SAND2014-4838C

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Assessing the Sensitivity of Thermal Battery Performance to Material Properties

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Motivation – Simulation Perspective

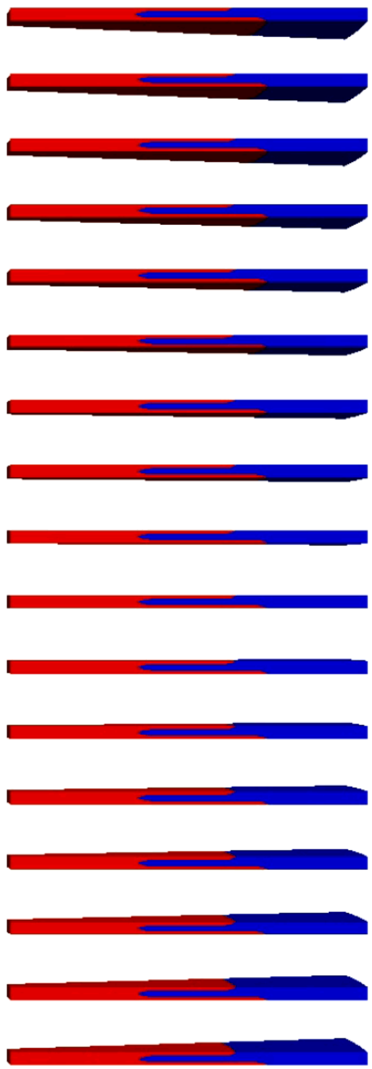
- A typical battery contains many materials, each with three important properties (from a thermal standpoint):
  - density
  - thermal conductivity (can be temperature-dependent and isotropic)
  - specific heat (generally temperature-dependent)
- Melting materials add:
  - latent heat
  - solidus and liquidus temperatures
- Measuring everything with high precision will be expensive and time-consuming
  - Sensitivity information from simulation can guide prioritization and precision of measurements

Motivation – Engineering Perspective

- Acceptance ranges are often defined for material properties
  - How do these ranges translate to performance measures?
  - Can interactions create a failed battery even when all materials are within bounds?
- The large number of samples required to explore the parameter space make a physical study time and cost prohibitive
  - Simulation can explore large spaces with little user intervention

Sensitivity of What?

- Can easily do temperature at a point
  - but must choose a point
- Center-fired batteries are reasonably uniform so a point at the axial midline of a separator would be good for rise time
  - radial location may give an indication of available capacity
- No clear choice for side-fired batteries due to non-axisymmetric geometry



Separator melt snapshot

Sensitivity of What?

Can also do max, min, or average temperature of a material

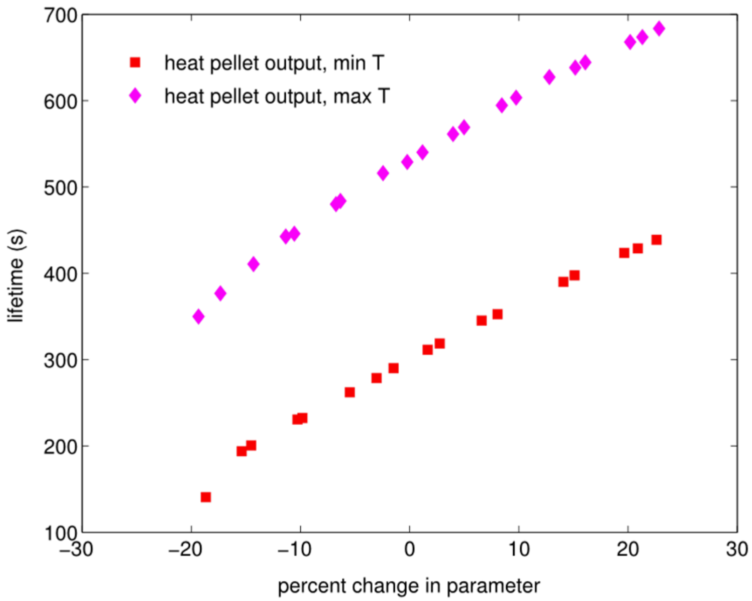
- Example: sensitivity of rise time
  - min temp of all separators > T_{melt} means *everyone completely* melted
    - most conservative
  - max temp of all separators > T_{melt} means *part* of *someone* melted
    - earliest
  - average temp of all separators > T_{melt}
    - somewhere in between
- When determining lifetime, roles are reversed
  - min temp < T_{melt} means someone froze somewhere
  - max temp < T_{melt} means everyone's completely frozen
- Max temp of anode could also be useful

How to Perturb Parameters?

- Fairly straightforward with constant values, but many parameters are given as tables or polynomials
- Adopted a “percent change” strategy
  - value multiplied by (1 + %change / 100)
  - allows very different parameters to be plotted together

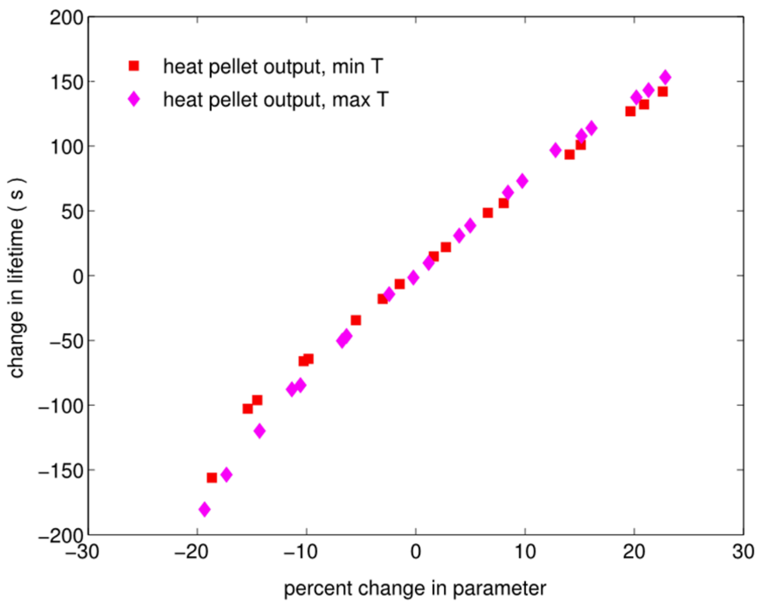
Lifetime of Large Side-Fired Battery

- Large difference between min temp and max temp definitions



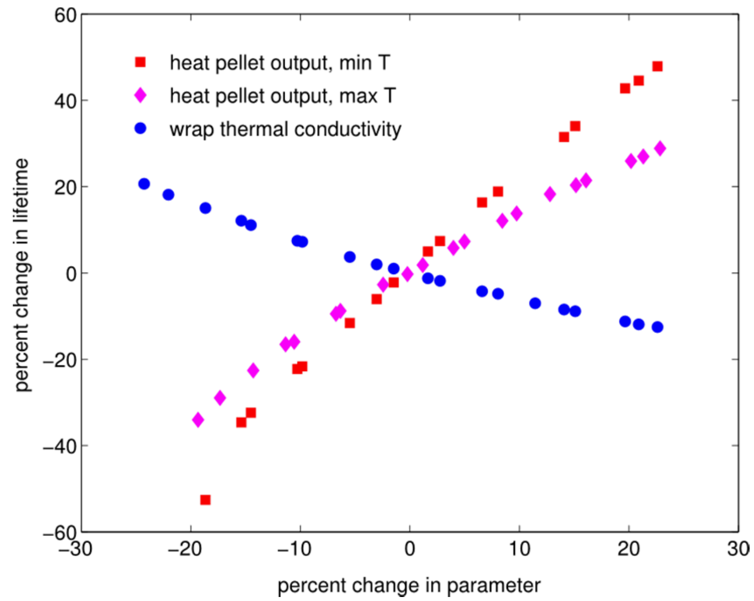
Lifetime of Large Side-Fired Battery

- Large difference between min temp and max temp definitions
- Collapses almost perfectly when plotted as a Delta



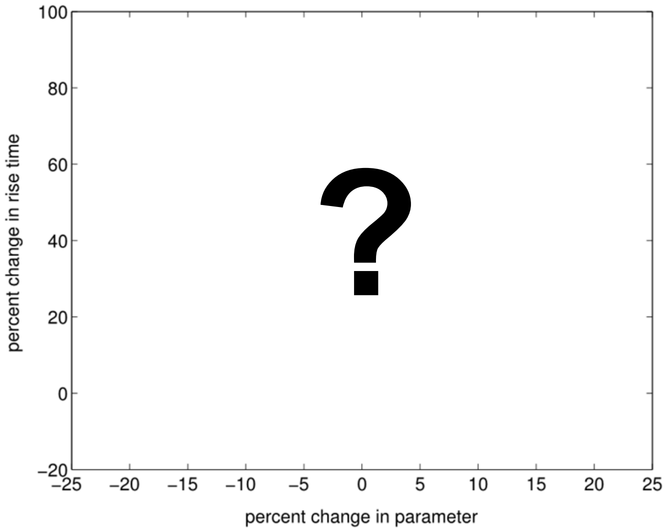
Lifetime of Large Side-Fired Battery

- Large difference between min temp and max temp definitions
- Collapses almost perfectly when plotted as a Delta
- Good collapse when given as a percent change from baseline
  - easier to compare across batteries



Rise Time of Small Center-Fired Battery

- Two obvious mediators of rise time:
  - burn rate
  - calorific output
- Acceptable ranges for these parameters specified for each pellet type.
- Which is more important to rise time?



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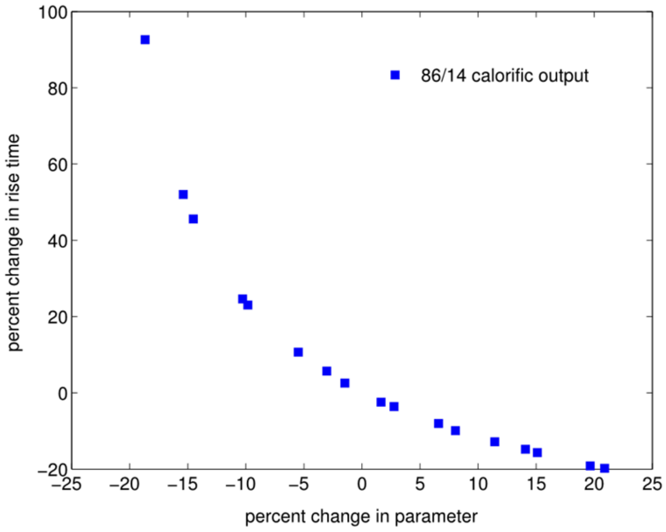
- Which is more important to rise time?
  - Very sensitive to calorific output



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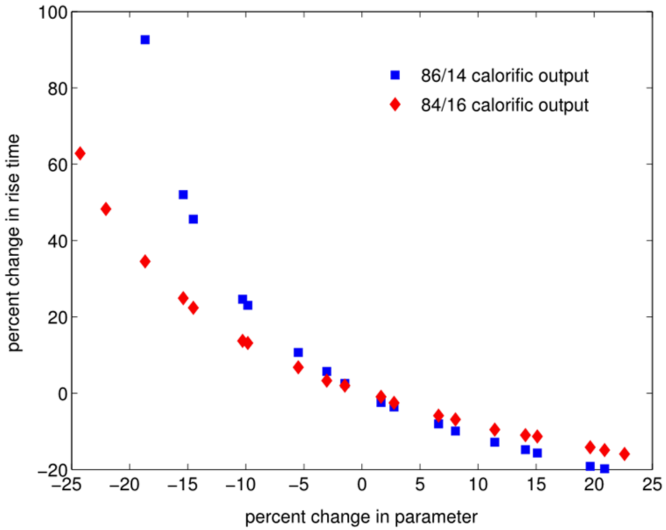
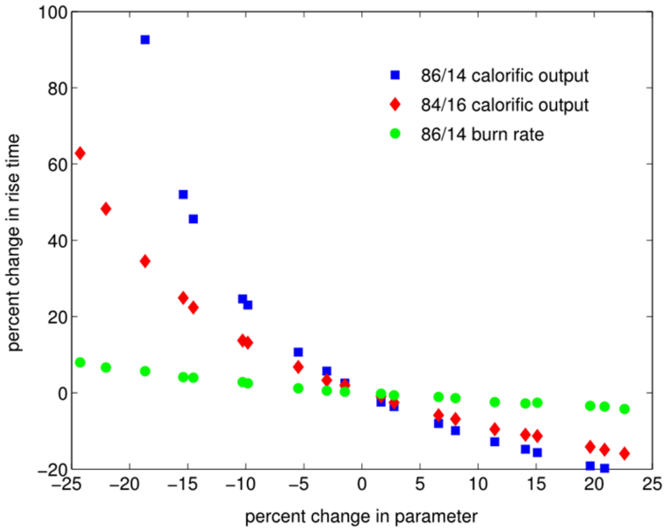
    - slightly less so for 84/16 (more energetic)



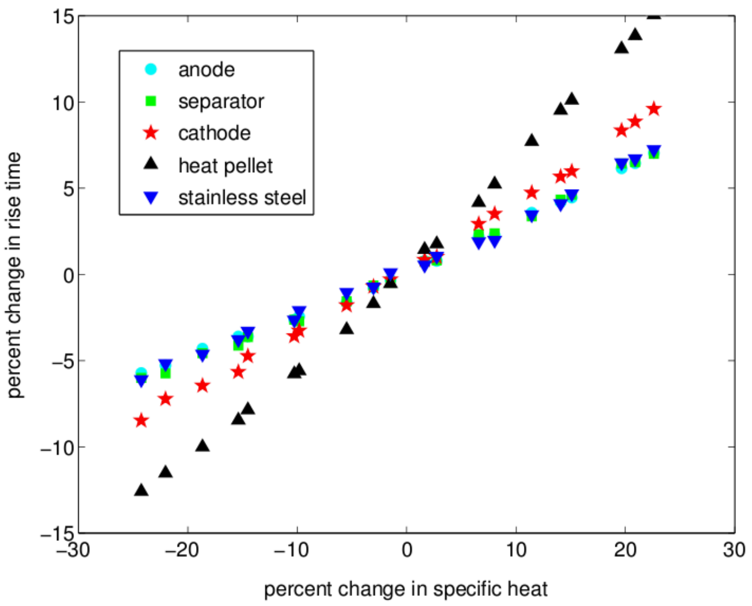
Rise Time of Small Center-Fired Battery

- Two obvious mediators of rise time:
  - burn rate
  - calorific output
- Acceptable ranges for these parameters specified for each pellet type.
- Which is more important to rise time?
  - Very sensitive to calorific output
    - slightly less so for 84/16 (more energetic)
  - Much less sensitive to burn rate



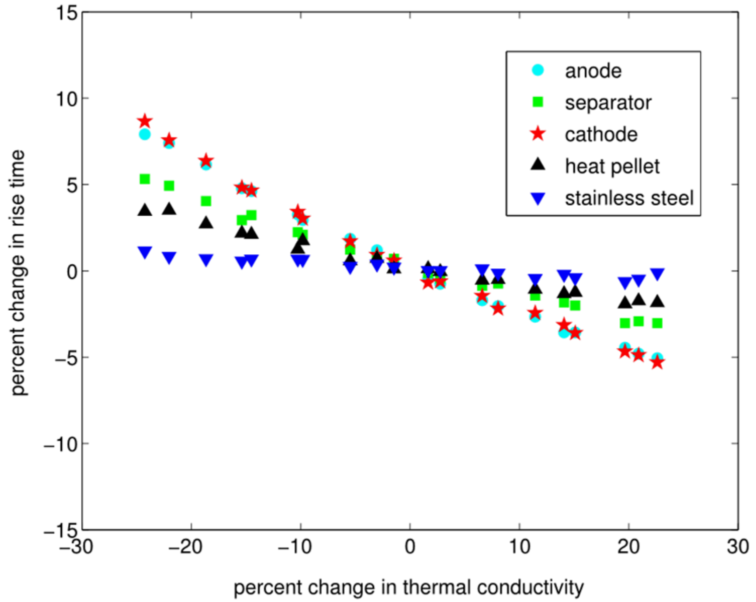
Rise Time of Small Center-Fired Battery

- Sensitivity to specific heat comparable to burn rate
- Sensitivity tracks heat capacity
  - specific heat x density x volume



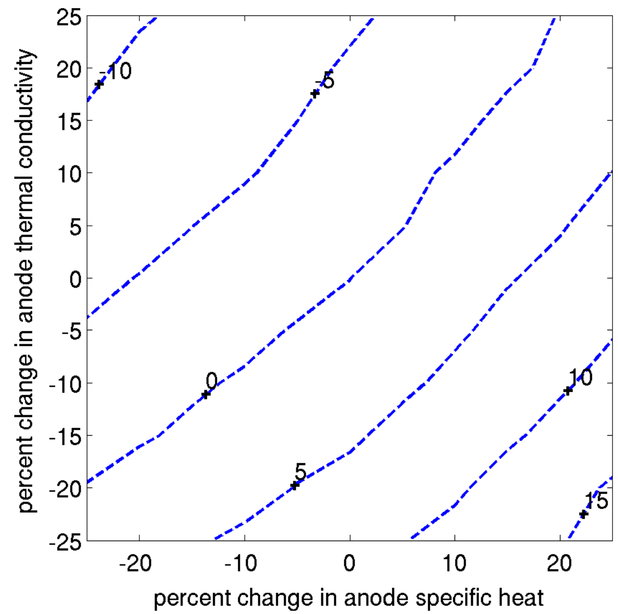
Rise Time of Small Center-Fired Battery

- Sensitivity to thermal conductivity comparable to specific heat
  - far less for heat pellet
  - somewhat more for anode and cathode
  - position with respect to the separator drives sensitivity
  - far, far less for steel collectors
    - makes sense because they are so thin



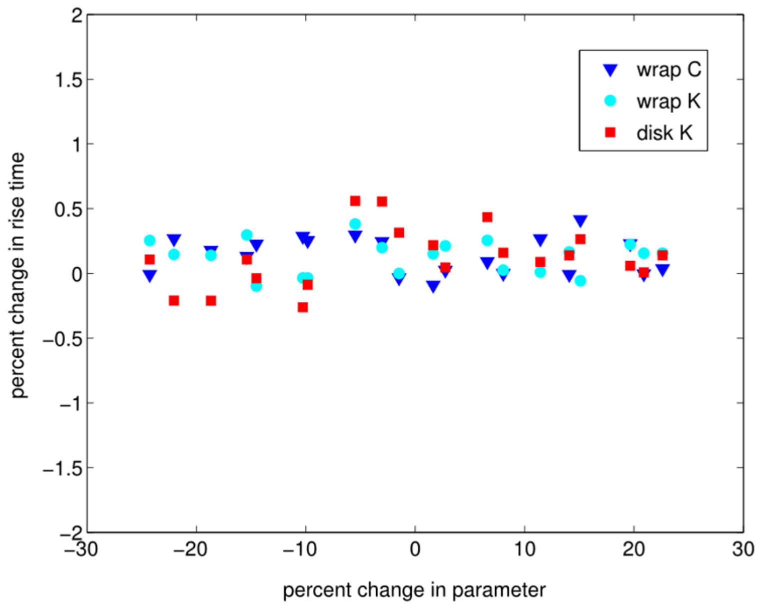
Rise Time of Small Center-Fired Battery

- To check for nonlinear interactions, a two-dimensional study can be run
  - Diagonal contours indicate independent effect
- Nothing interesting found for thermal conductivity and specific heat of anode



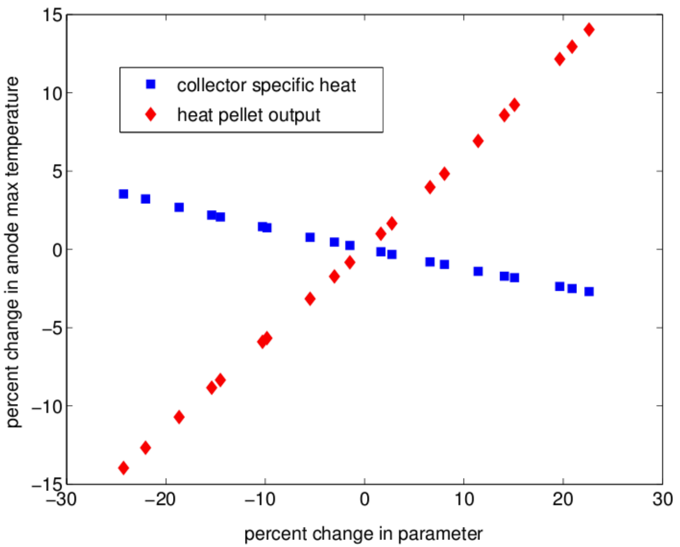
Rise Time of Small Center-Fired Battery

- Rise time is not sensitive to insulation
  - not surprising: the heat doesn't have much time to escape



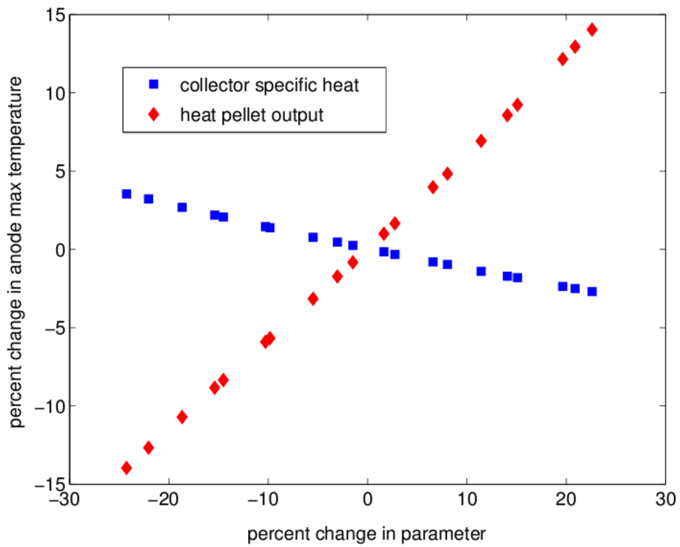
Max Anode Temperature in Small Battery

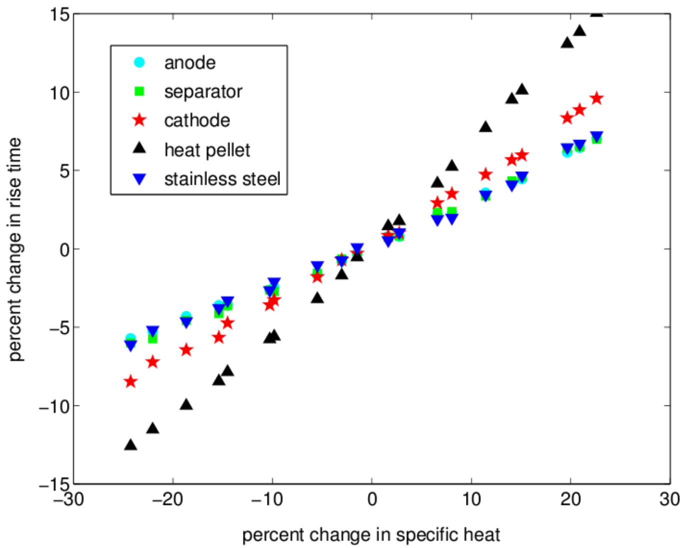
- Positive correlation with heat pellet output
- Negative correlation with collector specific heat
  - well-known buffering effect
  - opposite correlation to rise time



Max Anode Temperature in Small Battery

- Positive correlation with heat pellet output
- Negative correlation with collector specific heat
  - well-known buffering effect
  - opposite correlation to rise time
    - Can't add heat to reduce rise time, then fix anode temp by adding steel in this example.





Conclusion

- Sensitivity studies can help guide decisions on:
  - geometry
  - materials
  - property measurement
  - vendor requirements
- The large number of trials required for these studies make simulation attractive
- Automated exploration of parameter space and post-processing of results is very helpful
  - available through the open-source DAKOTA toolkit
    - dakota.sandia.gov