Accelerating Thermal Battery Design with Set-Based Concurrent Engineering

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Abstract

Set-based concurrent engineering (SBCE) methods, applied to thermal battery design, offers the promise of faster, cheaper design cycles when paired with complementary higher fidelity digital engineering tools. Using a limited subset of requirements, a reasonable first order thermal battery design can be optimized using set-based tools, which allows for rapidly exploration of design options before committing to either hardware builds or time intensive higher fidelity simulations. The model is described, with an example given to demonstrate functionality in the areas of mass, volume, thermal behavior and electrochemical performance.

Keywords

Thermal Battery; Design; Modeling

Introduction

Thermal battery development traditionally involves designing a battery to meet electrochemical and thermal requirements, realizing that design, and testing it to determine its mechanical and thermal response. This process, iterated until requirements are met, produces only a single point design and validates that design only to those specific requirements. These design-build-test iterations are very slow and expensive. Impacts can be minimized by only exploring designs similar to existing product and assuming equivalent reliability across similar environments. That approach becomes challenging as requirements evolve beyond those of current products. New tools are needed to rapidly screen larger design spaces for solutions that can meet requirements and determine what is practical in terms of cost, schedule, performance, and reliability.

Set-based concurrent engineering (SBCE) is one way to address these challenges. The commercial software tool *Success Assured* © [1] was chosen to build an SBCE model for design of thermal batteries due to ease of use, included visualization tools which support decision making, the ability to re-use models for multiple designs, and broad applicability during system and component design. Because the SBCE model is complementary to existing 3D finite element simulation capabilities (TABS), these two sets of tools enable informed evaluation across potential design spaces (SBCE) before simulating high fidelity point designs in selected configurations (FEA).

The current SBCE model addresses a typical subset of inter-related thermal battery performance requirements in three broad areas: mechanical envelope (mass and volume), thermal performance (thermal conductivity and temperature during use), and electrochemical performance (state of charge and current density). Mechanical and non-mechanical environments are not currently included. The design of a thermal battery for purposes of the model is assumed to include a cell stack, insulation and a case. A standard cell is composed of a heat pellet, anode, cathode, separator, and two collectors, while the stack is the sum total of all the cells in adjacent proximity (i.e. not separated by insulation). Axial and radial insulation fill the gap between a cell stack and the case, which is modeled as a header, base and thin-walled tube.

Model Description

In this SBCE model, mechanical envelope (ME) requirements are assumed to include only the outer dimensions and mass of the battery. Piece part dimensions and material choices (i.e. density) are the lowest level of decisions to compute these quantities. Volume and mass are computed for each piece part and then summed to create a standard cell, complete stack, and battery using the definitions illustrated in Figure 1. Although density of some parts (e.g. collectors, leads, case material) are dictated directly by the material choice, others like insulation and pellet density are not as straightforward. Insulation density depends on the level of compression applied by a closing force. Cell design requires additional considerations, such as performance characteristics of the heat pellet (handling strength, burn speed, ignition sensitivity) or electrochemical cell operation (anode and cathode wetting, deformation after activation). Theoretically all of these constraints could be modeled as discrete relationships, however historical values for compressed insulation density and pellet density were used for simplification.

Thermal performance within the SBCE model addresses the two most important aspects of thermal battery operation: the initial temperature after activation, and the final temperature at the end of the required activated life. The battery stack is approximated as a lumped mass. This enables an estimate of the average post-activated temperature by calculating the energy balance of a standard cell:

$$T_p = \sqrt{\left(\frac{Cp_b}{Cp_m}\right)^2 + \frac{2}{Cp_m}\left(\frac{q}{M} + \frac{1}{2}Cp_m T_i^2 + Cp_b T_i\right)} - Cp_b/Cp_m, \qquad (1)$$

where T_i is the required ambient starting temperature of the battery, q_{hp} is the energy per mass of the heat pellet, m is the mass of the standard cell in the battery, and c_p is the effective specific heat of the battery. Specific heat is assumed to be linear in temperature, defined by a slope (c_{pm}) and intercept (c_{pb}) with unique values depending on whether the battery has a small or large size. The lumped mass approximation implies the use of Newton's Law of Cooling, expressed as the exponential equation:

$$T_f = T_{env} + (T_p - T_{env})e^{-t_f/\tau}, \qquad (2)$$

where T_p is the starting temperature from Equation 1, T_{env} is the asymptotic environment temperature (melting temperature of the electrolyte salts), t_f is the elapsed time to the end of the activated life, and τ is a time constant. The time constant in Equation 2 functions similarly to a decay constant in an electrical circuit and controls the rate of thermal decay as the starting temperature cools to the environment temperature. In this case, τ is defined as:

$$\tau = hA/C, \qquad (3)$$

where h is a convection coefficient, A is the area through which the heat exchange occurs, and C is the thermal capacitance ($c_p * mass$). Although h is not straightforward to calculate, the heat loss through the different surfaces of the stack (top, bottom, side) can be treated as thermal resistors acting in parallel, yielding:

$$(hA)^{-1} \propto \frac{L_1}{k_1 A_1} + \frac{L_2}{k_2 A_2} + \cdots \qquad (4)$$

where *L* is the layer thickness, *k* is its thermal conductivity, and *A* is the area through which heat exchange occurs. The proportionality constant for Equation 4 was determined empirically by simulating several batteries using the TABS tool with a wide range of sizes and insulation configurations. Comparison of the thermal model (Equations 1 and 2) with TABS simulations demonstrates an agreement that almost always falls within 10%. An example is shown in Figure 2 for a long-life battery. TABS simulation results are shown in blue with ±10% error bars and the set-based formula results are shown in red.

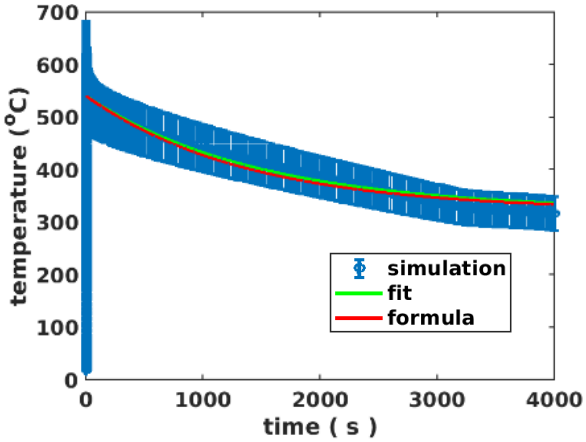


Figure 1. Set-based thermal model comparisons with TABS predictions for a long life thermal battery.

Electrochemical performance is the final part of the SBCE model, building on the decisions and relationships defined in the mechanical envelope and thermal areas. This capability predicts battery voltage given several other known or computed quantities: temperature (from the thermal model), current density (from required loads and cell diameter), duration (from required activated life), and state of charge (SOC) using capacity consumed (required loads and duration). These parameters can adequately define the polarization expected for a given cell chemistry if the discharge curves are known or computed across the entire parameter space. A full factorial design of experiments to obtain this data is not practical, so as an alternative, we have opted to simulate this performance space. This was done using the TABS single cell electrochemical model (LiSi/FeS2 chemistry with a LiCl/KCl electrolyte) calibrated against measured performance data [2, 3, 4]. In this way, several thousand constant current simulations were run across variations of pellet thicknesses, current density, temperature, and state of charge.

These TABS simulations were defined by eight (8) even spaced points between the minimum and maximum values for all parameters except capacity consumed. Since each simulation run yields voltages which could be extracted for an arbitrary number of points in capacity consumed space, twenty (20) values were selected in log space in order to produce

predictions for small capacity consumed, and fewer values at larger capacity consumed. Figure 3 shows some of these results, with cell voltage plotted against different parameters.

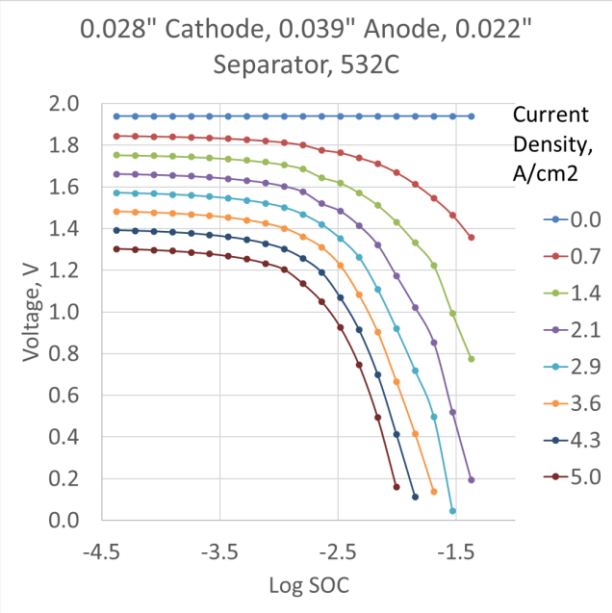


Figure 2. TABS single cell voltage predictions plotted against log(SOC).

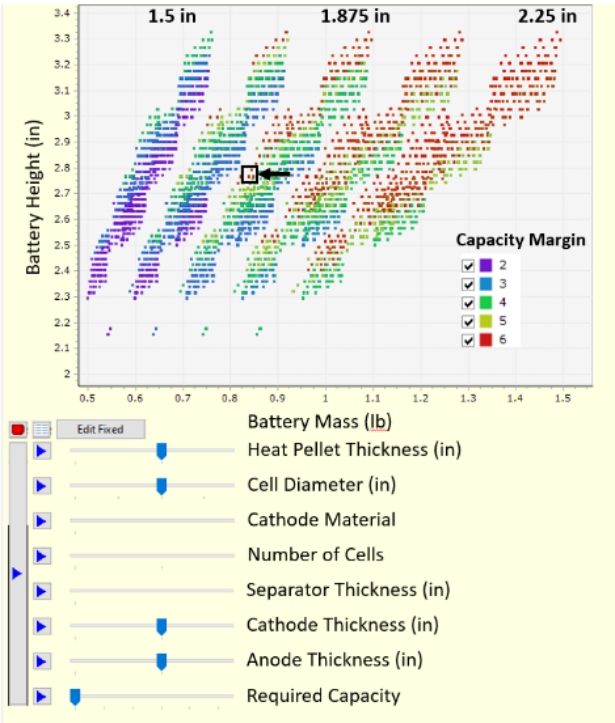
Exemplar

The SBCE model is capable of finding the complete set of solutions with all constraints and requirements enforced, but available computational resources can limit the ability to complete those calculations in a reasonable timeframe. Faster results were achieved by breaking the problem into more manageable sub-maps, wherein the solution space is narrowed down by a combination of set-based computation and engineering judgement. Three example design trade spaces are shown in Figure 4. Constraints enforced in these tradeoff charts are that the chemistry of a cell is a LiSi anode/FeS_2 cathode with coulombic capacities, respectively, of 1746 and 1206 $A \cdot s/g$ and a standard LiCl/KCl electrolyte ($T_m = 352°C$). Initial and post-activated temperature are $T_o = 25°C$ and $T_p = 550°C$, insulation is assumed to have a thermal conductivity and density properties 0.025 W/mK and 0.32 g/cc, and the maximum battery diameter is enforced to be no greater than 3 inches.

The capacity – ME tradeoff chart shown in Figure 4a shows that for a given cell diameter of 1.875 inches, a minimum height and mass can be achieved with a margin of 6x the required capacity. This design corresponds to pellet thicknesses (heat, cathode, anode) of 0.035, 0.020, 0.026 inches, respectively for a 15-cell stack. The thermal performance tradeoff chart (Figure 4b) predicts that this design will be above 450°C after an activated life of 4098 seconds, which is at least 100°C above the melting temperature of the electrolyte salts, if the axial and radial insulation thicknesses are set above 0.94 and 0.6 in, respectively. The rightmost boundary indicates a constraint from the maximum battery diameter. The voltage tradeoff chart (Figure 4c) illustrates that a 15-cell stack with this heat balance and cell design will be above 26.5V at the end of life given the predicted final temperatures and a capacity consumed of 97 mA-hr.

Conclusion

Development of this SBCE model required significant costs in time and labor to create the comprehensive model, collect data to populate the model, and identify gaps in knowledge. Completing the ME, thermal, voltage areas required an estimated 1.5 labor-years of work, using 3-5 experts, over the course of ~2 years. Subsequent activities are expected to take less time to implement. These three areas are working well and able to make accurate predictions about existing designs. The model is currently being used to assess new requirements and come up with performance, weight and sizing estimates within a developing project.



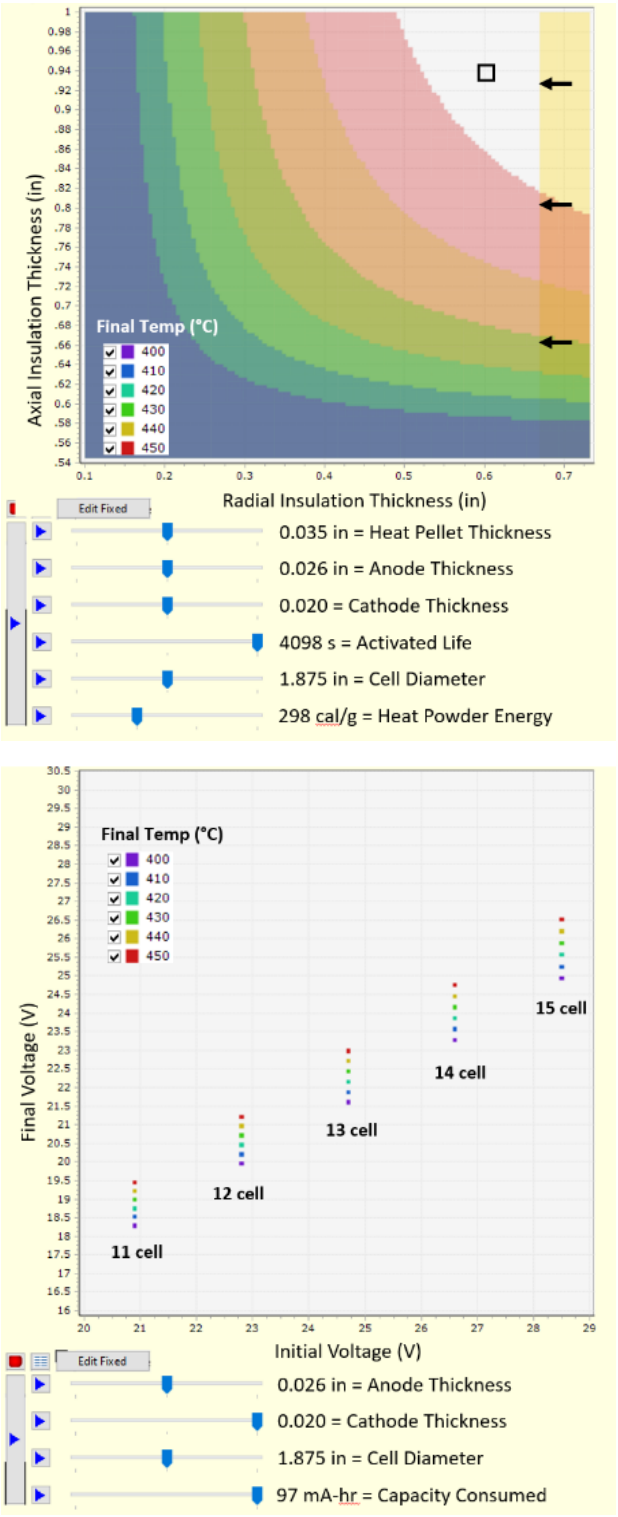


Figure 3. Tradeoff charts for (a) capacity, (b) final temperature and (c) final voltage.

Future developments include relationships for mechanical environments, manufacturing variability and reliability. These improvements will continue to imrove the overall agility of the design process and allow for a faster, more quantitative approach.

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