

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

Scott A. Roberts*, Adam V. Baca, Sylvain R. Bernard, Wesley A. Brooks, Ashley C. Fate, Emily Heintzelman, Edward S. Piekos, Tyler G. Voskuilen

Sandia National Laboratories, PO Box 5800, MS 0836, Albuquerque, NM, 87185-0828

*Corresponding Author: sarober@sandia.gov, (505) 844-7957

Abstract: *Predicting the thermal and electrical performance of a thermal battery using computer simulations has the potential to save significant time and cost in the battery development process. However, traditional battery models can have a high barrier to adoption, often limited to those with significant expertise in computational modeling. We have previously developed the Thermally Activated Battery Simulator (TABS) [1] as a user interface to wrap around models for thermal performance and single-cell electrochemical performance. This capability has enabled battery designers at Sandia and in the US Department of Defense to predict battery thermal performance and reduce design cycles. However, the barriers to adoption of the legacy TABS simulation were still significant.*

In a companion talk, we present a new, advanced model that couples thermal and electrochemical performance at a full thermal battery scale [2]. Because of this significant increase in predictive capability — and simultaneously the computational expense required to solve it — we took the opportunity to re-develop TABS as a modern, cloud-based web application with a significantly improved user experience. We performed in-depth user experience research, tightly coupled with the consistent design of a new user interface and implementation using modern web technologies. By using cloud computing technologies, we moved the computational expense off the user’s desktop and onto shared computing resources, allowing the user to focus on battery design and performance.

In this paper, we detail the development of version 6 of TABS. We discuss lessons learned from previous TABS deployments and from user experience research. We also demonstrate its ability to allow users to intuitively study the impact of battery design changes on performance while accurately simulating the electrical performance of complex battery designs.

Keywords: thermal battery; computational modeling

Introduction

Version 5 of TABS [1] has gained wide adoption amongst the thermal battery design and analysis community, including at Sandia National Laboratories and

the U.S. Department of Defense laboratories. However, this previous version had focused on two analysis scenarios - thermal analysis of full thermal batteries and electrochemical analysis of single cells. With the development of a full battery coupled thermal and electrochemical model [2], we must now consider the deployment of this novel capability to our users.

The previous version of TABS suffered from a number of barriers to even wider adoption. First is its reliance on the Linux operating system. While Sandia could deploy the software to Windows computer in virtual machine environment, this is less than ideal for a majority of our potential users. Secondly, while the user interface (UI) was fairly intuitive (especially when compared to building the simulation manually), it still required extensive training to learn its effective use.

TABS development process

TABS version 6 (v6) is developed from the ground up as a cloud-hosted web application to provide thermal and electrochemical modeling capabilities for full thermal batteries to our user base. Its development principles and technologies are outlined below.

User experience research: The goal of TABS v6 is to provide an updated user interface and incorporate improved functionality to positively impact the user experience. To achieve our goal, the TABS team needed a foundational understanding of the users and their needs rooted in user research. Users were identified as existing and prospective users (people who “should” be using the tool but are not) to identify: what is working well in the existing tool; opportunities for improvement; barriers to adoption; and gaps between user expectations of the new tool capability and design.

The foundational research helped identify five distinct use cases for the tool. Use cases help us understand the types of engineering question categories users are attempting to answer. This understanding leads to better system design because the team intentionally, and explicitly, targets satisfying the identified use cases. For example, “Ad-Hoc Curiosities” was identified as a use case where users wanted to be exploratory — they wanted to investigate engineering questions as a

means to building more informed research inquiries; “we don’t know what we don’t know.” Additionally, the foundational research helped define specific user types and their respective design drivers. We can consider the needs of each user type as the team works to design a tool to meet specific user needs. For example, a “Novice User” wants to “be empowered to investigate a whole manner of engineering questions.” To accomplish this driver, TABS v6 needs to provide; a clean, simple UI; an easily accessible tool; the ability to progress through standard and non-standard workflows; enable the user to answer their questions without tool subject matter expertise (SME) intervention; help grow the user’s expertise through exploration and access to support materials. When we understand ‘why’ behind user’s needs, we build better systems to meet those needs.

User interface design: The user research directs the UI design; once the user data is collected and user needs are understood, ideation and system design occur. During the initial design concept, key stakeholders are included to help ensure design concepts meet both user and customer requirements. Design concepts, presented as low- and high-fidelity mockups (figs. 1a and 1b), are presented to users as tangible hypotheses the research team looks to invalidate. Understanding how the design concept(s) fail to meet user needs allows for evolution of the design. The research team also focuses on task accomplishment — users are provided with tasks they should be able to accomplish if the system is designed correctly to meet their needs and expectations. This research method is called *usability testing*. During usability testing, if users are unable to successfully accomplish tasks, researchers identify patterns and findings as “usability issues.” New design concepts are created (fig. 1c) to help overcome usability issues and the new concepts are tested with users. The design, test, and refinement process is iterative and requires multiple rounds of feedback elicitation and testing throughout the development lifecycle.

User interface implementation: One of the goals of version 6 of TABS is to modernize the overall user experience while working in the TABS user interface. The UI has been upgraded from a Java Swing application to a Vue.js web application utilizing the Vuetify material design library. Vue.js is a progressive javascript framework built on top of HTML, CSS, and Javascript. It is a reactive, component based framework that also provides a compiler-optimized rendering system. Vuetify is a material design framework that provides a large selection of components that help give the UI a consistent look and feel. In addition, the UI makes use of Chart.js, Three.js, and Trame, for

2D and 3D modeling and results visualization. The UI has a back-end written in Node/Express that utilizes a MongoDB database and also interfaces with the tabs-api Kubernetes orchestrator.

Cloud computing infrastructure: By adopting cloud computing technologies, TABS will easily support on-demand simulation requests from the new web interface, via horizontal scaling. The various codes associated with TABS for backend computing are being containerized and then orchestrated on a Kubernetes cluster. We have developed a RESTful API to help with the management of these containers, allowing any client to submit jobs and retrieve results. Our containers are being developed and hosted on GitLab, leveraging continuous integration pipelines to build updated container images and push them onto our registry. Our Kubernetes deployment pulls these images directly from our registry for the API itself and the simulation codes. The on-demand simulations are ran as Kubernetes jobs. We are also leveraging a Simple Storage Service (S3) instance for an API-based data management solution. Thanks to that approach we are able to share data across the web application, the back-end API, and the multiple ad-hoc Kubernetes jobs.

TABS v6

It would be a near-impossible task to fully describe the advancements and features of TABS v6. Instead, in fig. 2 we briefly highlight some of the key innovations and design changes in this upcoming release.

When first entering the tool, users are greeted with a new landing page (fig. 2a) that more intuitively guides users towards their goal. On first use, a panel on the right orients the users to the workflow for building a battery. Templates are available to quickly jump-start simulations with battery designs that they might already be familiar with. Once users have their own projects, they are also presented a searchable, filterable list of their projects for quick access.

The battery design page (fig. 2b) will be familiar to previous users, but with significantly improved graphical layout and an improved 3D to-scale view of the battery (fig. 2c). Because of the addition of electrochemical physics to the model, fig. 2d allows specification of the voltage tap locations within the battery, along with specification of the transient load (current, voltage, or resistance) experienced by that tap.

The materials database experience has been completely revamped. To allow for carefree editing of material properties, upon entering the database editor (fig. 2e), the user is greeted with an orientation as to the hierarchy of material property databases. The reference database of material properties that comes

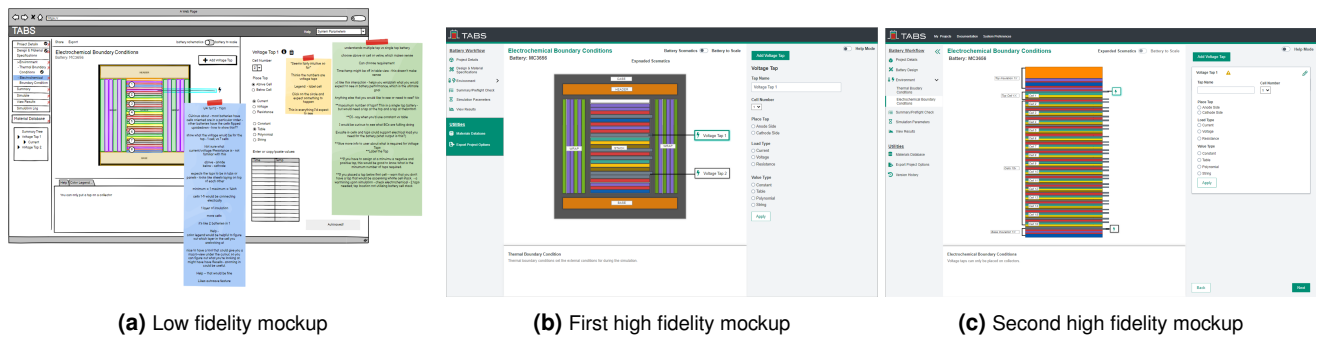


Figure 1. Evolution of electrochemical boundary condition specification feature from low fidelity (a) to high fidelity (b, c) mockups.

with TABS cannot be edited, but users can freely clone those materials and make modifications without fear of messing up other projects. For new materials that show promise, properties can be promoted to the user’s personal database for use in other projects (fig. 2f), or shared with the TABS developers for potential inclusion in the reference database. The materials are easily filterable and sortable.

Users have long asked for ways to make (and later compare) tweaks on the same battery design without creating new projects. In TABS v6, we are introducing two new concepts. First is the “design iteration” (fig. 2g), which allows users to start with a baseline battery design and make modifications to it (e.g., change constituent material thicknesses or material properties). Secondly, the user can define multiple “test conditions” for each design (fig. 2h), which includes things like initial battery temperature, external thermal boundary conditions, or loads on each tap. Each of these design iterations and test conditions have their own simulations, and the results can be compared on the same plot (fig. 2k).

Prior to running simulations, a series of pre-checks (fig. 2i) must be conducted to verify the validity of the design and to calculate certain statistics about the battery. The performance simulations themselves are performed simultaneously for all test conditions using secure cloud computing resources.

Finally, we have put significant investment into improving the ability to post-process and visualize the simulation results (fig. 2k). Line plots of key quantities of interest are available, and you can compare simulations for multiple design iterations and test conditions on the same plot, exporting the completed figures for use in reports and presentations. Users can also make multiple plots, customizing the content of

each one (fig. 2l). Two-dimensional plots of calculated variables are also available.

Summary

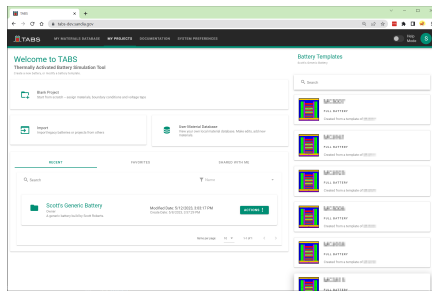
We expect that the advancements in TABS v6 (both in terms of model capability and interface usability) will be strongly desired by the thermal battery design community. We expect to complete development of the first production capability this year, with deployment to licensed users in early 2024.

Acknowledgments

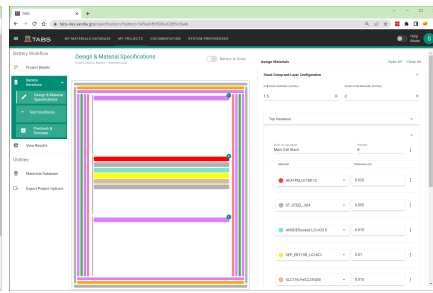
The authors gratefully acknowledge funding from the Joint Department of Defense/Department of Energy Munitions Technology Development Program. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525. The views expressed in this article do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

References

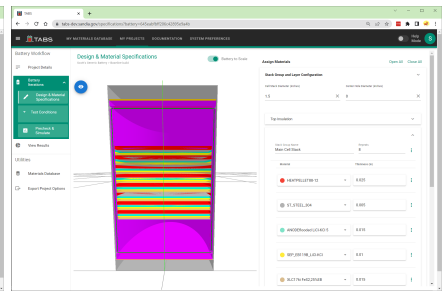
1. Roberts, S., C. Jove-Colon, H. Moffat, M. Neilsen, E. Piekos, B. Schroeder, B. Trembacki, and T. Voskuilen. “TABS : A Thermal Battery Desktop Design Tool.” *Proceedings of the 48th Power Sources Conference*, 2018.
2. Voskuilen, T. G., H. K. Moffat, N. W. Porter, and S. A. Roberts. “Coupled Thermal-Electrochemical Full Battery Modeling of LiSi/FeS₂ Batteries.” In *Proceedings of the 49th Power Sources Conference*, 2023.



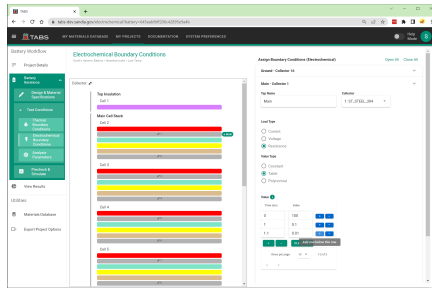
(a) Front landing page showing templates and user projects.



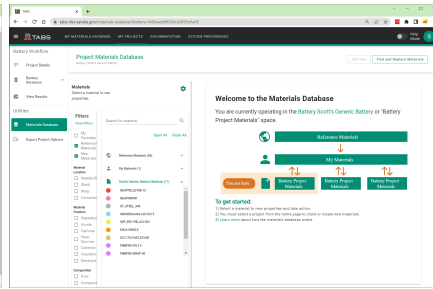
(b) Point-and-click battery design pulling materials from database.



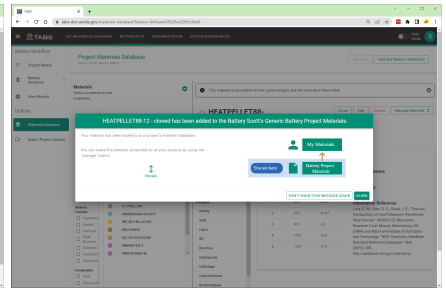
(c) View your battery design to scale in 3D.



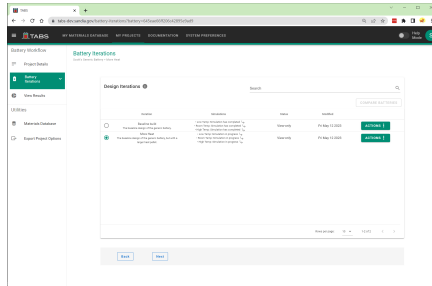
(d) Specification of voltage tap loads.



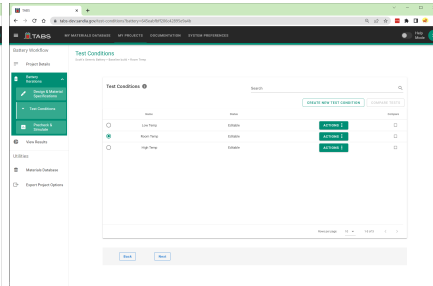
(e) Landing page for the materials database editor, showing the hierarchy of databases.



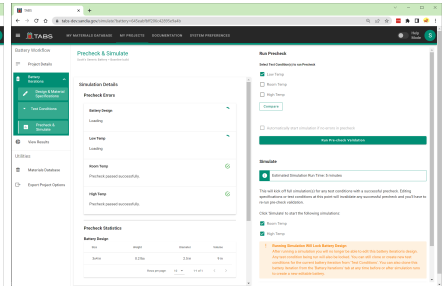
(f) Ability to promote properties to user database after editing.



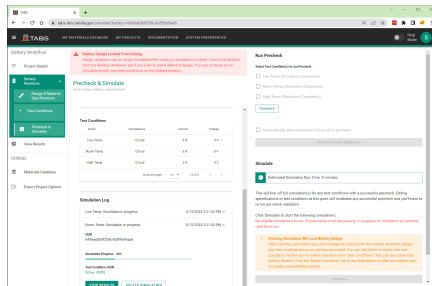
(g) Design iterations, allowing multiple simulations per design.



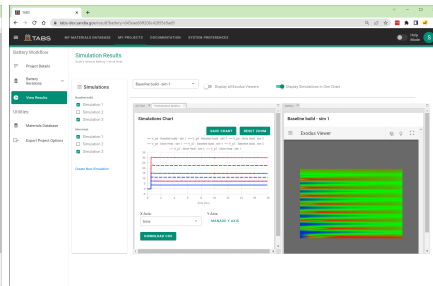
(h) Test conditions, allowing simulating multiple initial temperatures or boundary conditions simultaneously.



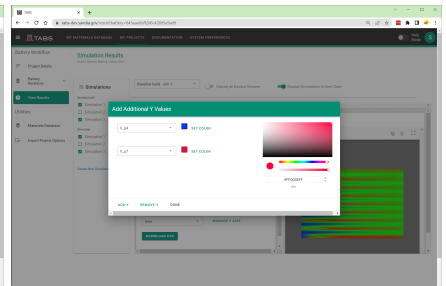
(i) Pre-simulation check calculates key metrics to provide feedback before a full simulation, ensuring it will run well.



(j) Run simulations using cloud computing resources and monitor progress.



(k) Visualize simulations using line plots and 2D viewer, comparing design iterations and test conditions simultaneously.



(l) Plots can be customized to choose which color to use for each variable.

Figure 2. Screenshots of the new TABS v6 tool highlighting new elements over previous TABS versions.