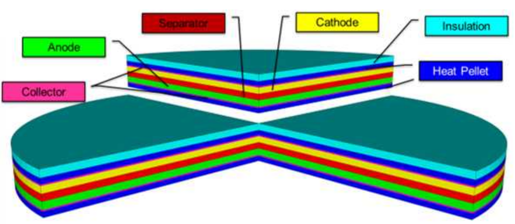
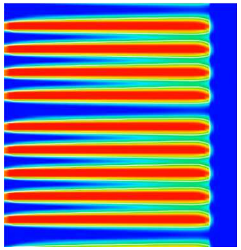
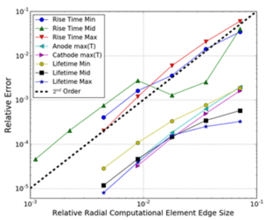
SAND2016-5705C

Uncertainty Quantification, Verification, and Validation of a Thermal Simulation Tool for Molten Salt Batteries







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47th Power Sources Conference
June 15, 2016

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Molten Salt Battery Overview

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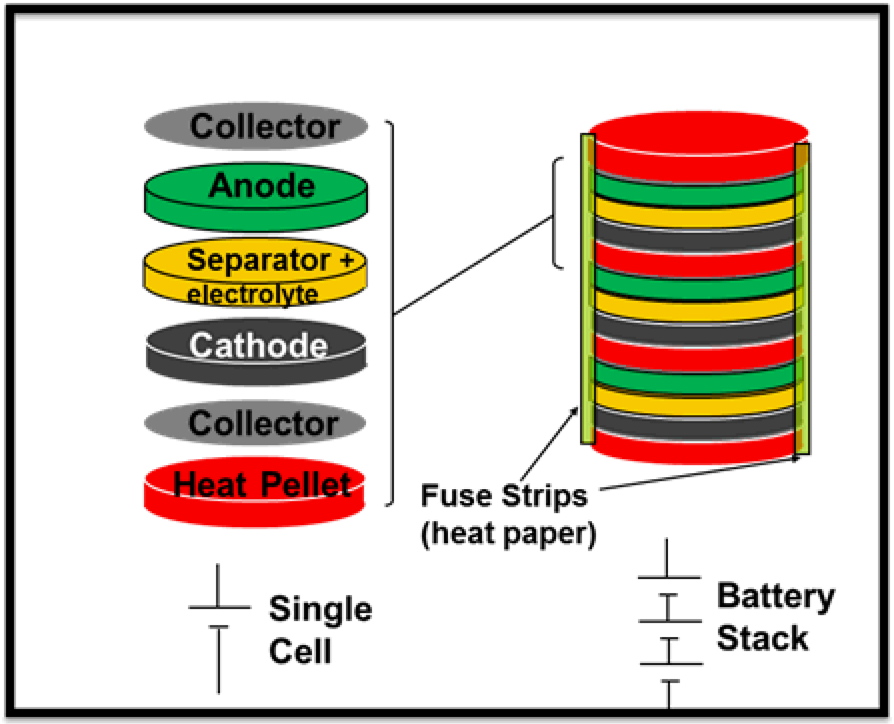
- Molten salt batteries are power sources that provide
  - Long shelf life
  - High voltage output
  - High current capacity
  - High power density
- Heat pellet burn releases large amounts of heat energy
- Solid electrolyte in separator melts and flows into porous electrodes, forming an electrochemical circuit and delivering power



Sandia's Thermally Activated Battery Simulator (TABS v3)

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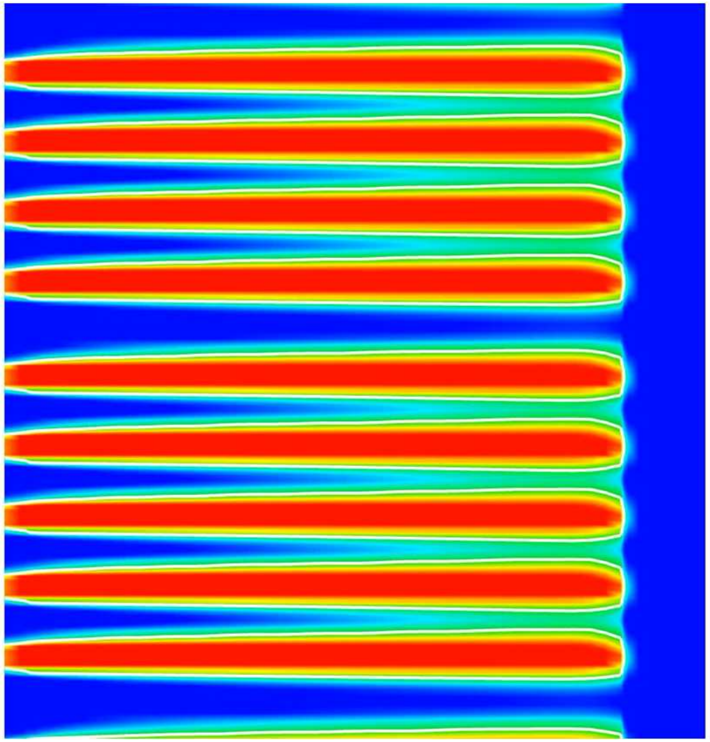
- Thermal management is critical for design of molten salt batteries
  - Heat generation and transport is the dominant process driving electrochemical performance
- Computational models widely used to aid design process
- TABS solves unsteady heat equation on 2D axisymmetric computational domain, using Sierra/Aria (FEM)

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot \kappa \nabla T + S_E$$

- Material properties are temperature dependent and have uncertainty
- Major energy source in S_{E} is burning of heat pellets. Burn front is tracked using a level-set method



Simulated battery activation

Stewart, J. R. and H. Edwards (2004); Notz, P.K. *et al* (2007); Piekos *et al* (2012)

Research Motivation and Focus

- Uncertainty Quantification: Determining the relationship between uncertain model inputs and probabilistic outputs
  - Yields more realistic simulation results and model validation
  - Allows design engineers to make informed decisions when specifying material property and manufacturing tolerances

- Verification: Ensuring models are being solved correctly

- Validation: Evaluating the models for accuracy by comparing simulations to experiments

Quantities of Interest (QOIs)

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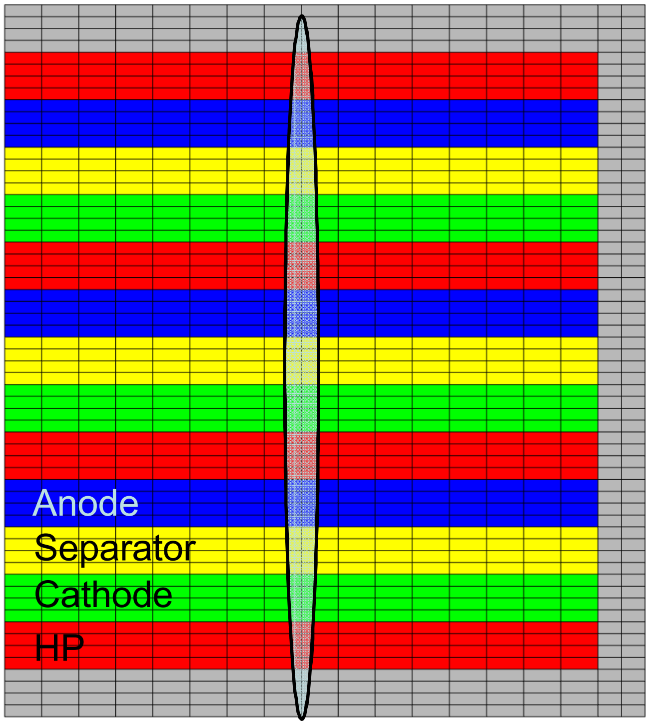
- Rise Time: Time between heat pellet ignition and delivery of useful electric power
- Lifetime: Time between heat pellet ignition and termination of useful power
- A translation between electrochemical power and temperature is made:
  - Melted electrolyte in separator region corresponds to activated battery
- QOIs
  - Battery rise time
    - **Rise Time Min**: Any point in separator region is above electrolyte melt temperature (T_{melt})
    - **Rise Time Mid**: Any column in separator is above T_{melt}
    - **Rise Time Max**: Entire separator is above T_{melt}
  - Battery lifetime
    - Inverse of three rise time metrics
  - Anode maximum temperature
  - Cathode maximum temperature



Rise Time Mid / Lifetime Mid
2D Axisymmetric Simplified Geometry

Uncertainty Quantification (UQ)

Uncertainty Quantification Methodology

- Each simulation parameter has nominal value and uncertainty range (shown in table)
- Uniform distribution assumed
- Latin Hypercube sampling used to run 500 unique thermal discharge simulations; QOIs calculated (Dakota toolkit)
- Collection of inputs and outputs used in a polynomial chaos UQ study
- Result is collection of uncertainty ranges and global sensitivity metrics for each output QOI w.r.t. each input parameter

Parameter	**Lower Bound**	**Upper Bound**
HP c_p	60%	140%
Separator c_p	60%	140%
Cathode c_p	60%	140%
Anode c_p	60%	140%
HP κ	10%	190%
Separator κ	10%	190%
Cathode κ	10%	190%
Anode κ	10%	190%
Insulation κ	10%	500%
HP Density (ρ)	97%	103%
HP Mass	99.5%	100.5%
HP Burn Speed	80%	100%
HP Heat Output	99%	101%
Ambient Temp	99.6%	100.4%
Emissivity (ϵ)	0	1

Results: QOI Value Ranges

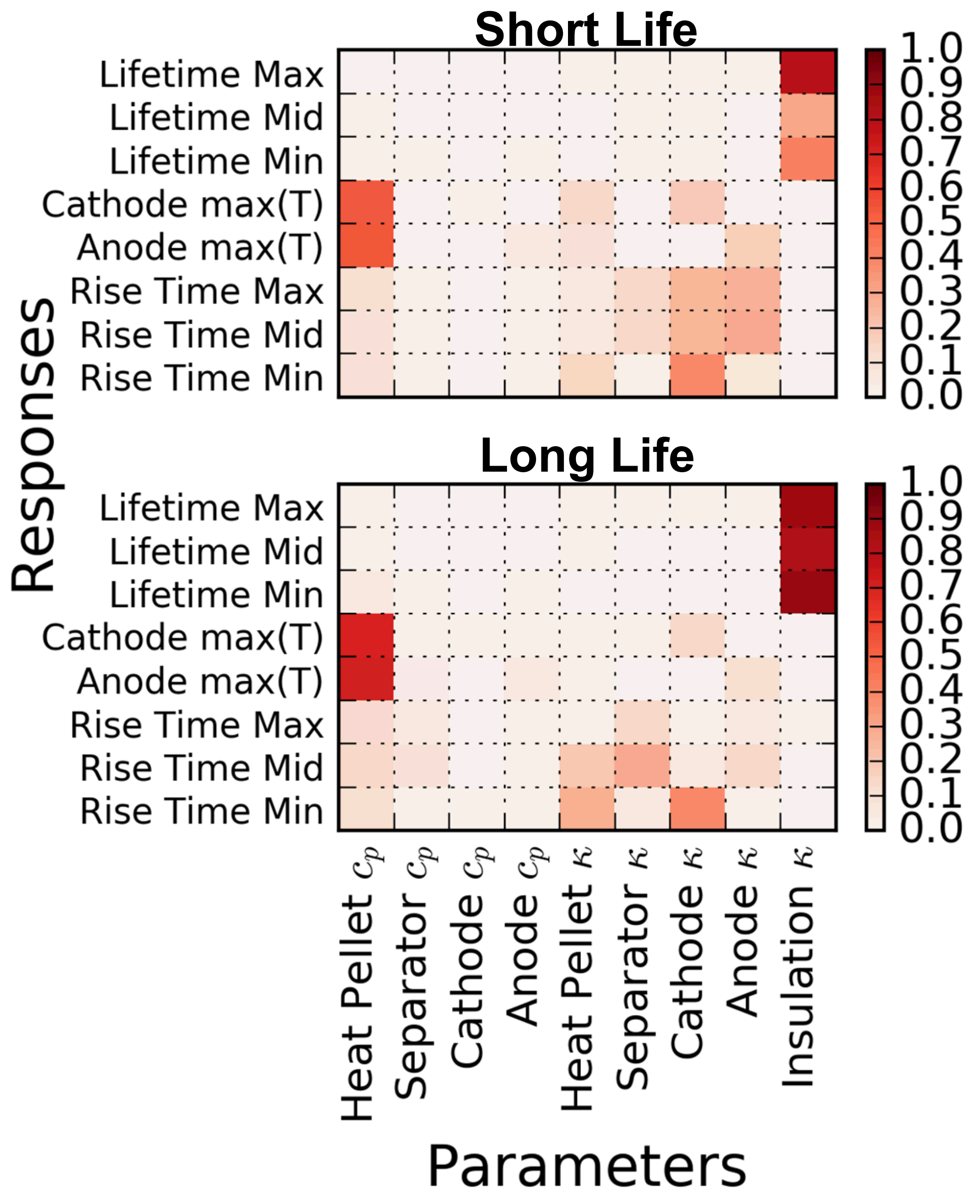
- Two types of batteries presented: long life and short life

QOI	Short Life	Long Life
Lifetime Max	44%	32%
Lifetime Mid	62%	30%
Lifetime Min	76%	54%
Cathode max(T)	12%	10%
Anode max(T)	12%	9%
Rise Time Max	35%	130%
Rise Time Mid	47%	53%
Rise Time Min	59%	64%

- Maximum standard deviation (σ) observed is 130% of the mean
- Maximum temperature QOIs show significantly smaller σ, indicating lower sensitivity to input uncertainties

Results: Sensitivity Index

- Sensitivity Index: Fraction of QOI uncertainty that results due to uncertainty in each input variable
  - Main effect sensitivity index shown here (no input variable interaction effects plotted)
- Darker red corresponds to larger effect of input uncertainty on output uncertainty
- Lifetime uncertainty mostly due to insulation κ
- Max temperatures largely depend on heat pellet c_p as well as electrode material κ
- Emissivity had large input range, but low sensitivity index



Verification and Validation (V&V)

Verification: Mesh Convergence

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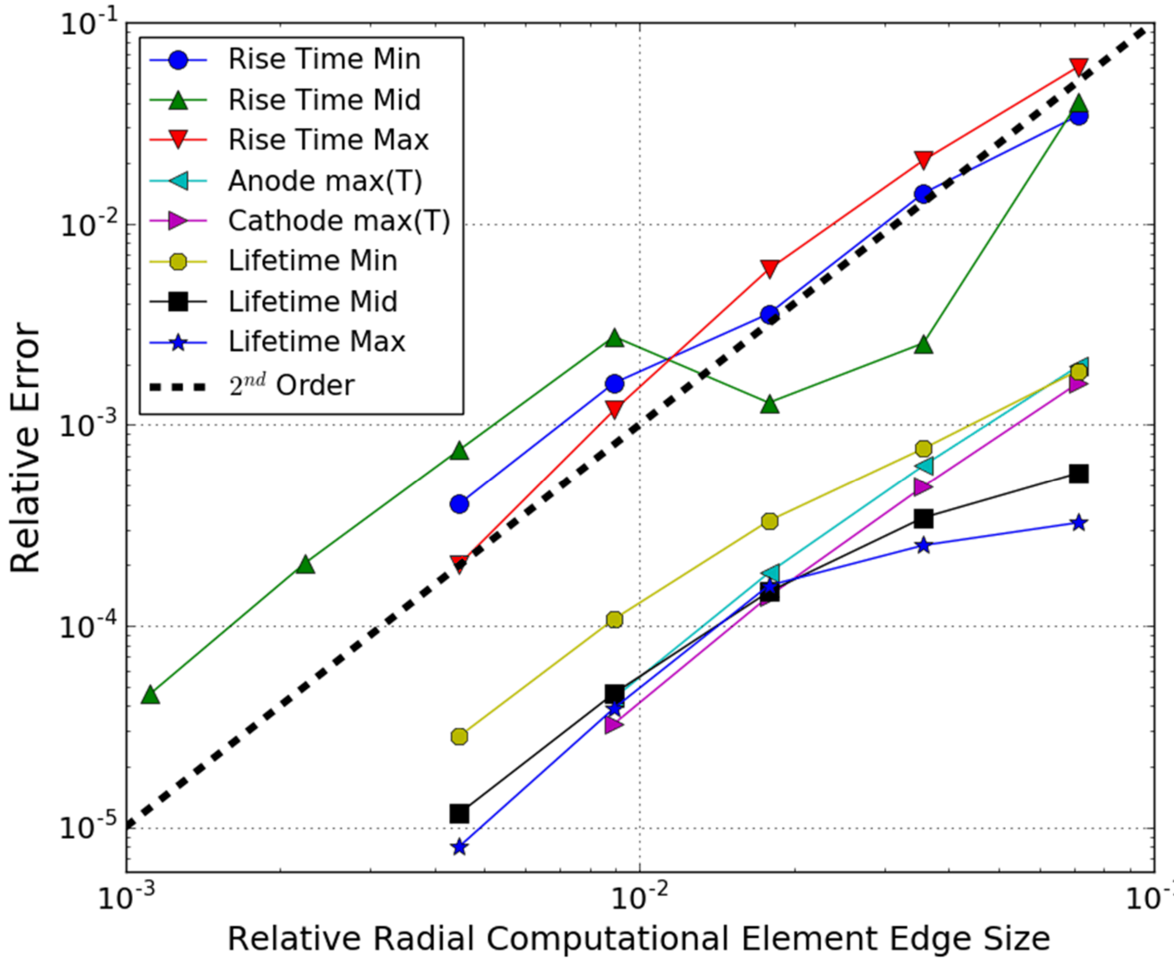
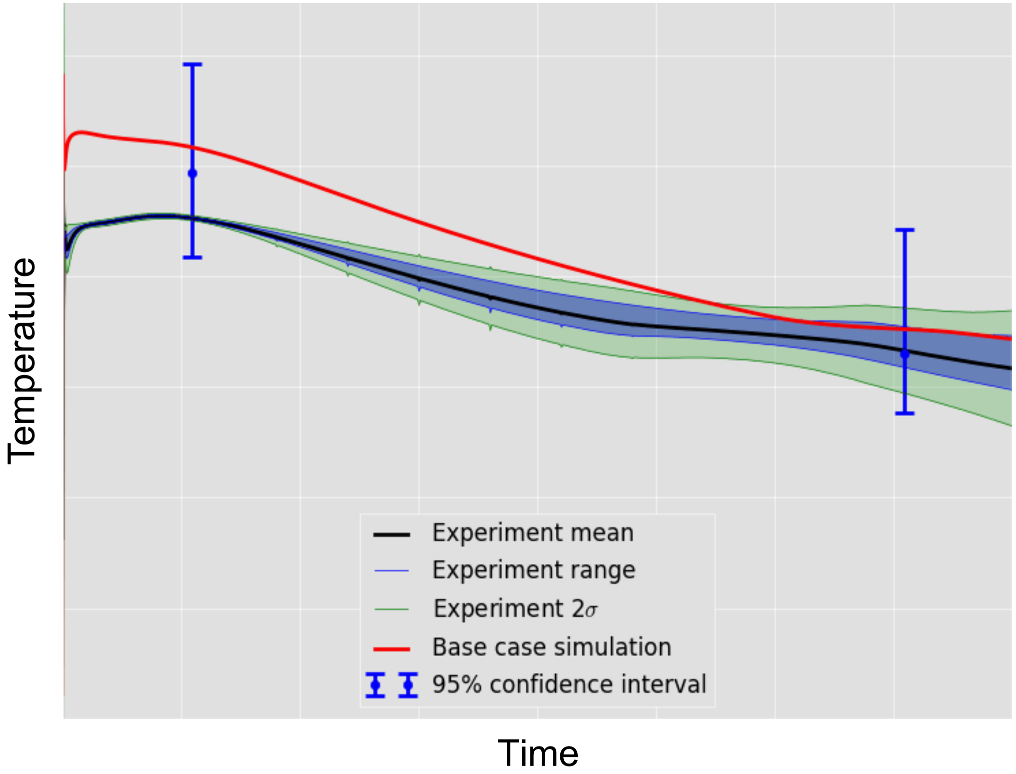
- Focus here on spatial discretization (mesh refinement) effects on QOIs
- Richardson Extrapolation used to determine relative error and calculate order of convergence
- All QOIs approach 2nd order convergence
- Rise time QOIs show largest relative errors (3-8% on coarsest mesh)
- Less than 1% error for other QOIs



Validation: Comparison to Instrumented Battery

- Three replications of instrumented battery (each with 15 thermocouples) activated to gather model validation temperature data
- Example validation plot for one thermocouple location:



- Experimental values fall within confidence interval range
- Working to improve nominal simulation accuracy and decreasing confidence interval

Conclusions and Ongoing Work

- Assessing effects of input uncertainties
  - Provides valuable information for battery design
  - Motivates experiments to reduce specific uncertainties
- DAKOTA toolkit allows for automated UQ and sensitivity studies
- Demonstrated efforts to both verify and validate our thermal model

- Ongoing/Future Work
  - Narrow uncertainty ranges with in-depth literature review and experiments
  - Incorporating electrochemistry and mechanics in addition to thermal
- Acknowledgments
  - Adam Hetzler, Richard Hills, Kenneth Hu
  - Sandia Power Sources Group
  - Advanced Simulation and Computing (ASC) Verification and Validation Program

Thank You