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

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TABS: The Thermally Activated Battery Simulator

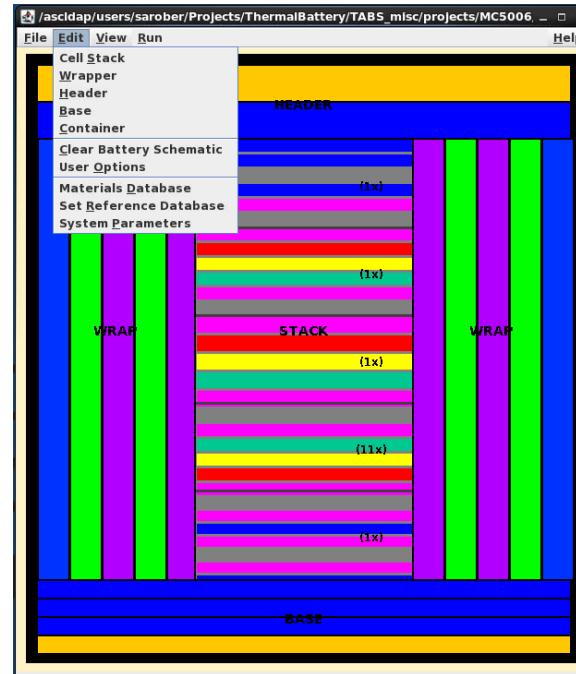
TABS design principles

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

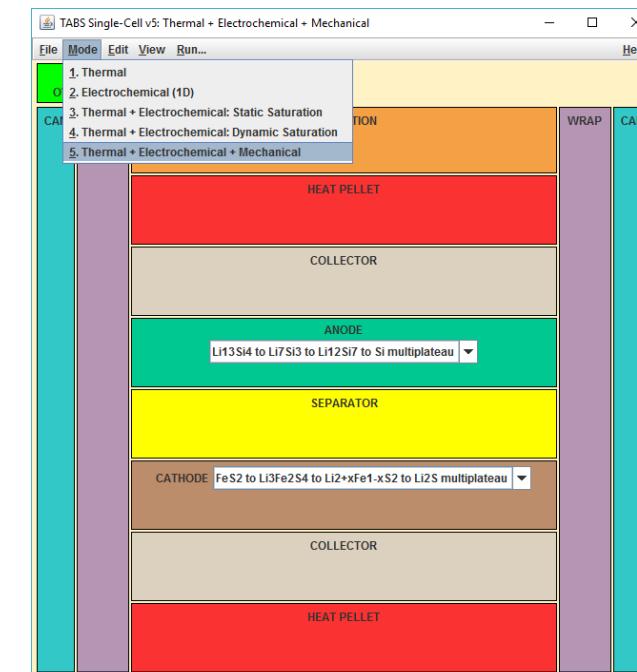
Present the user with the most **relevant quantities of interest**, yet enable them to explore more deeply

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



TABS-FB: Full Battery

- Thermal

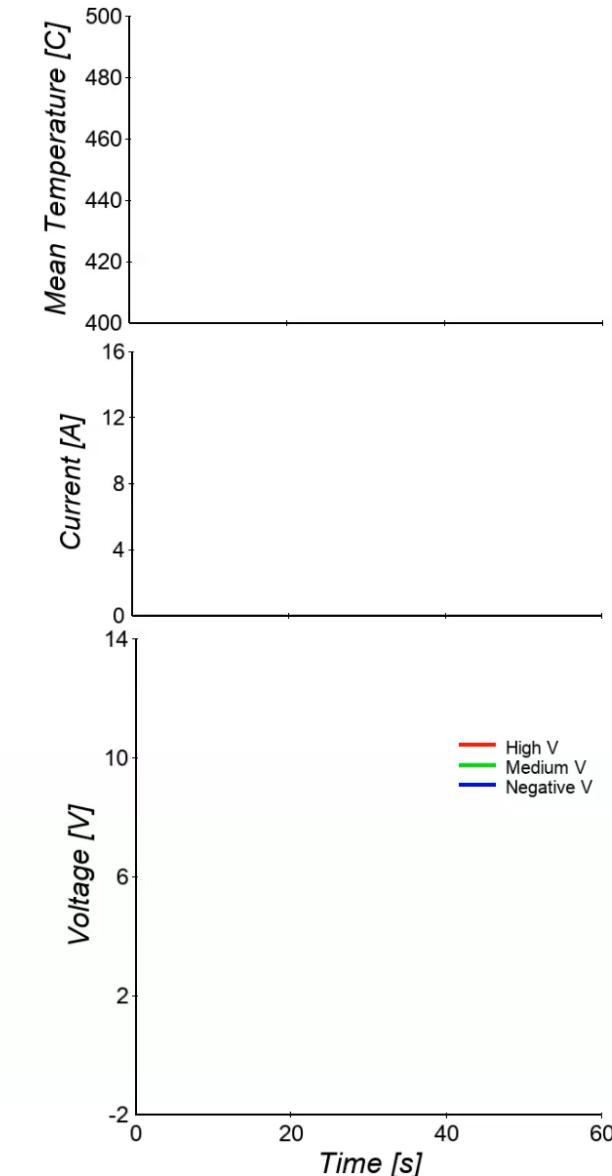
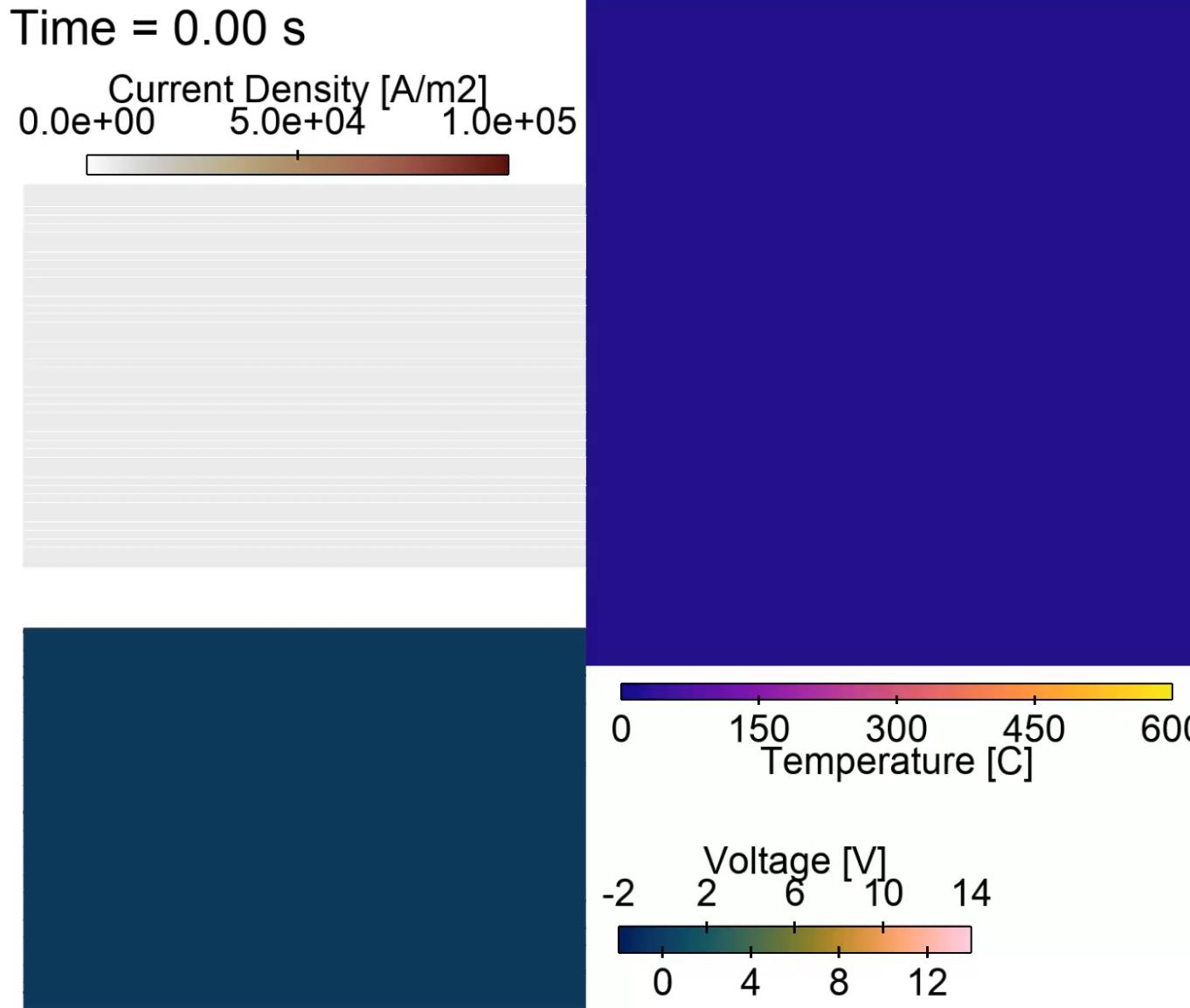


TABS-SC: Single Cell

- 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



So what's wrong with TABS?

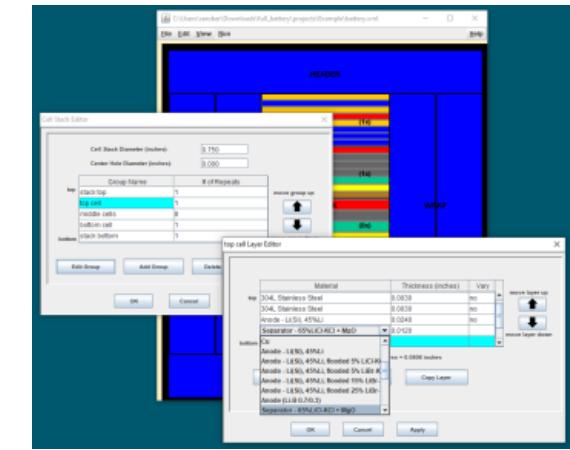


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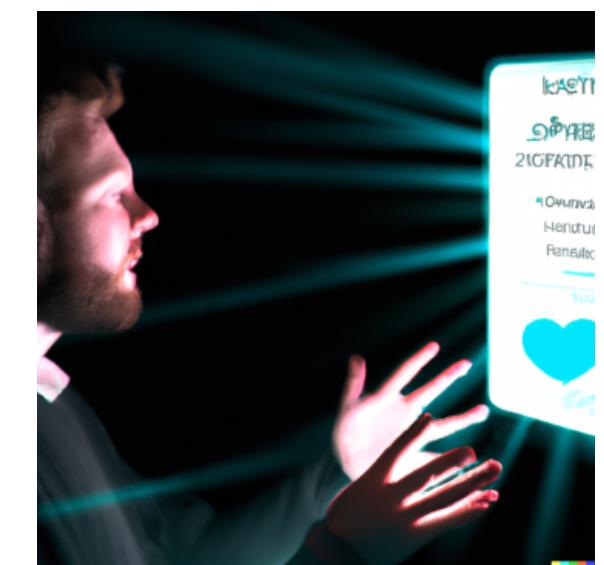
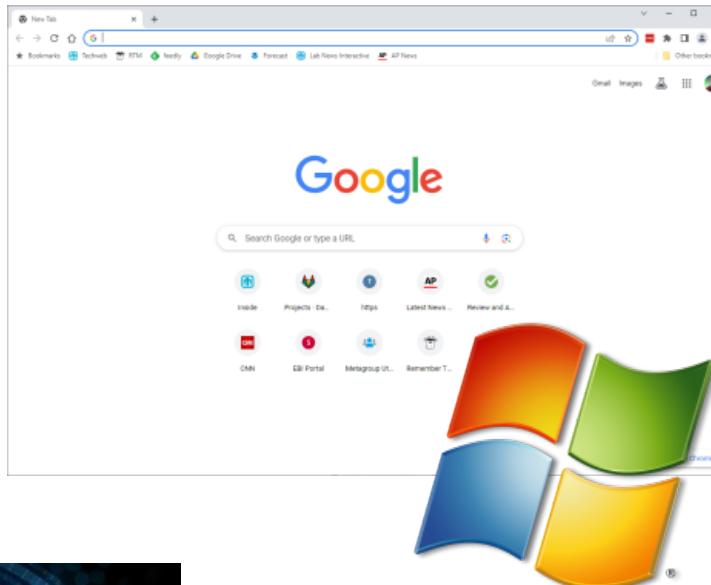




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TABS v6 designed from scratch to address prior deficiencies and provide an experience that delights our users

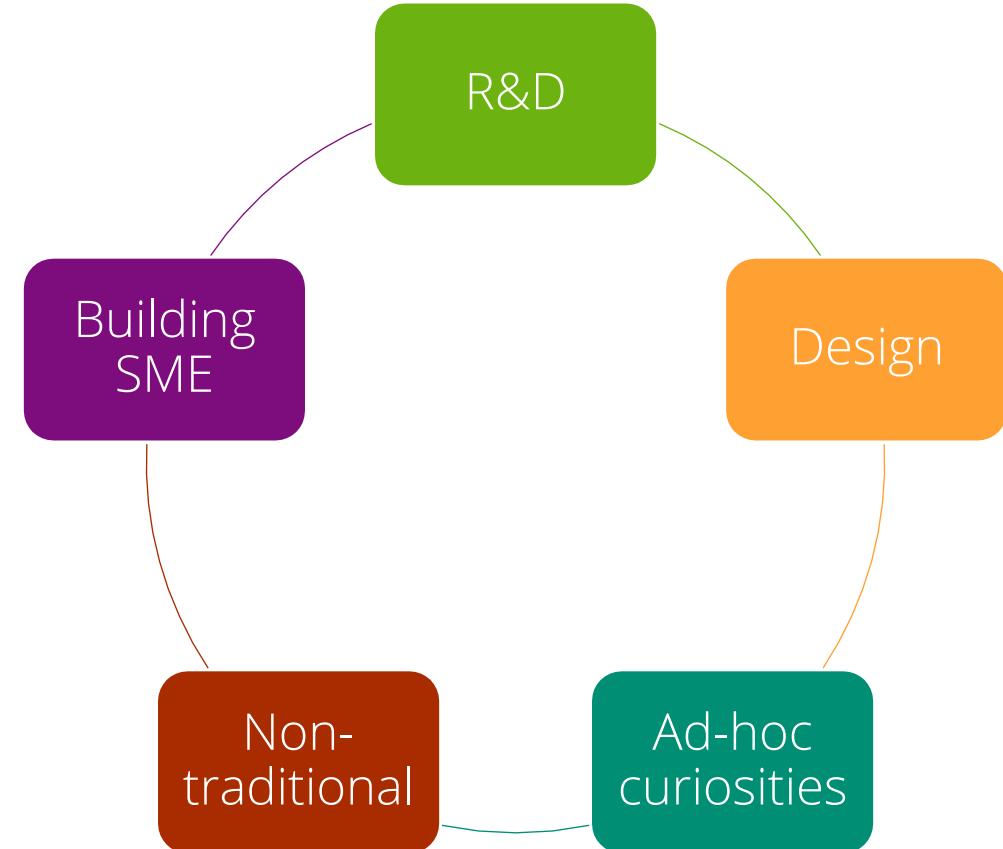


Embarked in foundational user experience research to design a tool that exceeds user's needs and desires

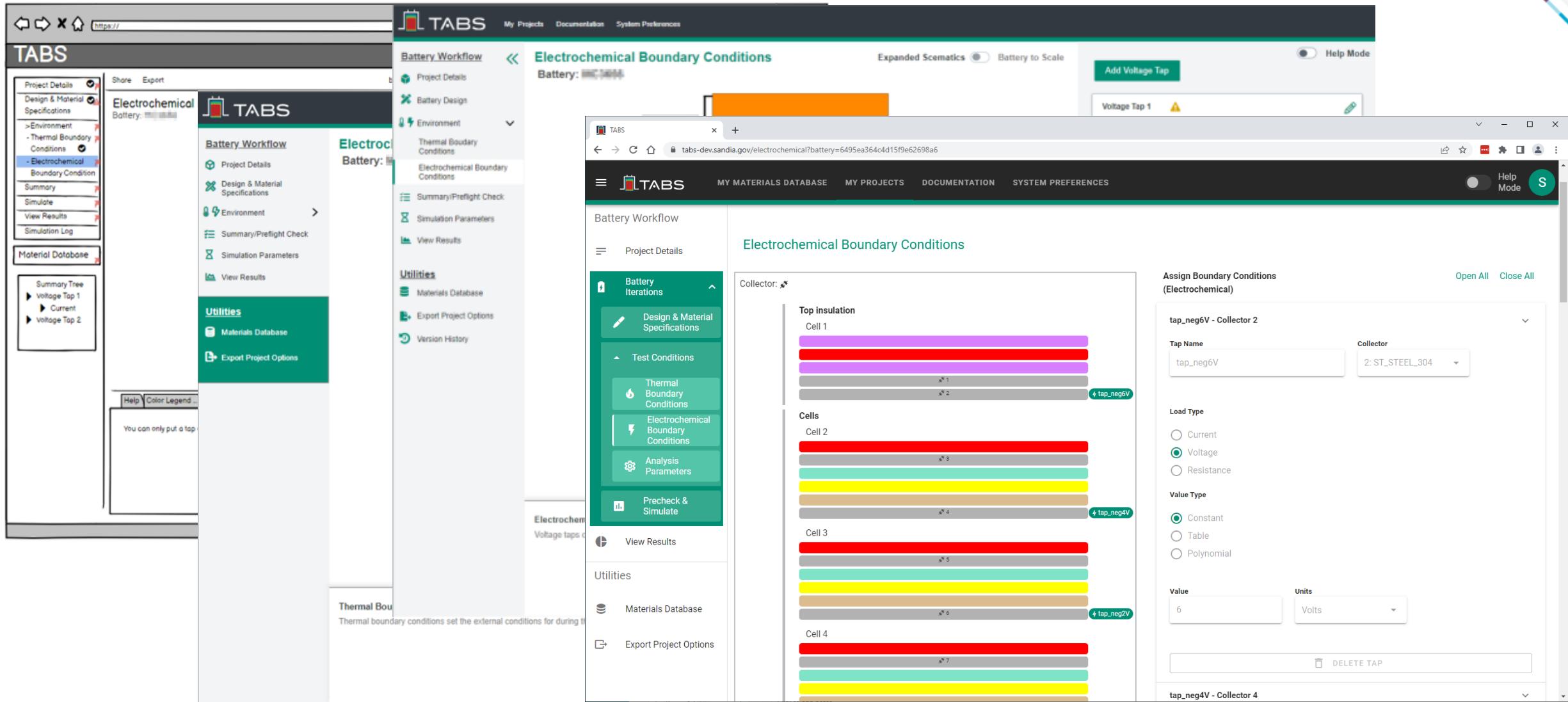
Interviewed current and prospective users (within Sandia, DOD, and AWE) to identify:



Identified 6 use cases:



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





TABS v6 highlights: Landing page with templates, recent projects

The screenshot shows the TABS v6 landing page with a dark theme. At the top, there is a navigation bar with tabs for 'MY MATERIALS DATABASE', 'MY PROJECTS', 'DOCUMENTATION', and 'SYSTEM PREFERENCES'. A 'Help Mode' toggle and a user profile icon are also present. The main content area is titled 'Welcome to TABS' and 'Thermally Activated Battery Simulation Tool'. It features three main sections: 'RECENT' (listing 'Scott's Generic Battery' with details: Owner, Modified Date: 6/22/2023, 12:50:57 PM, Create Date: 6/22/2023, 12:17:15 PM, and an 'ACTIONS' button), 'FAVORITES' (empty), and 'SHARED WITH ME' (empty). To the right, a 'Battery Templates' section is displayed, showing a search bar and a list of five 'FULL BATTERY' templates, each with a thumbnail image and a 'Created from a template of' link.

RECENT

FAVORITES

SHARED WITH ME

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 < >

Battery Templates

Search

FULL BATTERY

Created from a template of [REDACTED]

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

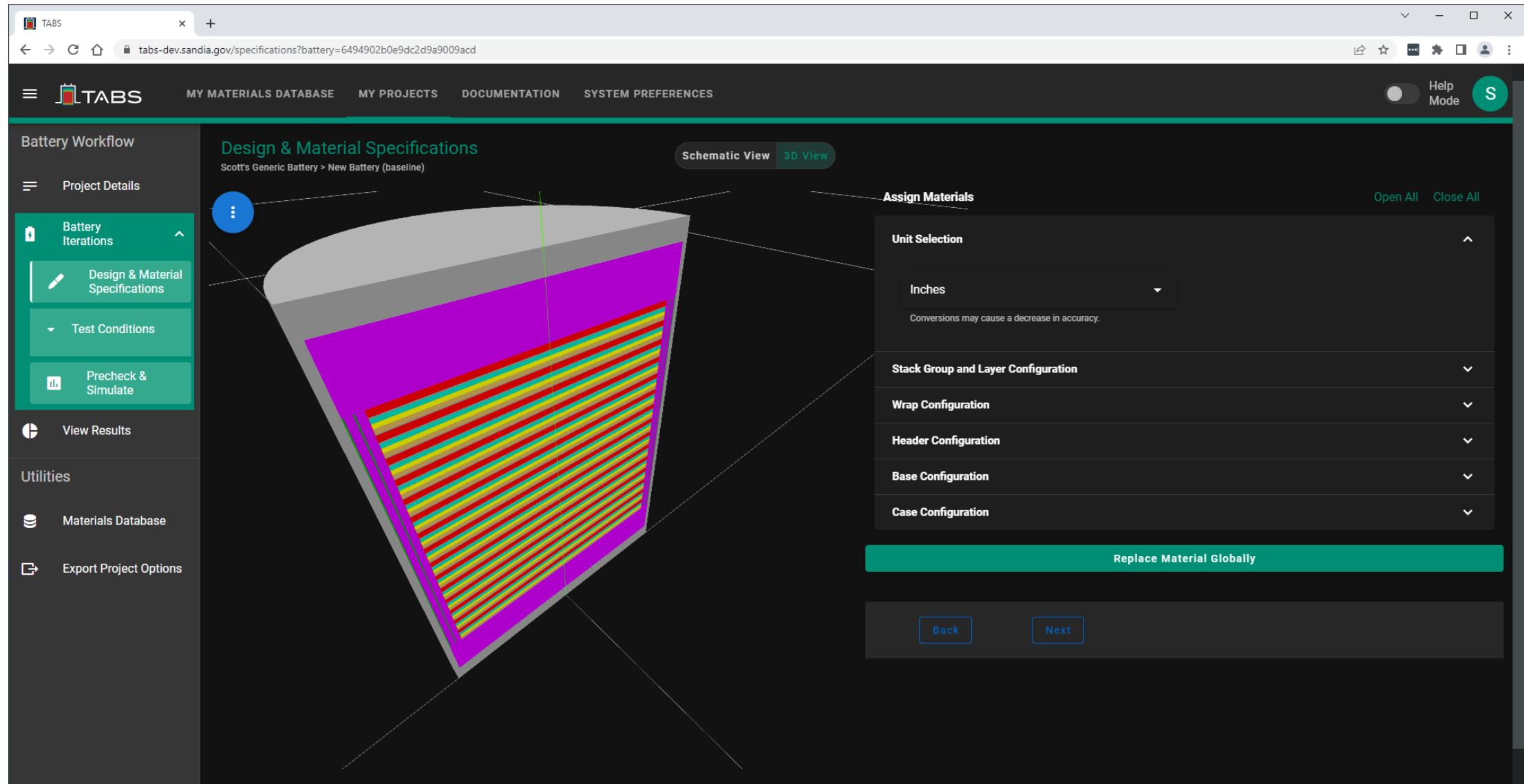
The screenshot shows the TABS v6 Materials Database interface. The left sidebar includes 'Project Details', 'Battery Iterations', and 'View Results'. Under 'Utilities', 'Materials Database' is selected. The main area features a 'Filters' sidebar with 'My Favorites', 'Reference', 'Materials', and 'New Materials' checked. A 'Search for material' bar is present. A central modal window displays a success message: 'HEATPELLET86-14 - b has been added' and 'HEATPELLET86-14 - b has been added to the Battery Scott's Generic Battery Project Materials'. It also says, 'You can make this material accessible to all your projects by using the "manage" button.' Below this, a 'Manage Material' button is shown. A 'My Materials' section indicates 'You are here' and lists 'Battery Project Materials'. A table lists material properties: IdealCapacity (6, 903, 0.205), CellVoltage (7, 960, 0.22), CaloriesPerGram (8, 985, 0.223), BurnFrontSpeed (9, 1010, 0.222), and MoleFractionLi. A note at the top right of the main area states: 'This material is accessible for the current project, but not currently in More heat'.

		Value	Uncertainty	Uncertainty Reference
	Value	0.105	None	
	Value	0.119	15%	Uncertainty
	Value	0.136		Uncertainty Reference
	Value	0.156		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/
	Value	0.172		
	Value	0.188		

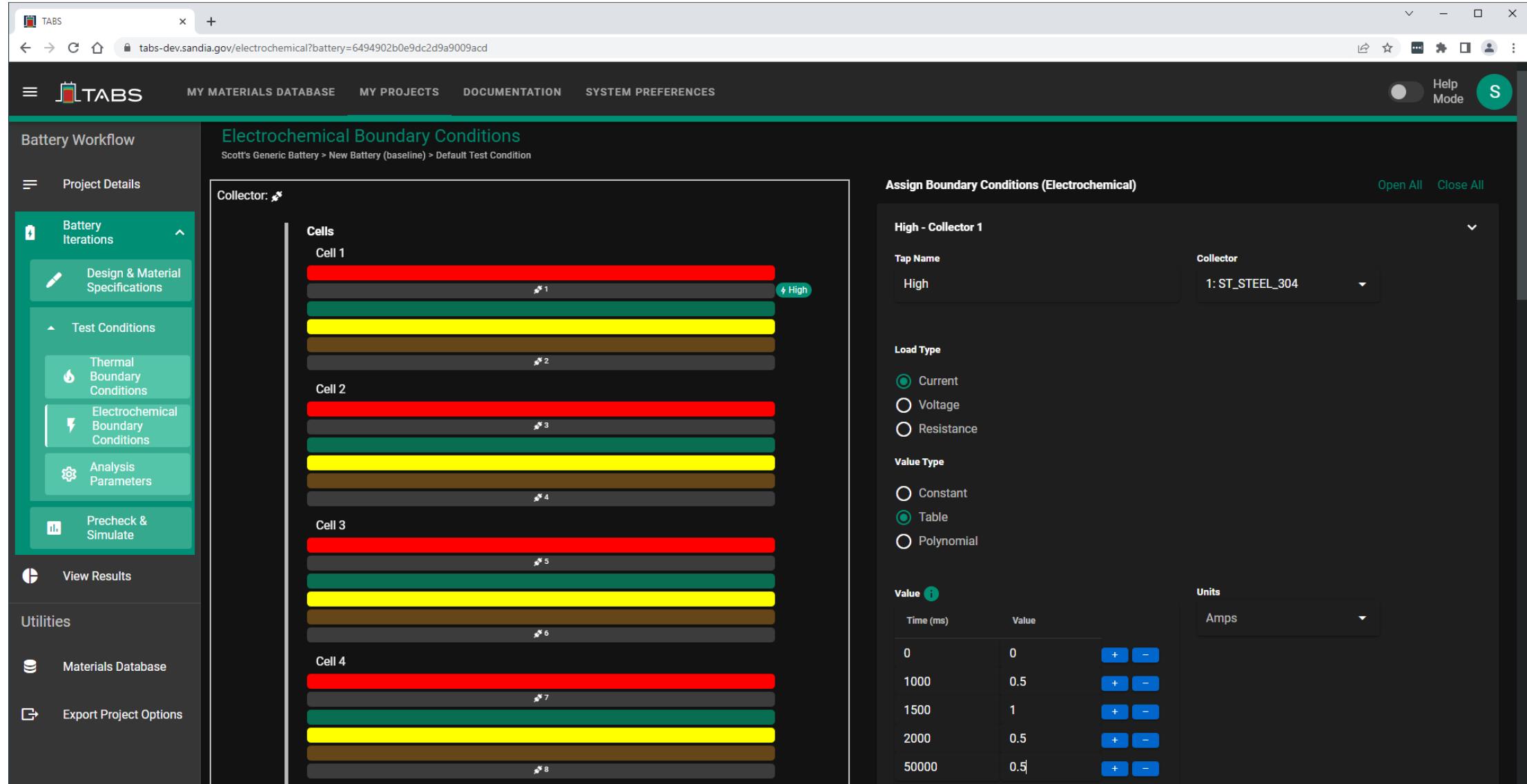
TABS v6 highlights: Building a battery from scratch in < 5 minutes

The screenshot shows the TABS v6 software interface for battery design. The main title is "Design & Material Specifications" for "Scott's Generic Battery > New Battery (baseline)". The interface includes a "Schematic View" (selected) and a "3D View" tab. On the left, a sidebar titled "Battery Workflow" lists "Project Details" (selected), "Battery Iterations" (with "Design & Material Specifications" highlighted), "Test Conditions", and "Precheck & Simulate". Other options include "View Results", "Utilities", "Materials Database", and "Export Project Options". The central area displays a schematic diagram of a battery cell with labels: "Case", "Header", "Wrap", "Stack", "Wrap", "Case", "Base", and "Case". To the right, the "Assign Materials" panel is open, showing "Unit Selection" (Inches) and "Stack Group and Layer Configuration" (with five items: "Wrap Configuration", "Header Configuration", "Base Configuration", and "Case Configuration", each with a red exclamation mark icon). A large green "Replace Material Globally" button is at the bottom. Top navigation includes "MY MATERIALS DATABASE", "MY PROJECTS", "DOCUMENTATION", "SYSTEM PREFERENCES", "Help Mode", and a user profile icon.

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



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



Electrochemical Boundary Conditions
Scott's Generic Battery > New Battery (baseline) > Default Test Condition

Assign Boundary Conditions (Electrochemical)

High - Collector 1

Tap Name	Collector
High	1: ST_STEEL_304

Load Type

Current

Voltage

Resistance

Value Type

Constant

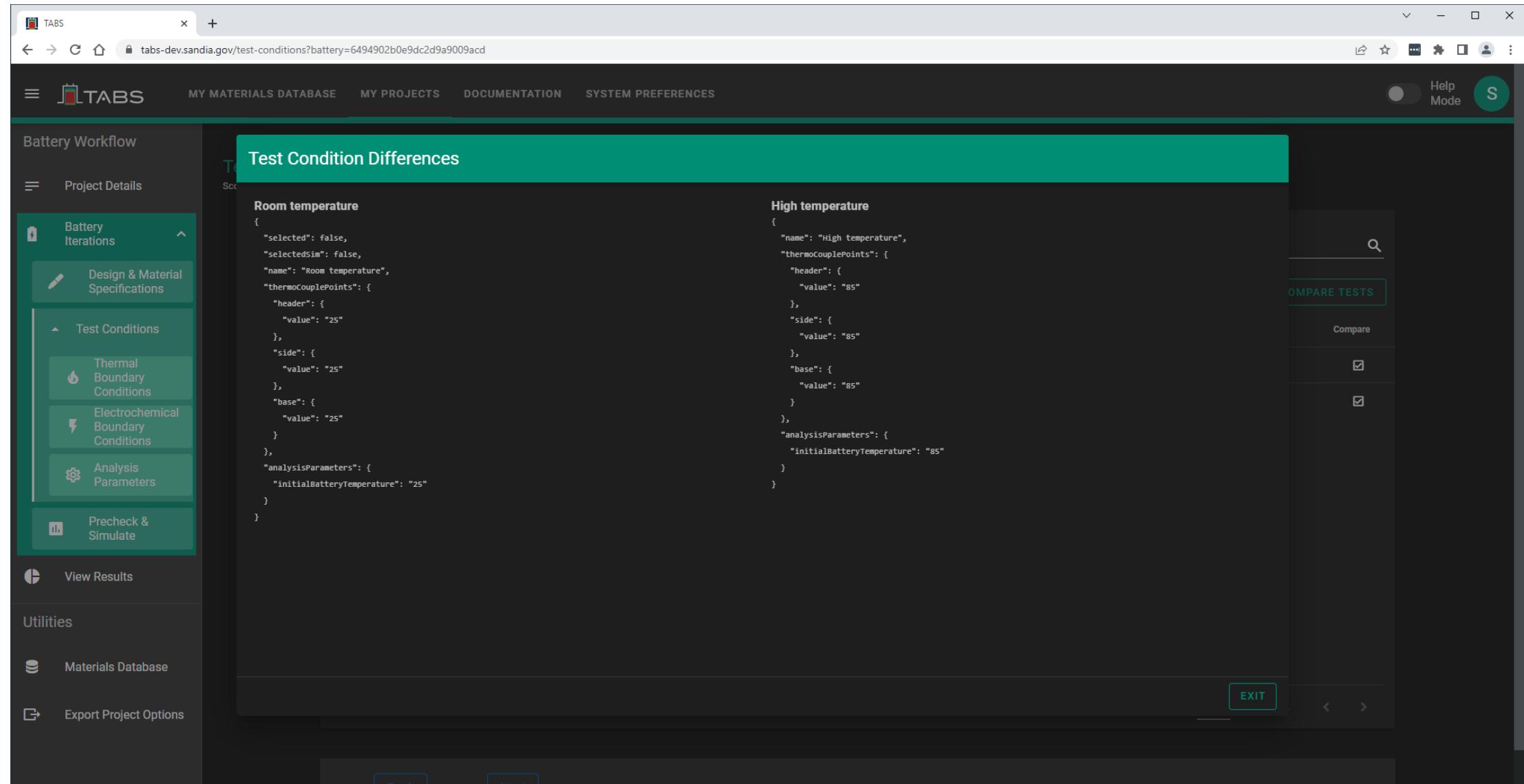
Table

Polynomial

Value

Time (ms)	Value	Units
0	0	Amps
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

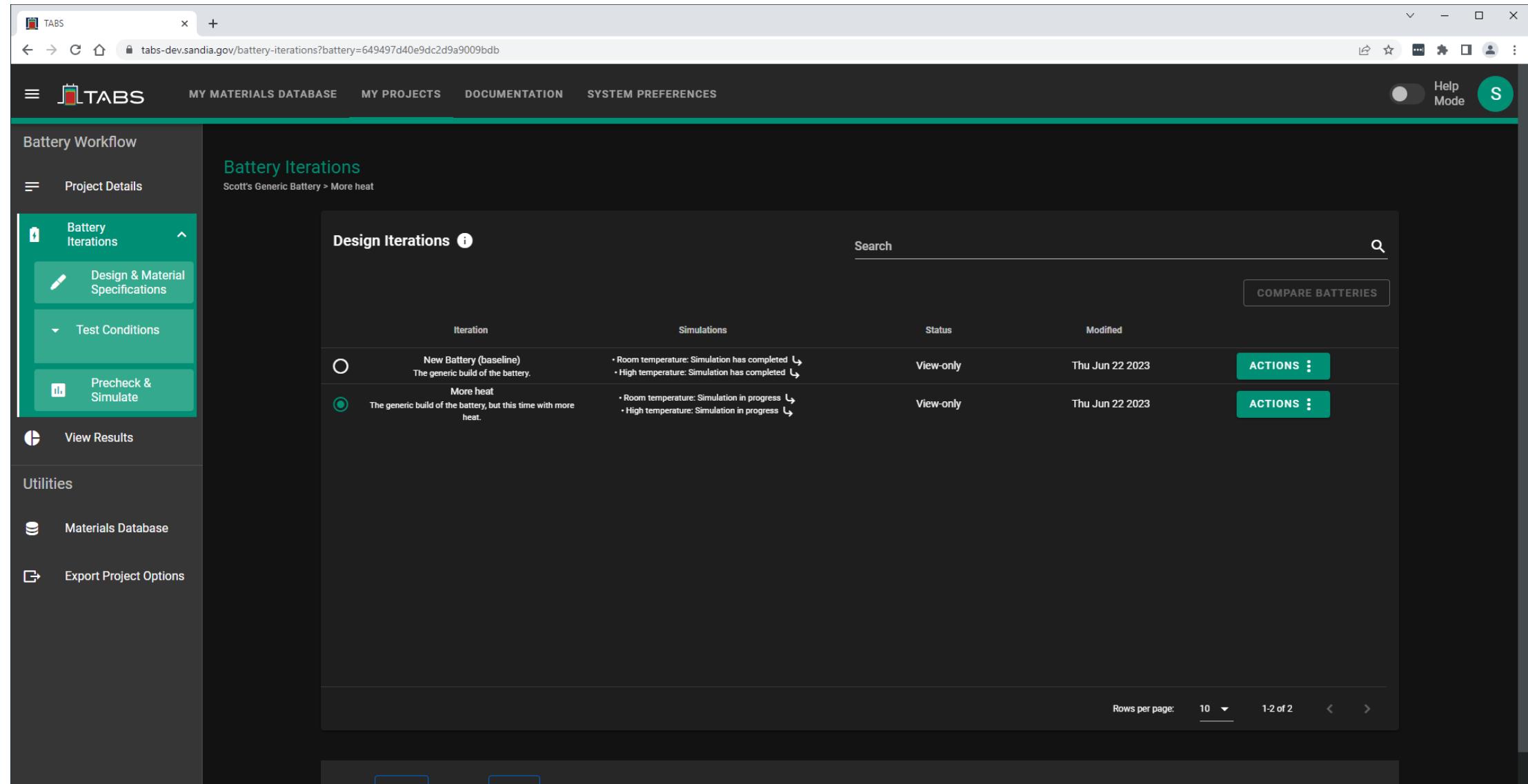


The screenshot shows the TABS v6 software interface. The top navigation bar includes tabs for 'MY MATERIALS DATABASE', 'MY PROJECTS', 'DOCUMENTATION', and 'SYSTEM PREFERENCES'. A 'Help Mode' toggle and a user profile icon are also present. The left sidebar, titled 'Battery Workflow', contains sections for 'Project Details', 'Battery Iterations', 'Test Conditions' (which is currently selected), 'Analysis Parameters', and 'Precheck & Simulate'. The main content area is titled 'Test Condition Differences' and displays two JSON objects side-by-side: 'Room temperature' and 'High temperature'. Both objects define 'thermocouplePoints' with 'header' and 'side' values of 25 and 85 respectively, and an 'analysisParameters' section with an 'initialBatteryTemperature' of 25. A 'COMPARE TESTS' button is visible on the right. The bottom right corner of the window has an 'EXIT' button.

```
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"
  }
}
```

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



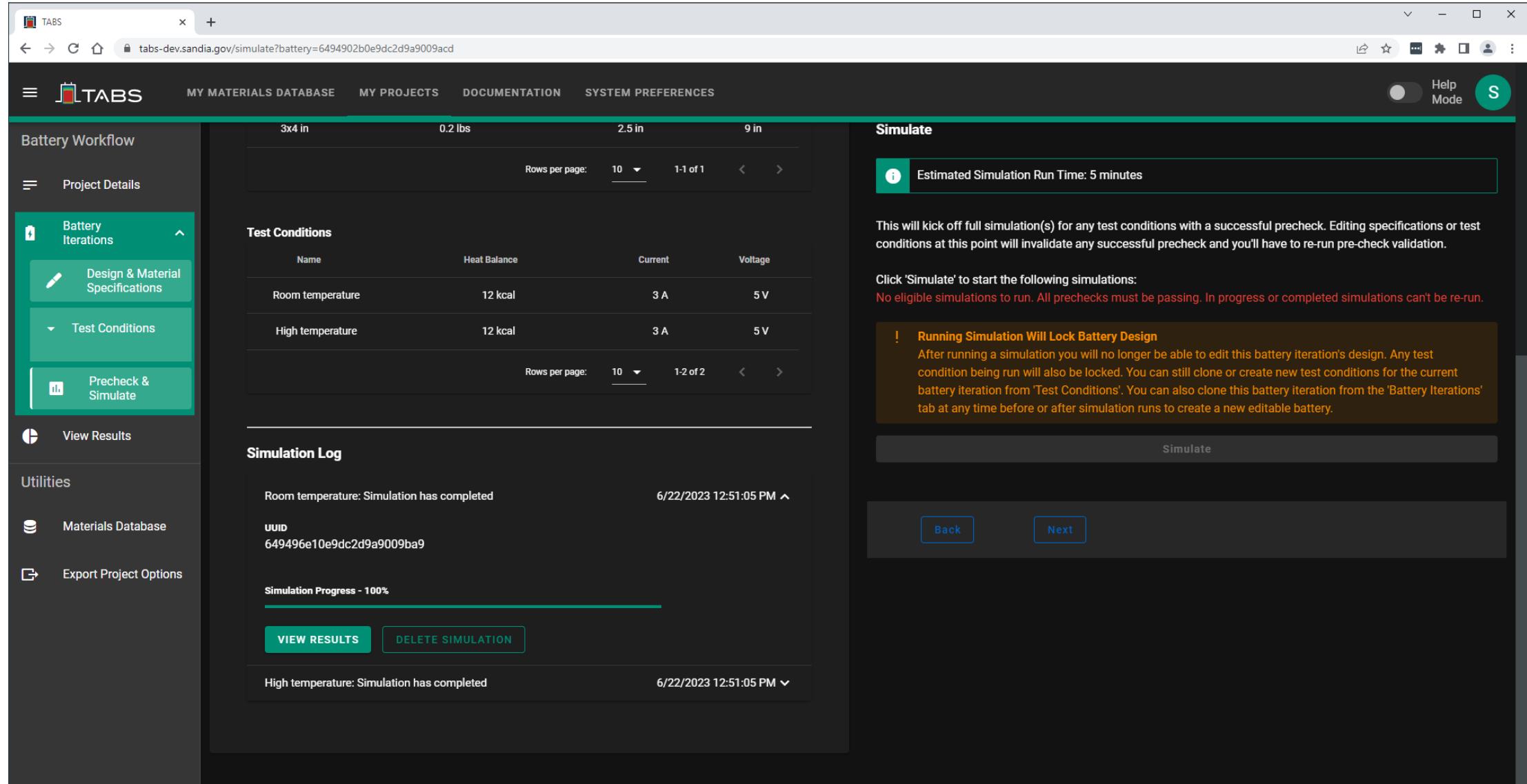
Battery Iterations
Scott's Generic Battery > More heat

Design Iterations

Iteration	Simulations	Status	Modified	Actions
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

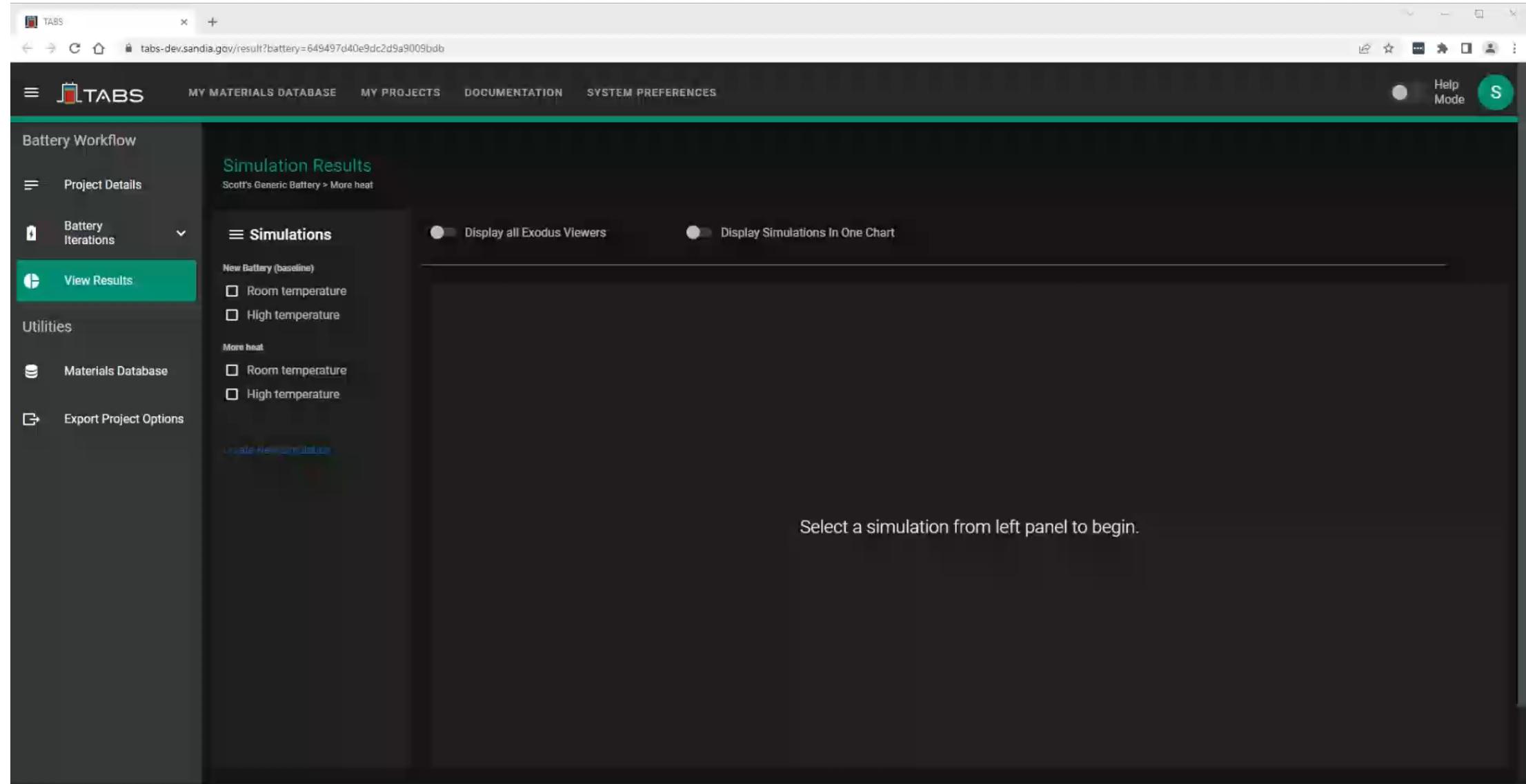
Rows per page: 10 1-2 of 2

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



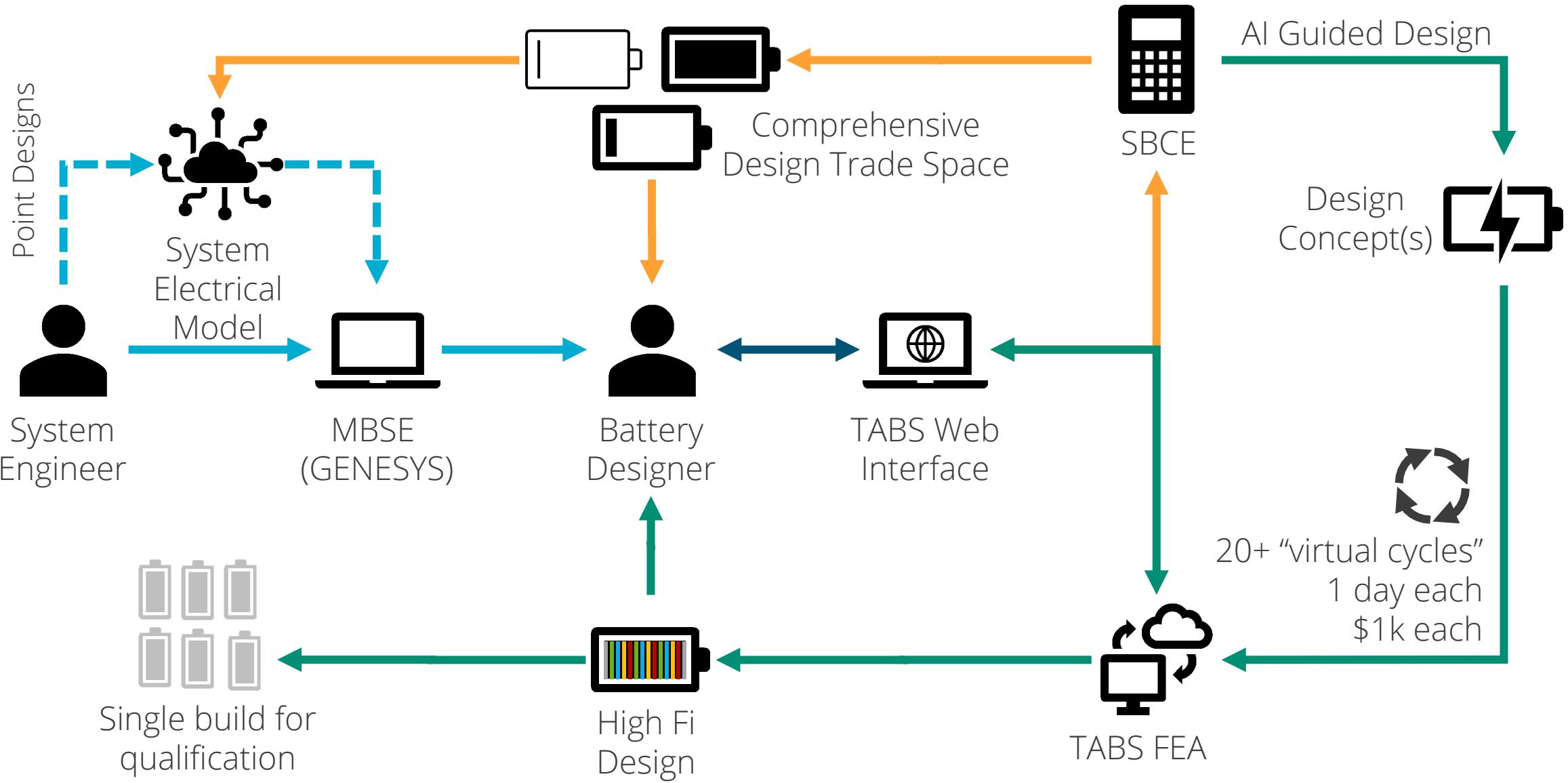
The screenshot shows the TABS v6 web interface for battery simulation. The left sidebar includes 'Project Details' (Battery Iterations, Design & Material Specifications, Test Conditions, Precheck & Simulate, View Results), 'Utilities' (Materials Database, Export Project Options), and a 'Battery Workflow' section. The main content area shows 'Test Conditions' for 'Room temperature' and 'High temperature' with parameters: 12 kcal, 3 A, 5 V. The 'Simulation Log' section shows two completed simulations: 'Room temperature: Simulation has completed' on 6/22/2023 at 12:51:05 PM and 'High temperature: Simulation has completed' on the same date. A 'Simulate' button is present, along with 'Back' and 'Next' buttons. A note states: '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.' A warning box notes: 'Running Simulation Will Lock Battery Design' and '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.'

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



The screenshot shows the TABS v6 web interface. The top navigation bar includes tabs for 'TABS', 'MY MATERIALS DATABASE', 'MY PROJECTS', 'DOCUMENTATION', 'SYSTEM PREFERENCES', 'Help Mode' (with a green 'S' icon), and a user profile icon. The left sidebar, titled 'Battery Workflow', contains 'Project Details', 'Battery Iterations' (selected), and 'View Results' (highlighted in green). The 'Utilities' section includes 'Materials Database' and 'Export Project Options'. The main content area is titled 'Simulation Results' for 'Scott's Generic Battery > More heat'. It features a 'Simulations' section with two radio buttons: 'Display all Exodus Viewers' (selected) and 'Display Simulations In One Chart'. Below this are two groups of simulation options: 'New Battery (baseline)' and 'More heat', each with 'Room temperature' and 'High temperature' checkboxes. A 'Create New Simulation' button is at the bottom. A text overlay at the bottom right says '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

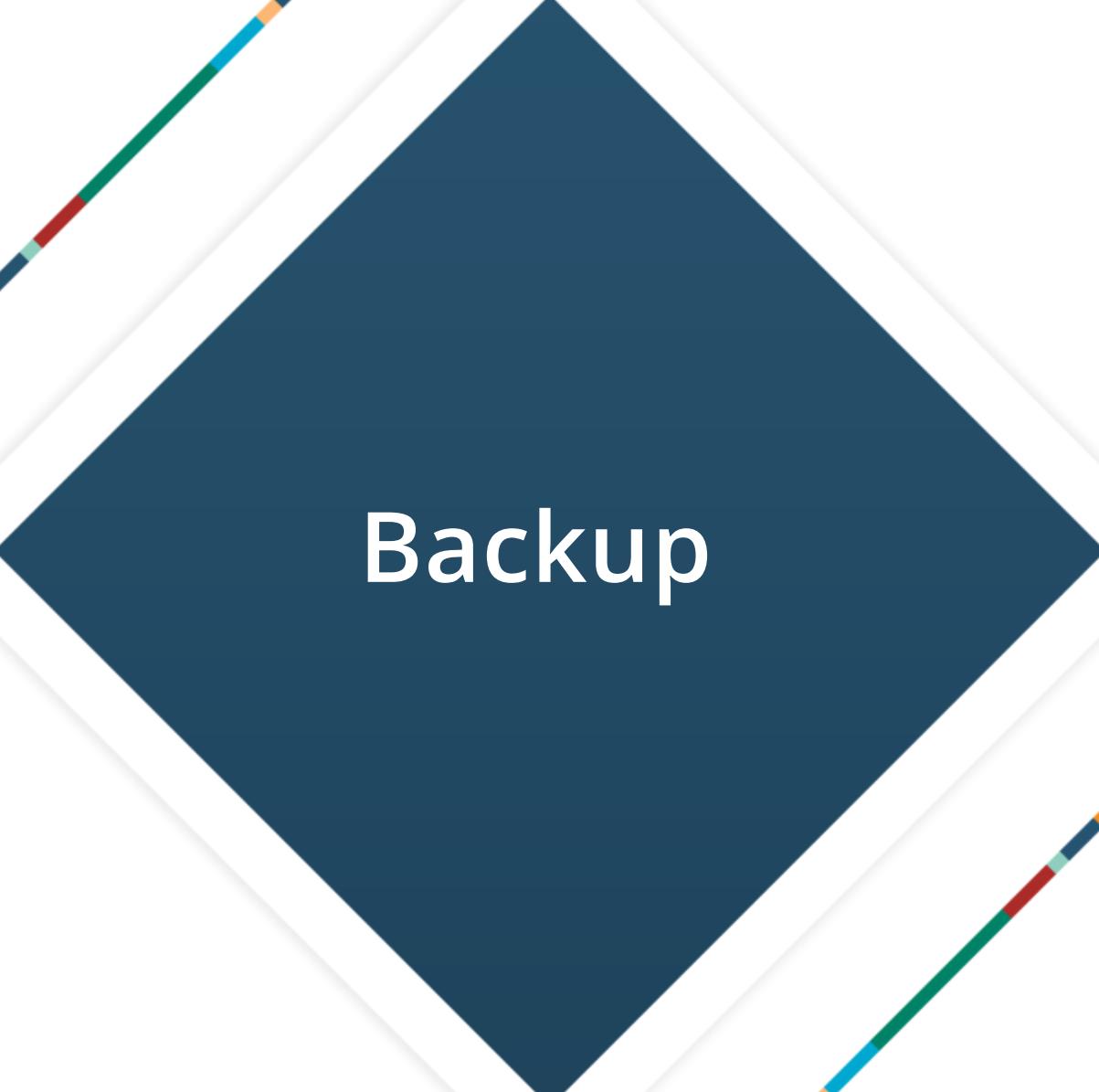
TABS v6 will be available to U.S. government organizations and their contractors

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

Contact Scott A. Roberts for more information:

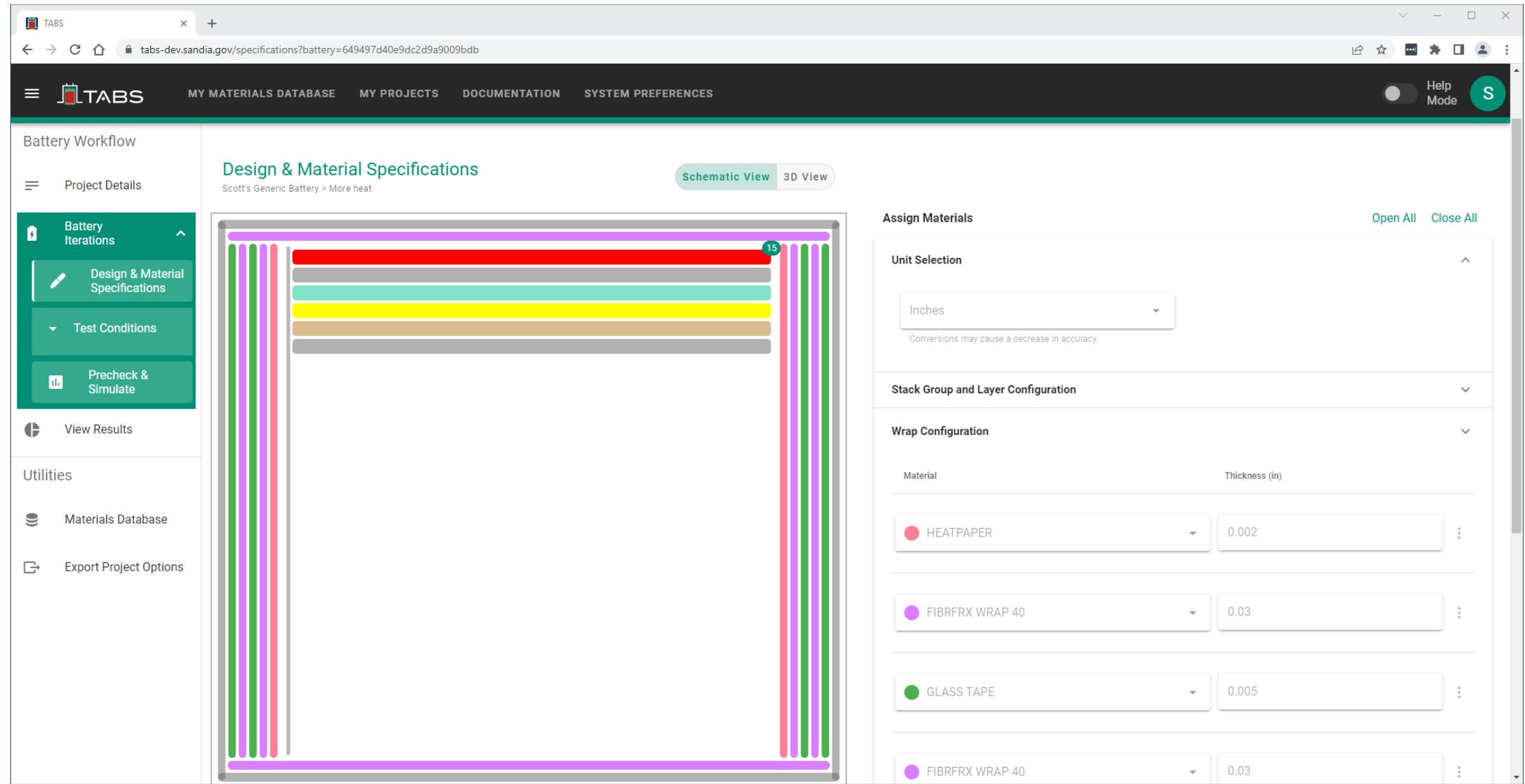
- NIPR: sarober@sandia.gov,
SIPR: sarobers@sandia.doe.sgov.gov,
JWICS: Scott.Roberts@doe.ic.gov
- Phone: (505) 844-7957





Backup

Light mode



Design & Material Specifications
Scott's Generic Battery > More heat

Schematic View **3D View**

Assign Materials

Unit Selection
Inches

Conversions may cause a decrease in accuracy.

Stack Group and Layer Configuration

Wrap Configuration

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

Open All **Close All**

Results - comparison

TABS x + tabs-dev.sandia.gov/result?battery=649497d40e9dc2d9a9009bdb Help Mode S

MY MATERIALS DATABASE MY PROJECTS DOCUMENTATION SYSTEM PREFERENCES

Battery Workflow

Project Details

Battery Iterations

View Results

Utilities

Materials Database

Export Project Options

Simulation Results

Scott's Generic Battery > More heat

Simulations

New Battery (baseline) - Room t...

Room temperature

High temperature

More heat

Room temperature

High temperature

2D Plot: x

Display all Exodus Viewers

Display Simulations In One Chart

Simulations Chart

SAVE CHART RESET ZOOM

29.6
25
15
10
5
0
-2.4

time (ms)

X-Axis: time
Y-Axis: MANAGE Y AXIS

DOWNLOAD CSV

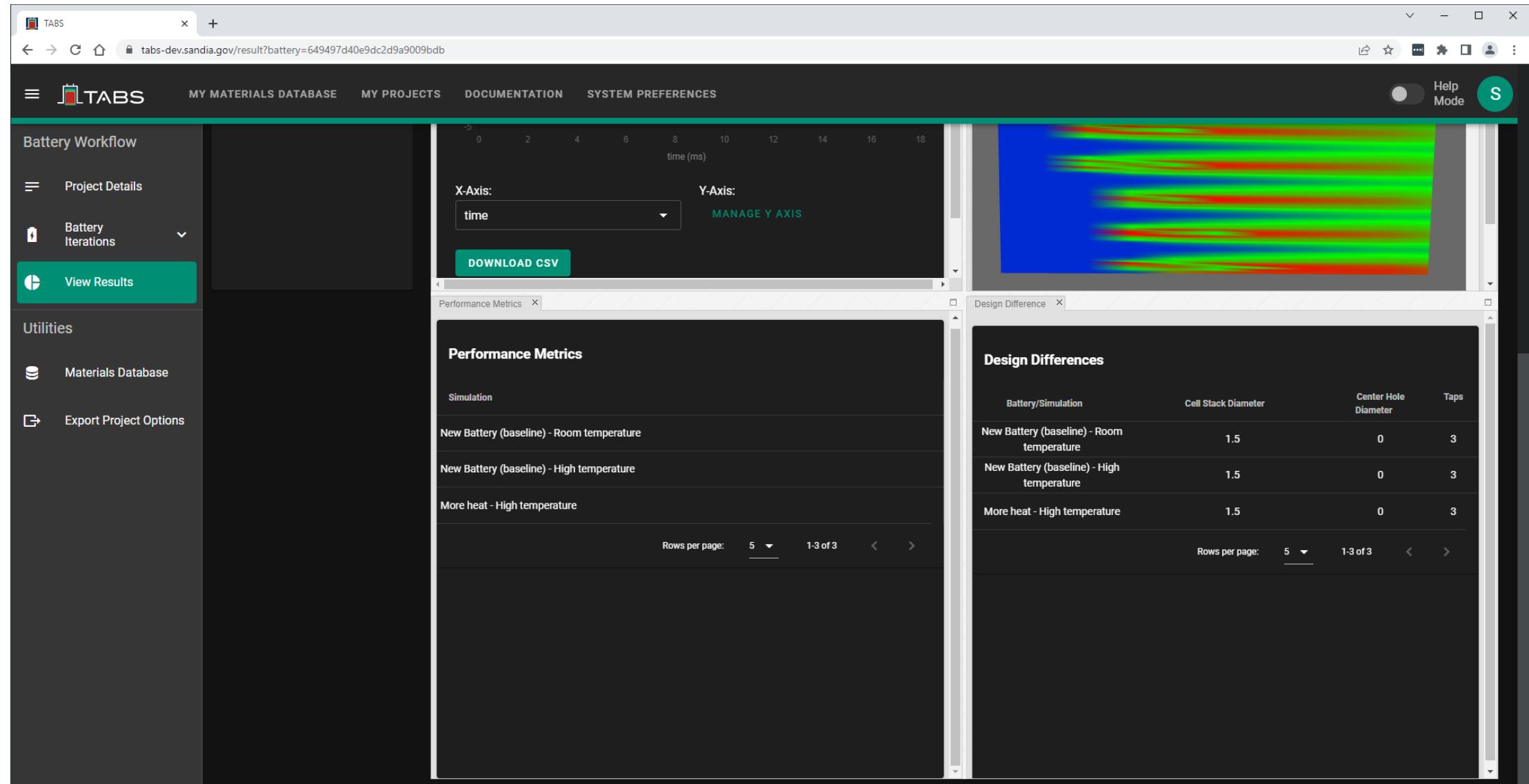
New Battery (baseline) - Room temperature

Exodus Viewer

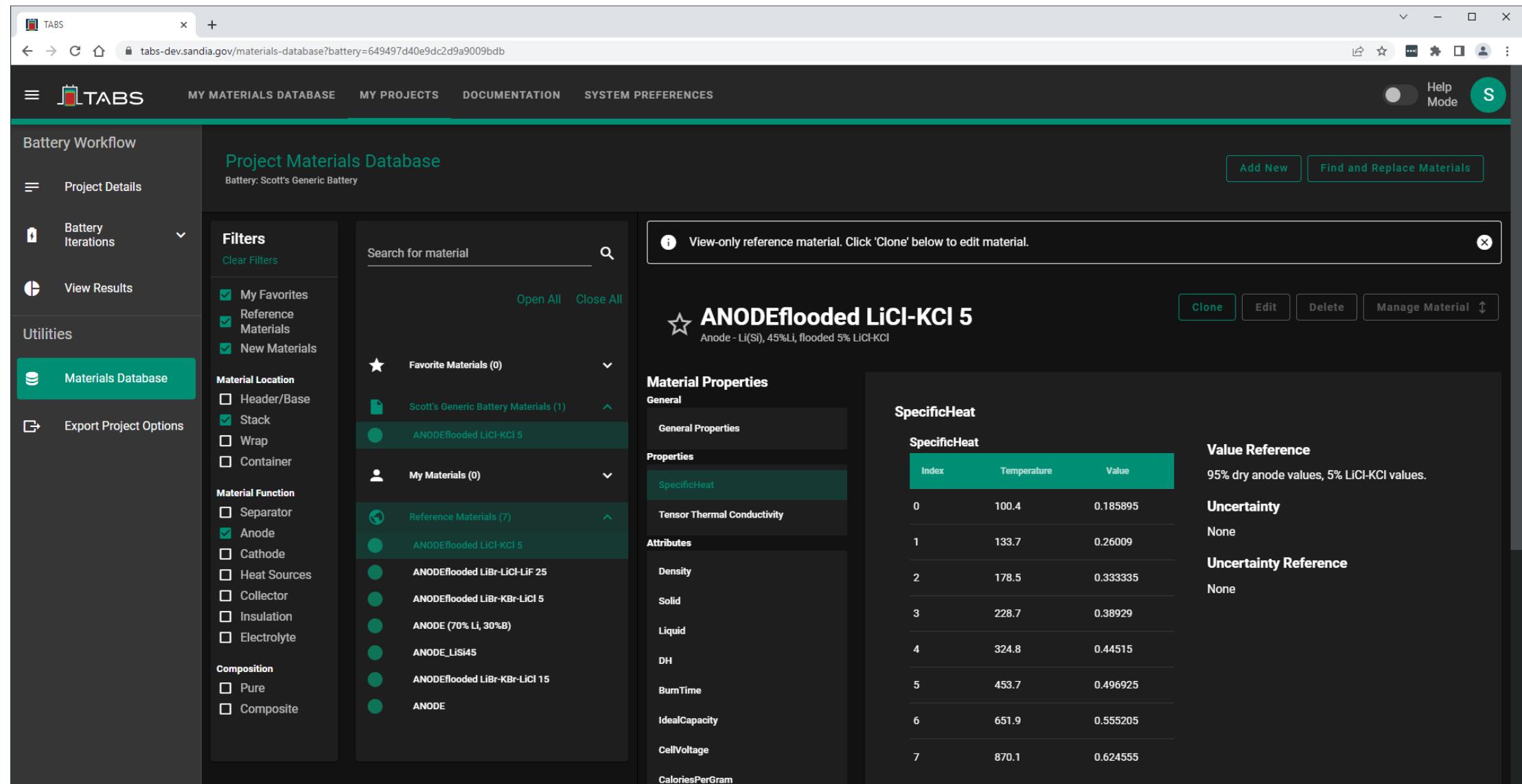
Performance Metrics x

Design Difference x

Results - metrics



Database - filter



The screenshot shows the TABS Project Materials Database interface. The left sidebar includes 'Battery Workflow' (Project Details, Battery Iterations, View Results), 'Utilities' (Materials Database, Export Project Options), and a 'Filters' section with checkboxes for 'My Favorites', 'Reference', 'Materials', and 'New Materials'. The main area displays the 'Project Materials Database' for 'Battery: Scott's Generic Battery'. A search bar and a note about view-only reference material are present. The central focus is on the 'ANODEflooded LiCl-KCl 5' material, which is identified as 'Anode - Li(Si), 45%Li, flooded 5% LiCl-KCl'. The 'Material Properties' section shows 'General' properties like 'General Properties', 'Properties' (with 'SpecificHeat' selected), and 'Attributes'. A table for 'SpecificHeat' lists values for index 0 to 7. To the right, sections for 'Value Reference' (95% dry anode values, 5% LiCl-KCl values) and 'Uncertainty' (None) are shown. The bottom right corner features a large 'S' icon.

Project Materials Database
Battery: Scott's Generic Battery

Filters

Search for material

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

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

Material Properties

General

Properties

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

TABS

tabs-dev.sandia.gov/materials-database?battery=649497d40e9dc2d9a9009bdb

MY MATERIALS DATABASE MY PROJECTS DOCUMENTATION SYSTEM PREFERENCES Help Mode S

Find and Replace

Find a specific material used in your project's battery design and replace with another material.

Find: (materials used in project)
HEATPELLET86-14

Replace With: (materials applicable to at least 1 location.)
HEATPELLET86-14 - b

Project: Scott's Generic Battery **Battery:** More heat

Locations in this project:
Stack - Cells Group(0) - Layer(0) - Repeats(15)

Reference
Glaub, J. E. "Thermal Properties of Iron/Potassium Perchlorate Heat-Generating Compounds." U.S. Patent 3,173,317, Monsanto Research Corp: St. Louis, MO (1965) and National Bureau of Standards and Technology. "NIST Standard Reference Database 16: Book Standard Reference Data." (2016). URL: www.nist.gov/chemistry/

Find and Replace Materials

Project: Scott's Generic Battery Battery: More heat

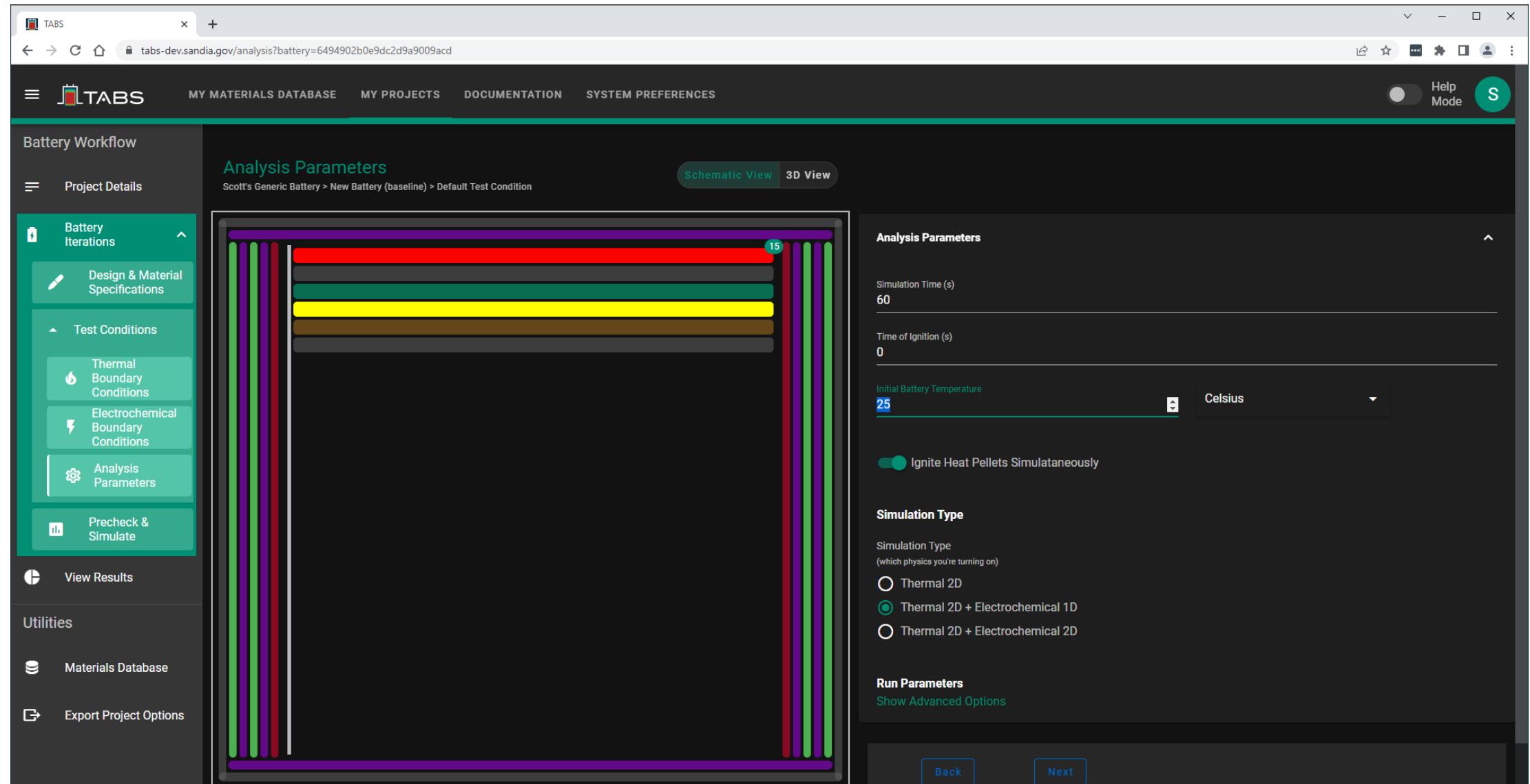
Stack - Cells Group(0) - Layer(0) - Repeats(15)

CLOSE REPLACE SELECTED REPLACE ALL

Reference

er, D. E., Glaub, J. E. "Thermal Properties of Iron/Potassium Perchlorate Heat-Generating Compounds." U.S. Patent 3,173,317, Monsanto Research Corp: St. Louis, MO (1965) and National Standards and Technology. "NIST Standard Reference Database 16: Book Standard Reference Data." (2016). URL: www.nist.gov/chemistry/

Analysis parameters



The screenshot shows the TABS software interface for battery analysis. The top navigation bar includes tabs for 'TABS', 'MY MATERIALS DATABASE', 'MY PROJECTS', 'DOCUMENTATION', 'SYSTEM PREFERENCES', 'Help Mode' (with a 'S' icon), and a user profile. The left sidebar, titled 'Battery Workflow', contains sections for 'Project Details' (selected), 'Battery Iterations', 'Design & Material Specifications', 'Test Conditions' (with sub-options for 'Thermal Boundary Conditions', 'Electrochemical Boundary Conditions', 'Analysis Parameters' (selected), and 'Precheck & Simulate'), 'View Results', 'Utilities', 'Materials Database', and 'Export Project Options'. The main content area is titled 'Analysis Parameters' and shows a schematic view of a battery cell with various components and a value '15' highlighted. The 'Analysis Parameters' section includes fields for 'Simulation Time (s)' (60), 'Time of Ignition (s)' (0), 'Initial Battery Temperature' (25, Celsius), and a toggle for 'Ignite Heat Pellets Simultaneously'. The 'Simulation Type' section offers three options: 'Thermal 2D' (selected), 'Thermal 2D + Electrochemical 1D', and 'Thermal 2D + Electrochemical 2D'. The 'Run Parameters' section includes a 'Show Advanced Options' link. Navigation buttons 'Back' and 'Next' are at the bottom.

Project details

TABS

MY MATERIALS DATABASE MY PROJECTS DOCUMENTATION SYSTEM PREFERENCES

Help Mode S

Battery Workflow

Project Details

Scott's Generic Battery > New Battery (baseline)

Sensitivity Level: UUR

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