TABS: A Thermal Battery Desktop Design Tool

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Abstract: *The Thermally Activated Battery Simulator (TABS) is a computer modeling tool for assisting thermal battery designers in assessing design performance. This tool has been designed to run efficiently on a desktop computer and to present the user with an intuitive interface, allowing the designer to keep focused on the battery design, not the simulation details. The traditional TABS tool has been previously demonstrated to positively impact the battery design process at Sandia National Laboratories and has been integrated into regular workflows.*

In this paper, we demonstrate significant advancements to the capabilities and efficiencies of TABS. The traditional full-battery thermal model has been rebranded as TABS Full Battery (TABS-FB). Additionally, we have developed a second component to the modeling suite, dubbed TABS Single Cell (TABS-SC). This model focuses on a single thermal battery cell, providing the ability to predict the electrochemical performance (voltage and current) of the cell, with contributions from mechanical deformation, electrolyte flow, and thermal transport. A new materials database editor has also been developed that enables time-evolving properties for composite materials.

Keywords: Molten salt battery; modeling; simulation

The TABS Concept

The overarching goal of the TABS project is to create a computational tool to support thermal battery designers in creating and testing their designs virtually, reducing the number of design-build-test cycles required for qualification. Pursuing this goal, TABS is designed using the following principles:

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

Two separate TABS modules are available in the current release (version 5.0, released May 2018). TABS-FB is a full battery thermal simulator (without electrochemistry or other physics), calculating the battery's internal temperature distribution from ignition to freeze-out. TABS-SC is a multiphysics simulator at a single-cell level, with the intent of predicting electrochemical performance by simulating heat generation and transport, mechanical deformation, two-phase porous electrolyte flow and species transport, electrical transport, and electrochemical reactions.

A typical TABS workflow is illustrated in Figure 1. The primary graphical user interface (GUI) is shown in the top-middle of Figure 1. Using this GUI, the user defines their battery design graphically and intuitively. After specifying the battery design dimensions, TABS automatically creates a discretized mesh using Cubit [1].

TABS contains a built-in, extensible database of thermophysical properties, shown via a series of snapshots in Figure 2. The database distributed with TABS is pre-populated with properties for many of the materials commonly used in thermal batteries. Through the editor window shown in Figure 2a, the user can add new materials or edit any of the properties of existing materials. Pressed-pellet materials common to the electrochemical cell are considered to be composite materials (editor shown in Figure 2b) comprised of solid, liquid (electrolyte), and gas phases, with each of these having its own distinct properties specified separately (Figure 2c). Additionally, the solid phase can be comprised of multiple materials (e.g. FeS_2, MgO, and Li_2O). This composite material behavior enables the properties to evolve over the course of the simulation (e.g. as electrolyte flows during startup, the cathode swells during discharge, etc.). In addition, the database contains the ability to store uncertainty values (for later use in uncertainty quantification studies) for each property and references for these values and uncertainties.

The mesh is combined with thermophysical properties for a physics simulation using Sierra/Aria [2]. For computational efficiency, the mesh and simulation are created assuming 2D axisymmetry common to most

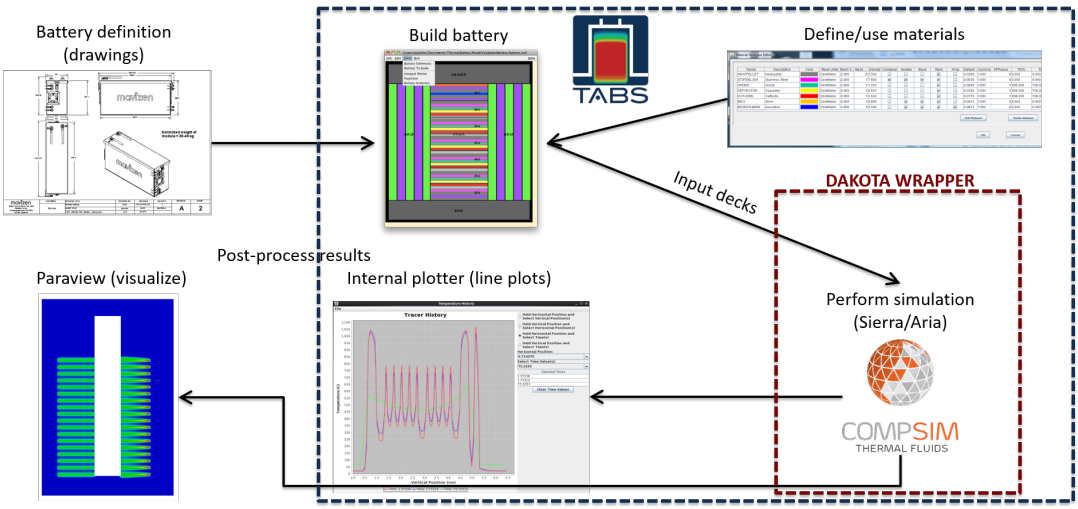
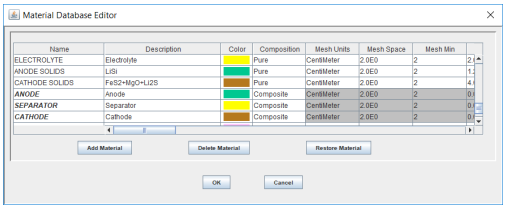
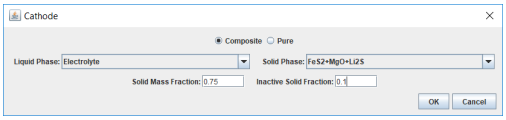


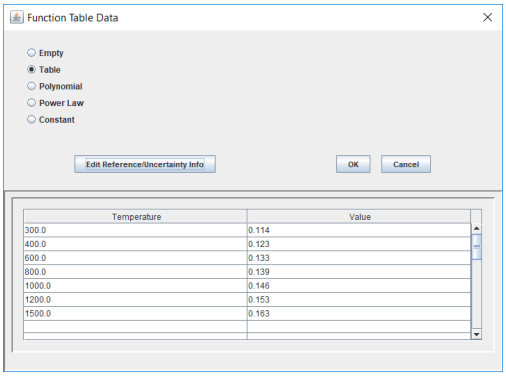
Figure 1. Overview of the TABS workflow showing steps to go from battery definition to solution



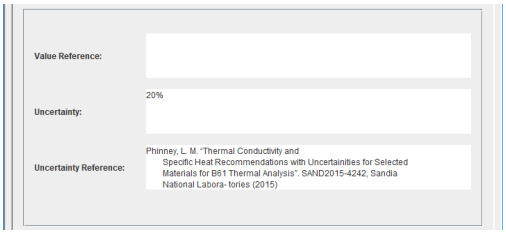
(a) Main database editor window



(b) Composite material editor



(c) Property entry editor



(d) Reference and uncertainty editor

Figure 2. Materials database editor

thermal batteries (which are typically right-circular cylinders). Depending on the resolution and physics chosen, simulations typically take less than one hour on a desktop workstation computer.

The fundamental output from a TABS simulation is a history of every fundamental physics quantity included in the simulation at every spatial point in the geometry for every time simulated. A number of convenient post-processing options are provided through the TABS GUI. First, global scalar quantities, such as battery rise and life times, are displayed directly in the TABS GUI window. Second, time-dependent scalar quantities, such as cell voltage and current, are saved as a comma-separated values (CSV) file viewable in spreadsheet editors. Additionally, TABS-FB contains a built-in plot generator, enabling spatial and temporal interrogation of the solution in the form of line plots. This plotting feature is currently under development for the next release of TABS-SC. Finally, Paraview [3] can be used for exploring the results in great detail, creating colored 2D images and movies.

TABS-FB: Full Battery Thermal Simulator

The original component to TABS is the TABS-FB full battery thermal simulator, whose main window is shown in Figure 3. The cell stack is designated as the combination of individual cells comprised of any number of materials, including heat pellets, collectors, cathodes, separators, and anodes. Identical cells may be repeated multiple times (note the “8x” in Figure 3) and combined with individually specified cells which are not identical. Radial insulation and wraps, axial insulation, header, footer, and can complete the battery definition. Center-hole fired or side-fired batteries can be specified.

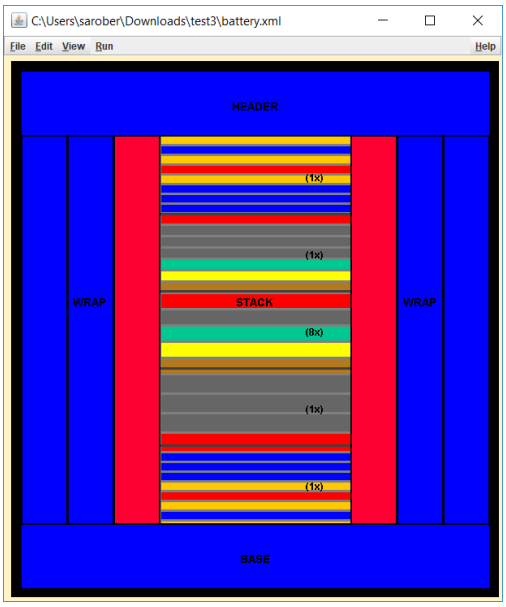


Figure 3. TABS-FB main window

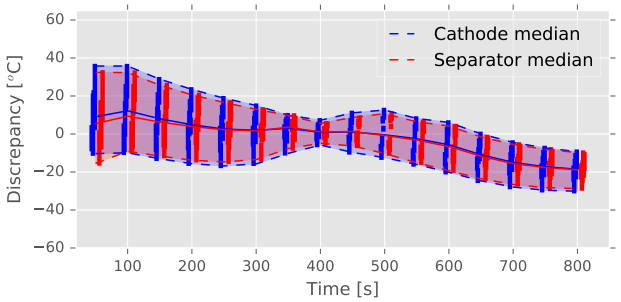


Figure 4. Example plot of TABS-FB experimental validation showing discrepancies between experimental data and nominal temperature for cathode and anode temperatures. The solid curves in the middle represent the median difference between experiment and simulation and the bands represent the range of values.

The TABS-FB physics model consists of heat generation and transport and has been previously described in detail [4]. For center-hole fired batteries, all heat pellets are simultaneously ignited at their centers. Side-fired batteries are initiated at the center of the heat pellet nearest the header, which then burns to ignite heat paper strips that burn axially and ignite the remaining heat pellets. Heat is lost through the can due to conduction, convection, and radiation.

The primary global scalar quantities of interest (QOIs) resulting from TABS-FB simulations are rise time, life time, and the maximum temperature in the cathode and anode. These QOIs are immediately available to the user through the TABS GUI without further post-processing. Additional temperature plots can also be easily created.

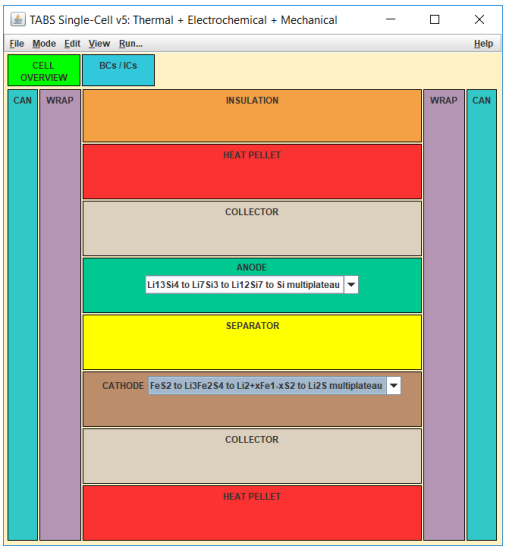


Figure 5. TABS-SC main window

TABS-FB has been subjected to a rigorous credibility assessment [4]. The underlying physics code has been verified using known solutions, and battery-specific problems have been subjected to solution verification, showing expected order-of-convergence with mesh resolution and time step size. These verification activities informed the default numerical parameters found in TABS-FB. Parameter uncertainties were quantified and propagated through the model. Resulting QOI uncertainties are relatively large due to highly uncertain values for insulation thermal conductivities, an area of active research [5]. Validation was performed against data from thermocouples embedded in a purpose-built model validation battery. The discrepancy between experiment and simulation (an example of which is shown in Figure 4) is always less than 50 °C, and typically much less (nominally 20 °C) during the majority of the battery's operational time.

TABS-SC: Single Cell Multiphysics Simulator

The newest component of TABS is the TABS-SC single cell multiphysics simulator, shown in Figure 5. The primary intent of this module is to predict the electrochemical performance of a battery cell. To do this, heat generation and transport, mechanical deformation, two-phase porous flow and species transport, electrical transport, and electrochemical reactions are modeled. Due to the complexity of these coupled physics, TABS-SC implements this capability only for single electrochemical cells. For the sake of computational efficiency, multiple levels of physics fidelities are offered in the form of simulation fidelity modes [6]. The electrochemical reactions are driven by specifying the cell load, either in the form of a current, voltage, or load resistance.

A large number of QOIs are available from TABS-SC in each of the physics areas simulated, both global and time-dependent scalars. Battery performance is primarily captured through the cell voltage and current, which are readily viewable in the output CSV file. Progress and spatial distribution of each electrochemical reaction, electrolyte distribution, and many other parameters are also available.

Credibility assessments of TABS-SC are ongoing. Code and solution verification show expected results and parametric uncertainties are quantified. Validation against experimental single-cell test data has also been completed, but agreement is currently poor, leading to ongoing research investments in improving the calibration of a number of electrochemical parameters [7]. More complete documentation of the TABS-SC physics model and credibility assessment is pending.

Obtaining and Using TABS

TABS is export controlled under EAR99 and is available to entities of the U.S. Government and their prime contractors from Sandia National Laboratories under a Government Use Notice. Concurrent licenses for Cubit [1] and Sierra/Aria [2] are also required.

TABS and its supporting codes are designed to be run natively under a Linux-based operating system, including MacOS. Windows computing environments can be supported via multiple non-native implementations, including virtual machines and the Windows Subsystem for Linux. TABS is capable of parallel processing, and the developers recommend running on a reasonably powerful multi-core desktop workstation for the best experience, although TABS-FB has been successfully run on laptop computers.

The Future of TABS

TABS continues to be actively developed. A minor version release (v5.1) is planned for the end of 2018, bringing additional post-processing capabilities to TABS-SC, improved electrochemical calibration, and an ability to use TABS-FB thermal profiles to define the temperature in TABS-SC. TABS v6.0 is slated for deployment in 2020 and will bring basic electrical simulation capabilities to the full battery scale. Future versions will improve the fidelity of full-battery electrochemistry and mechanics, including the ability to model battery performance in dynamic mechanical environments.

Acknowledgments

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