5



TABS v6 highlights: Multiple test conditions can be simulated for a single consistent battery design

The screenshot displays the TABS v6 web application interface. The browser address bar shows the URL: `tabs-dev.sandia.gov/test-conditions?battery=6494902b0e9dc2d9a9009acd`. The application has a dark theme with a sidebar on the left containing navigation options: Battery Workflow, Project Details, Battery Iterations, Design & Material Specifications, Test Conditions (expanded), Thermal Boundary Conditions, Electrochemical Boundary Conditions, Analysis Parameters, Precheck & Simulate, View Results, Utilities, Materials Database, and Export Project Options. The main content area is titled "Test Condition Differences" and compares two configurations: "Room temperature" and "High temperature".

Room temperature

```
{
  "selected": false,
  "selectedSim": false,
  "name": "Room temperature",
  "thermocouplePoints": {
    "header": {
      "value": "25"
    },
    "side": {
      "value": "25"
    },
    "base": {
      "value": "25"
    }
  },
  "analysisParameters": {
    "initialBatteryTemperature": "25"
  }
}
```

High temperature

```
{
  "name": "High temperature",
  "thermocouplePoints": {
    "header": {
      "value": "85"
    },
    "side": {
      "value": "85"
    },
    "base": {
      "value": "85"
    }
  },
  "analysisParameters": {
    "initialBatteryTemperature": "85"
  }
}
```

On the right side of the comparison window, there is a search bar, a "COMPARE TESTS" button, a "Compare" button, and two checkboxes, both of which are checked. At the bottom right of the window, there is an "EXIT" button and navigation arrows.

TABS v6 highlights: Battery iterations allow testing tweaks to design, materials while keeping previous simulation pedigree

The screenshot displays the TABS v6 web application interface. The browser address bar shows the URL: `tabs-dev.sandia.gov/battery-iterations?battery=649497d40e9dc2d9a9009bdb`. The application has a dark theme with a teal accent color.

Navigation Bar:

- Left: TABS logo, menu icon.
- Center: MY MATERIALS DATABASE, MY PROJECTS, DOCUMENTATION, SYSTEM PREFERENCES.
- Right: Help Mode toggle, user profile icon (S).

Left Sidebar (Battery Workflow):

- Project Details
- Battery Iterations (selected, with expand/collapse arrow)
 - Design & Material Specifications
 - Test Conditions
 - Precheck & Simulate
- View Results
- Utilities
 - Materials Database
 - Export Project Options

Main Content Area:

Battery Iterations
Scott's Generic Battery > More heat

Design Iterations ⓘ

Search

[COMPARE BATTERIES](#)

	Iteration	Simulations	Status	Modified	
○	New Battery (baseline) The generic build of the battery.	• Room temperature: Simulation has completed ↗ • High temperature: Simulation has completed ↗	View-only	Thu Jun 22 2023	ACTIONS ⋮
●	More heat The generic build of the battery, but this time with more heat.	• Room temperature: Simulation in progress ↗ • High temperature: Simulation in progress ↗	View-only	Thu Jun 22 2023	ACTIONS ⋮

Rows per page: 10 1-2 of 2 < >



TABS v6 highlights: Simulations run in cloud-computing resources, with multiple simultaneous simulations possible

TABS

MY MATERIALS DATABASEMY PROJECTSDOCUMENTATIONSYSTEM PREFERENCES

Battery Workflow

Project Details

Battery Iterations

Design & Material Specifications

Test Conditions

Precheck & Simulate

View Results

Utilities

Materials Database

Export Project Options

3x4 in0.2 lbs2.5 in9 in

Rows per page: 101-1 of 1

Test Conditions

Name	Heat Balance	Current	Voltage
Room temperature	12 kcal	3 A	5 V
High temperature	12 kcal	3 A	5 V

Rows per page: 101-2 of 2

Simulation Log

Room temperature: Simulation has completed6/22/2023 12:51:05 PM

UUID649496e10e9dc2d9a9009ba9

Simulation Progress - 100%

VIEW RESULTSDELETE SIMULATION

High temperature: Simulation has completed6/22/2023 12:51:05 PM

Simulate

Estimated Simulation Run Time: 5 minutes

This will kick off full simulation(s) for any test conditions with a successful precheck. Editing specifications or test conditions at this point will invalidate any successful precheck and you'll have to re-run pre-check validation.

Click 'Simulate' to start the following simulations:
No eligible simulations to run. All prechecks must be passing. In progress or completed simulations can't be re-run.

Running Simulation Will Lock Battery Design

After running a simulation you will no longer be able to edit this battery iteration's design. Any test condition being run will also be locked. You can still clone or create new test conditions for the current battery iteration from 'Test Conditions'. You can also clone this battery iteration from the 'Battery Iterations' tab at any time before or after simulation runs to create a new editable battery.

Simulate

BackNext

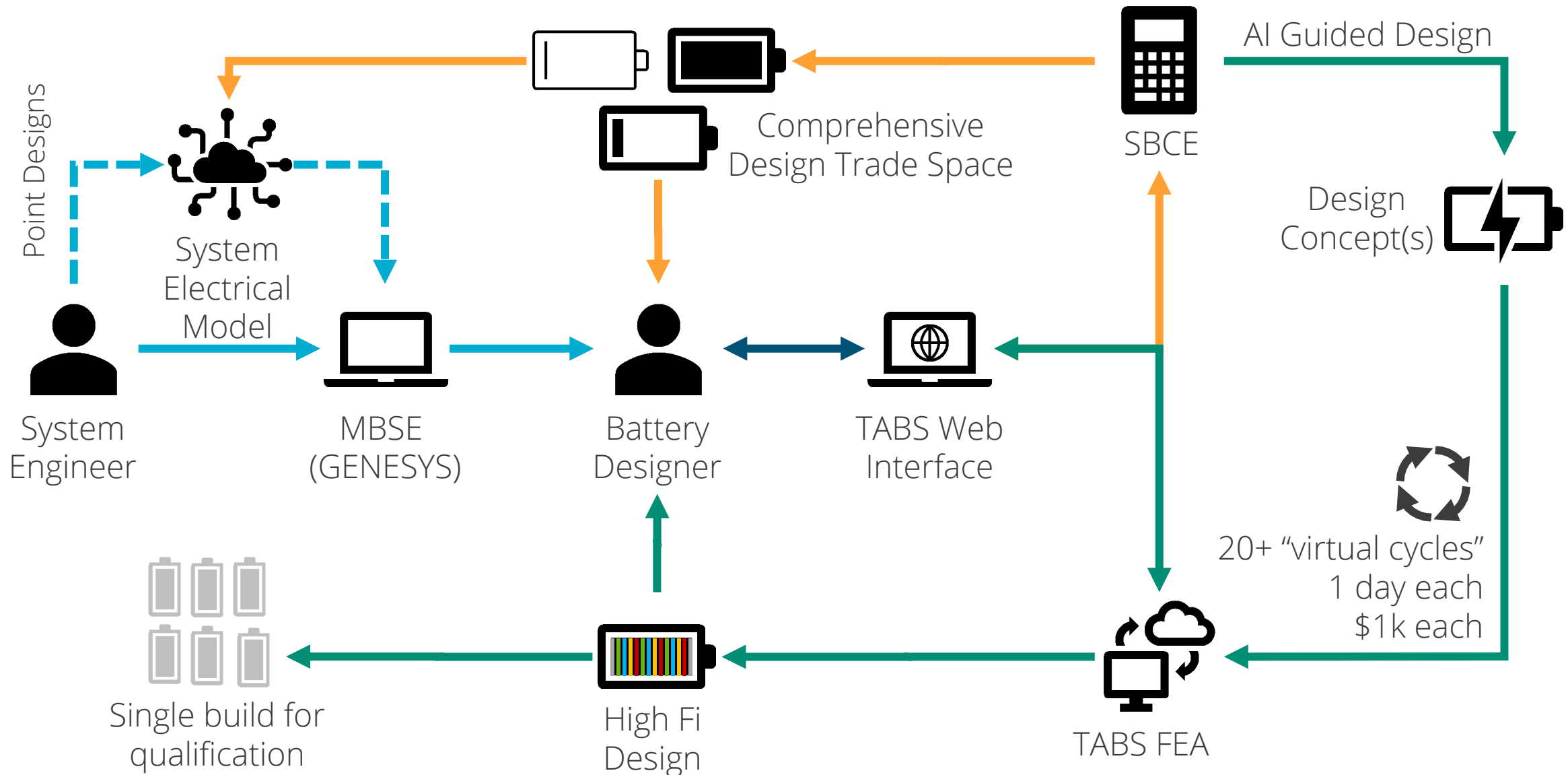


TABS v6 highlights: Results visualized in-browser, with comparison between battery iterations and test conditions

The screenshot displays the TABS v6 web application interface. The browser address bar shows the URL: `tabs-dev.sandia.gov/result?battery=649497d40e9dc2d9a9009bdb`. The application has a dark theme with a green accent color. The top navigation bar includes links for "MY MATERIALS DATABASE", "MY PROJECTS", "DOCUMENTATION", and "SYSTEM PREFERENCES". A "Help Mode" button with a user icon is on the right. The left sidebar, titled "Battery Workflow", contains sections for "Project Details", "Battery Iterations" (with a dropdown arrow), and "Utilities". The "View Results" option under "Battery Iterations" is highlighted in green. The main content area is titled "Simulation Results" and shows the path "Scott's Generic Battery > More heat". It features a "Simulations" panel on the left with checkboxes for "Room temperature" and "High temperature" under two categories: "New Battery (baseline)" and "More heat". Two toggle switches are present: "Display all Exodus Viewers" and "Display Simulations In One Chart". The main plot area is currently empty, displaying the text "Select a simulation from left panel to begin."



Future State: Fully-Integrated Digital Workflow



Wow! How can I use TABS v6?



Initial TABS v6 capability development nearly complete

- Deployment at Sandia scheduled October 2023
- Deployment to external partners (DOD) scheduled early 2024
- Continual improvements through 2024 and beyond

TABS v6 will be available to U.S. government organizations and their contractors

- License requirements and costs depends on your organization and deployment details

Contact Scott A. Roberts for more information:

- NIPR: sarober@sandia.gov,
SIPR: sarobers@sandia.doe.sgov.gov,
JWICS: Scott.Roberts@doe.ic.gov
- Phone: (505) 844-7957



Backup

Light mode

TABS

MY MATERIALS DATABASEMY PROJECTSDOCUMENTATIONSYSTEM PREFERENCES

Help Mode

Battery Workflow

Project Details

Battery Iterations

Design & Material Specifications

Test Conditions

Precheck & Simulate

View Results

Utilities

Materials Database

Export Project Options

Design & Material Specifications

Scott's Generic Battery > More heat

Schematic View3D View

Assign Materials

Open AllClose All

Unit Selection

Inches

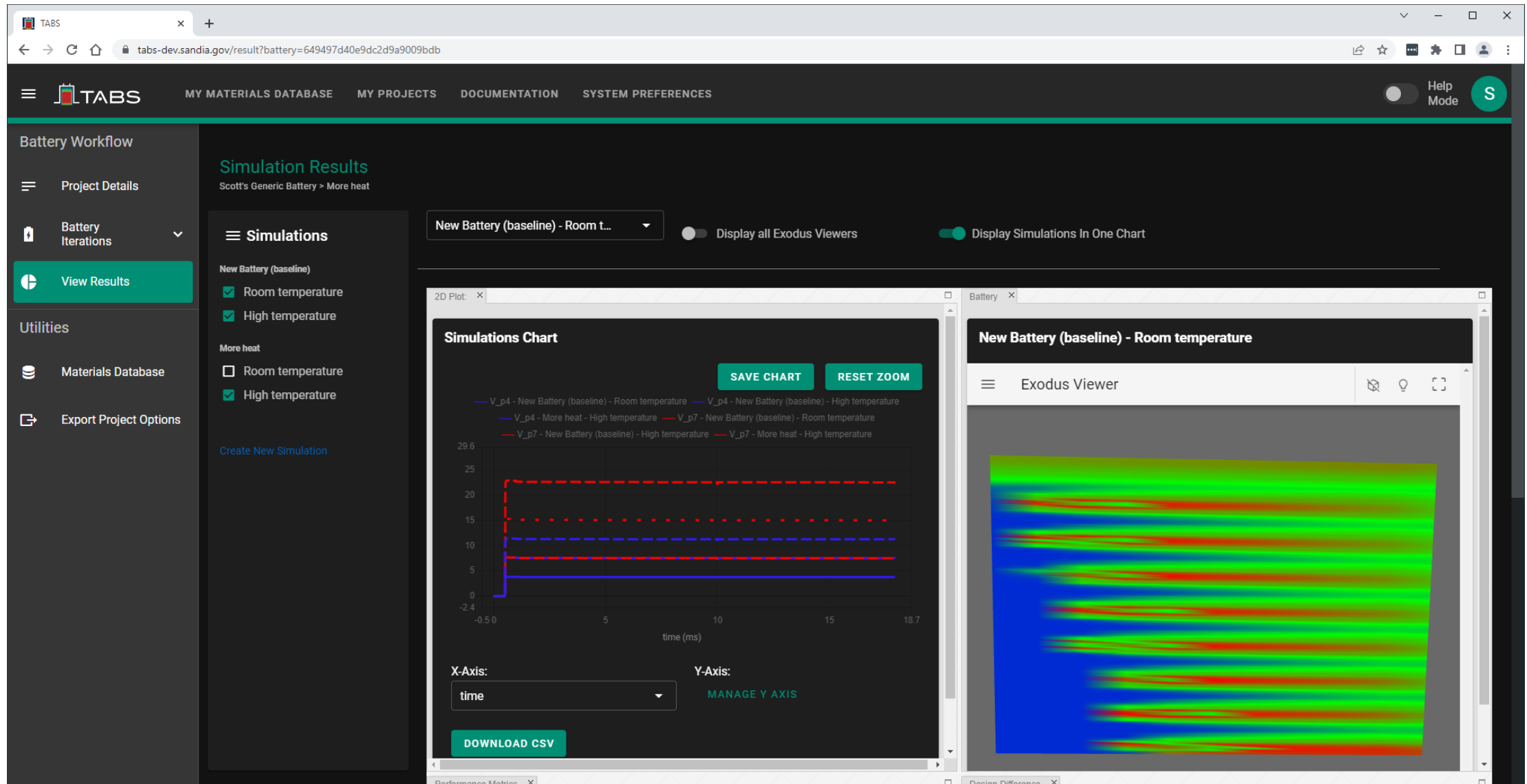
Conversions may cause a decrease in accuracy.

Stack Group and Layer Configuration

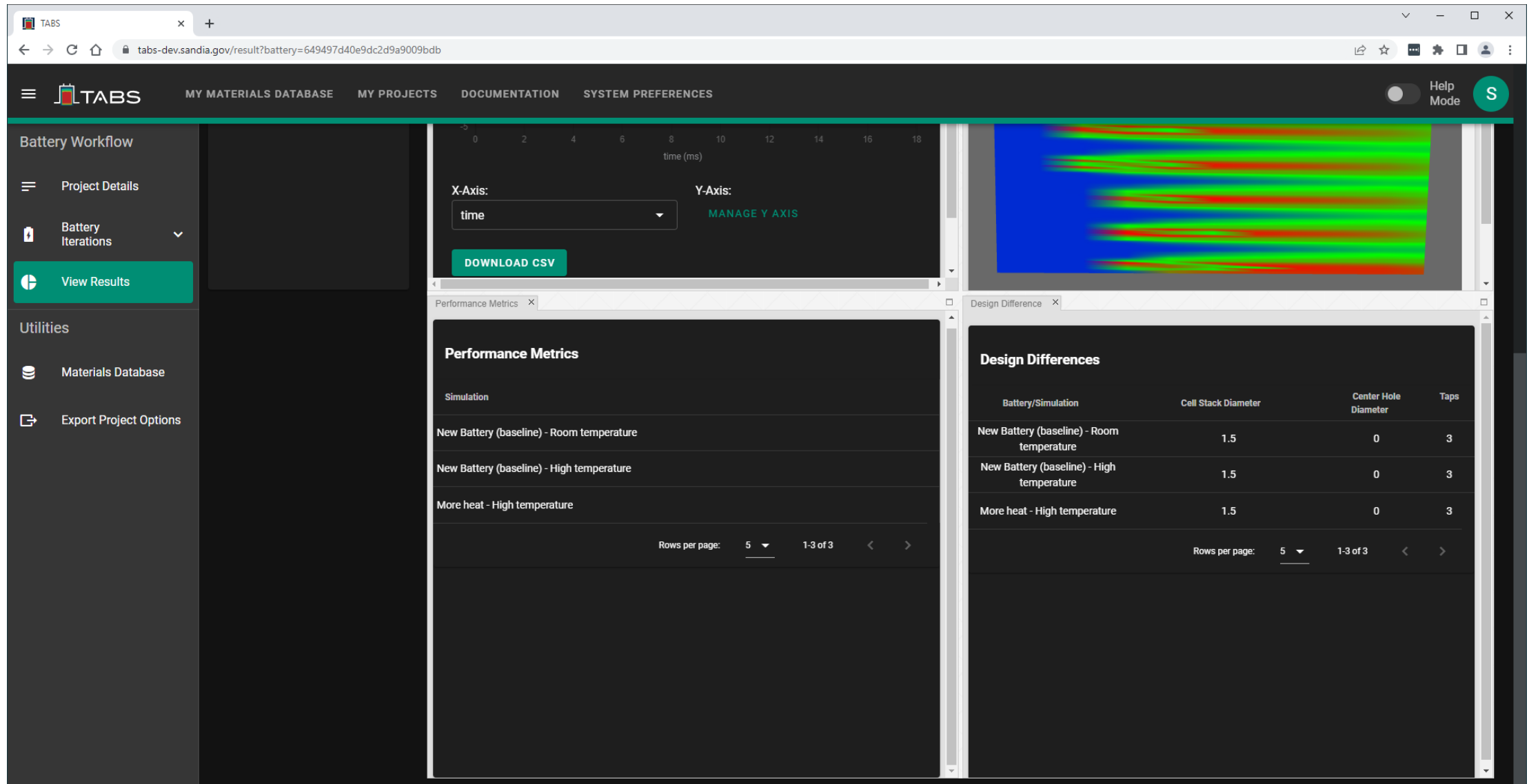
Wrap Configuration

Material	Thickness (in)
HEATPAPER	0.002
FIBRFRX WRAP 40	0.03
GLASS TAPE	0.005
FIBRFRX WRAP 40	0.03

Results - comparison



Results - metrics



Database - filter

TABS

MY MATERIALS DATABASEMY PROJECTSDOCUMENTATIONSYSTEM PREFERENCES

Battery Workflow

Project Details

Battery Iterations

View Results

Utilities

Materials Database

Export Project Options

Project Materials Database

Battery: Scott's Generic Battery

Add NewFind and Replace Materials

Filters

Clear Filters

☒ My Favorites

☒ Reference Materials

☒ New Materials

Material Location

☐ Header/Base

☒ Stack

☐ Wrap

☐ Container

Material Function

☐ Separator

☒ Anode

☐ Cathode

☐ Heat Sources

☐ Collector

☐ Insulation

☐ Electrolyte

Composition

☐ Pure

☐ Composite

Search for material

Open AllClose All

★ Favorite Materials (0)

📄 Scott's Generic Battery Materials (1)

ANODEflooded LiCl-KCl 5

👤 My Materials (0)

🌐 Reference Materials (7)

ANODEflooded LiCl-KCl 5

ANODEflooded LiBr-LiCl-LiF 25

ANODEflooded LiBr-KBr-LiCl 5

ANODE (70% LI, 30%B)

ANODE_LiSi45

ANODEflooded LiBr-KBr-LiCl 15

ANODE

View-only reference material. Click 'Clone' below to edit material.

★ ANODEflooded LiCl-KCl 5

Anode - Li(Si), 45%Li, flooded 5% LiCl-KCl

CloneEditDeleteManage Material

Material Properties

General

General Properties

Properties

SpecificHeat

Tensor Thermal Conductivity

Attributes

Density

Solid

Liquid

DH

BurnTime

IdealCapacity

CellVoltage

CaloriesPerGram

SpecificHeat

SpecificHeat

Index	Temperature	Value
0	100.4	0.185895
1	133.7	0.26009
2	178.5	0.333335
3	228.7	0.38929
4	324.8	0.44515
5	453.7	0.496925
6	651.9	0.555205
7	870.1	0.624555

Value Reference

95% dry anode values, 5% LiCl-KCl values.

Uncertainty

None

Uncertainty Reference

None



Database – find and replace

The screenshot shows the 'Find and Replace' dialog in the TABS Materials Database. The interface is dark-themed with a teal header bar for the dialog. The left sidebar contains navigation options: Battery Workflow, Project Details, Battery Iterations, View Results, Utilities, Materials Database (selected), and Export Project Options. The main area is titled 'Find and Replace' and contains the following sections:

- Find:** (materials used in project) - HEATPELLET86-14
- Replace With:** (materials applicable to at least 1 location.) - HEATPELLET86-14 - b
- Locations in this project:** ☒ Stack - Cells Group(0) - Layer(0) - Repeats(15)

The central visualization shows a battery cell structure with 15 repeating units. The top unit is highlighted in red, and the bottom unit is highlighted in yellow. The right sidebar contains a 'Find and Replace Materials' button, a 'Delete' button, and a 'Manage Material' button. The bottom of the dialog has three buttons: 'CLOSE', 'REPLACE SELECTED', and 'REPLACE ALL'. The bottom status bar shows 'Reference Materials (50)' and 'CaloriesPerGram'.

Analysis parameters

The screenshot displays the TABS web application interface. The browser address bar shows the URL: `tabs-dev.sandia.gov/analysis?battery=6494902b0e9dc2d9a9009acd`. The application header includes the TABS logo and navigation links: MY MATERIALS DATABASE, MY PROJECTS, DOCUMENTATION, and SYSTEM PREFERENCES. A user profile icon with the letter 'S' and a 'Help Mode' toggle are also present.

The left sidebar contains a 'Battery Workflow' section with the following options: Project Details, Battery Iterations (expanded), Design & Material Specifications, Test Conditions (expanded), Thermal Boundary Conditions, Electrochemical Boundary Conditions, Analysis Parameters (selected), Precheck & Simulate, View Results, Utilities, Materials Database, and Export Project Options.

The main content area is titled 'Analysis Parameters' and shows the configuration for 'Scott's Generic Battery > New Battery (baseline) > Default Test Condition'. It features two tabs: 'Schematic View' (active) and '3D View'. The schematic view displays a battery cell diagram with various layers and components, including a red layer labeled '15'.

The right sidebar contains the 'Analysis Parameters' configuration panel, which includes the following settings:

- Simulation Time (s):** 60
- Time of Ignition (s):** 0
- Initial Battery Temperature:** 25 (Celsius)
- Ignite Heat Pellets Simultaneously:** ☒
- Simulation Type:** Thermal 2D + Electrochemical 1D (selected)
- Run Parameters:** [Show Advanced Options](#)

At the bottom of the right sidebar, there are 'Back' and 'Next' buttons.

Project details

The screenshot displays the TABS web application interface. The browser address bar shows the URL: `tabs-dev.sandia.gov/details?battery=6494902b0e9dc2d9a9009acd`. The application has a dark theme with a teal accent color.

Navigation Bar:

- Left: TABS logo, menu icon.
- Center: MY MATERIALS DATABASE, MY PROJECTS, DOCUMENTATION, SYSTEM PREFERENCES.
- Right: Help Mode toggle, user profile icon with 'S'.

Left Sidebar (Battery Workflow):

- Project Details (highlighted in teal)
- Battery Iterations (with a dropdown arrow)
- View Results

Left Sidebar (Utilities):

- Materials Database
- Export Project Options

Main Content Area:

Project Details

Scott's Generic Battery > New Battery (baseline)

Sensitivity Level

UUR [X] [v]

Project Name

Scott's Generic Battery

Project Description

A thermal battery made up by Scott Roberts.

Describing Battery Project

Technical Specifications / Battery Options

Battery Firing Configuration

☒ Side Fire

☐ Center Fire

Simulation Type
(which physics you're turning on)

☐ Thermal

☒ Thermal + Electrochemical