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Characterizing Heat Transfer from Venting Li-ion Batteries Undergoing Thermal Runaway with Inverse Techniques

Andrew Kurzawski, Alex Bates, Lucas Gray, Loraine Torres-Castro, Timothy Walsh, John Hewson

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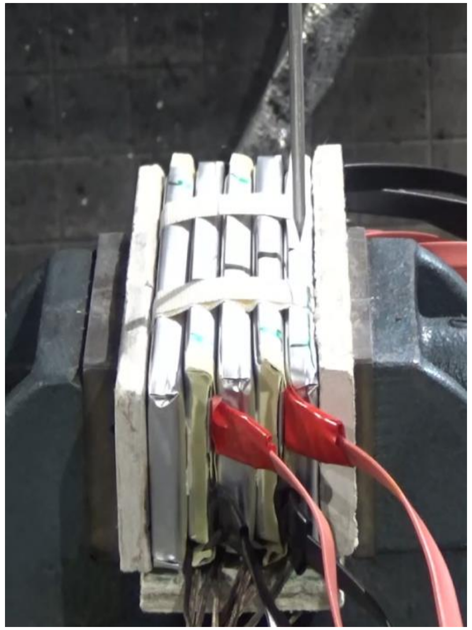
U.S. DEPARTMENT OF ENERGY

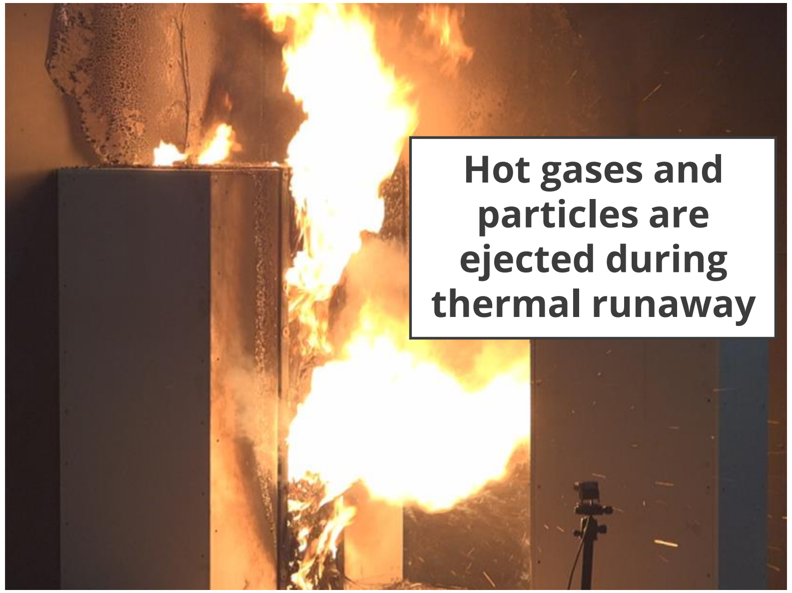
NNSA

MOTIVATION

- Li-ion batteries are becoming more prevalent in larger systems
  - Electric vehicles
  - Energy storage systems
- Thermal runaway is a major safety concern
  - Manufacturing defects
  - Improper use
  - Mechanical damage
- Thermal runaway can spread to other cells and through the system if not contained.
- Literature has focused on propagation via conduction, less exists on heat transfer from vented gases and solid ejecta.

Propagation through conduction



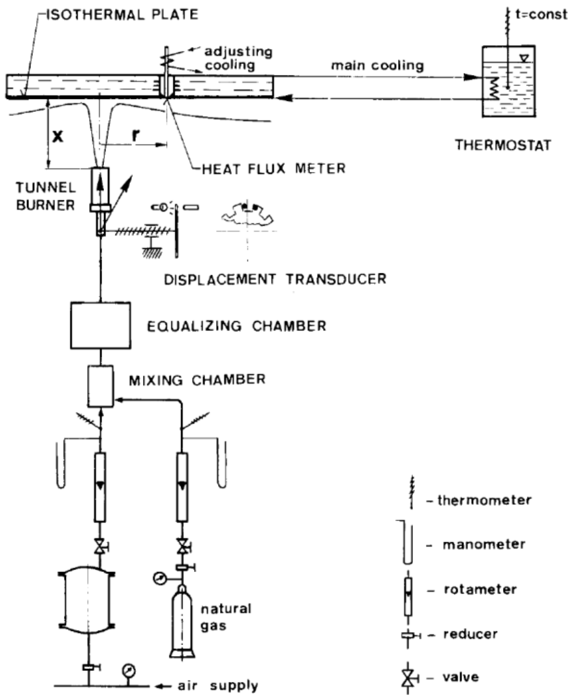


Source: https://www.ul.com/news/ul-9540a-battery-energy-storage-system-ess-test-method

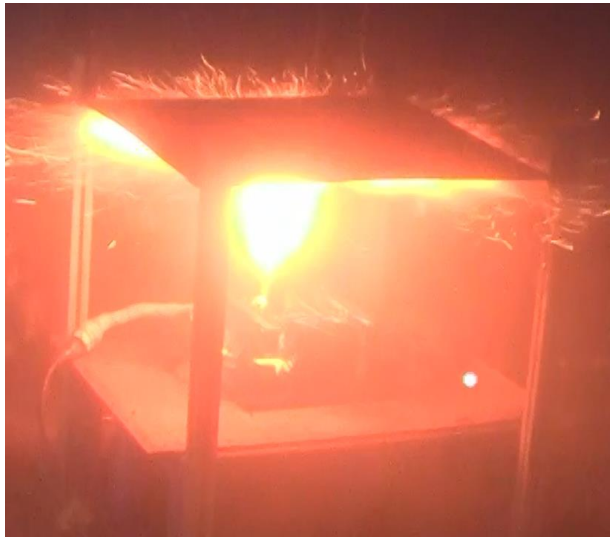
VENTING HEAT TRANSFER

Goal: we want to design an apparatus to measure heat flux of a venting jet impinging on a flat surface.

- Typically, jet heat transfer correlations are created with well-controlled steady state systems.
- High energy density batteries can vent in 10 – 30 seconds, meaning we need to make transient measurements.



Cylindrical and prismatic cells have vent ports

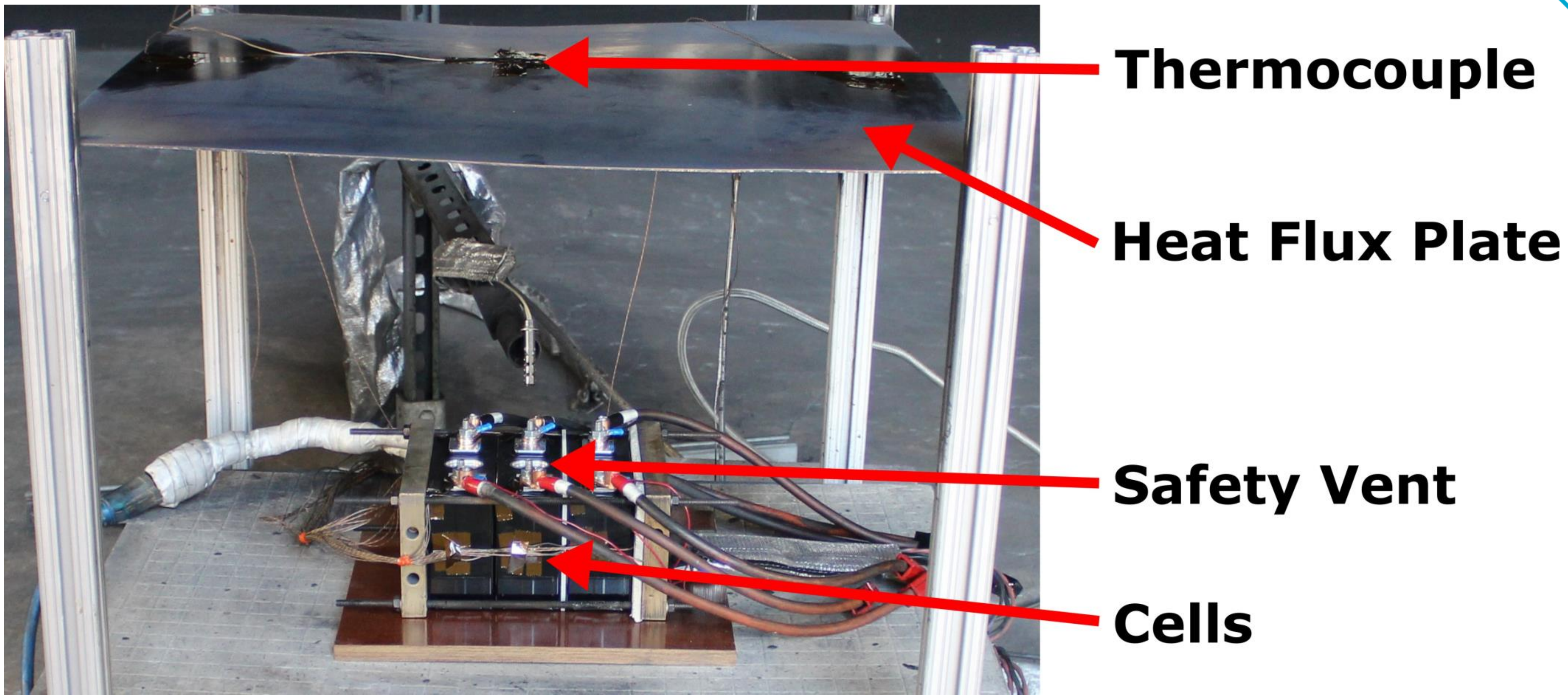


Venting prismatic cell ejecting particles and gas

In this work: we use simulations motivated by preliminary experiments to design a heat flux measurement apparatus.

Image source: Popiel, C. O., Van der Meer, T. H., and Hoogendoorn, C., "Convective heat transfer on a plate in an impinging round hot gas jet of low reynolds number," International journal of heat and mass transfer, 23(8), pp. 1055–1068 (1980)

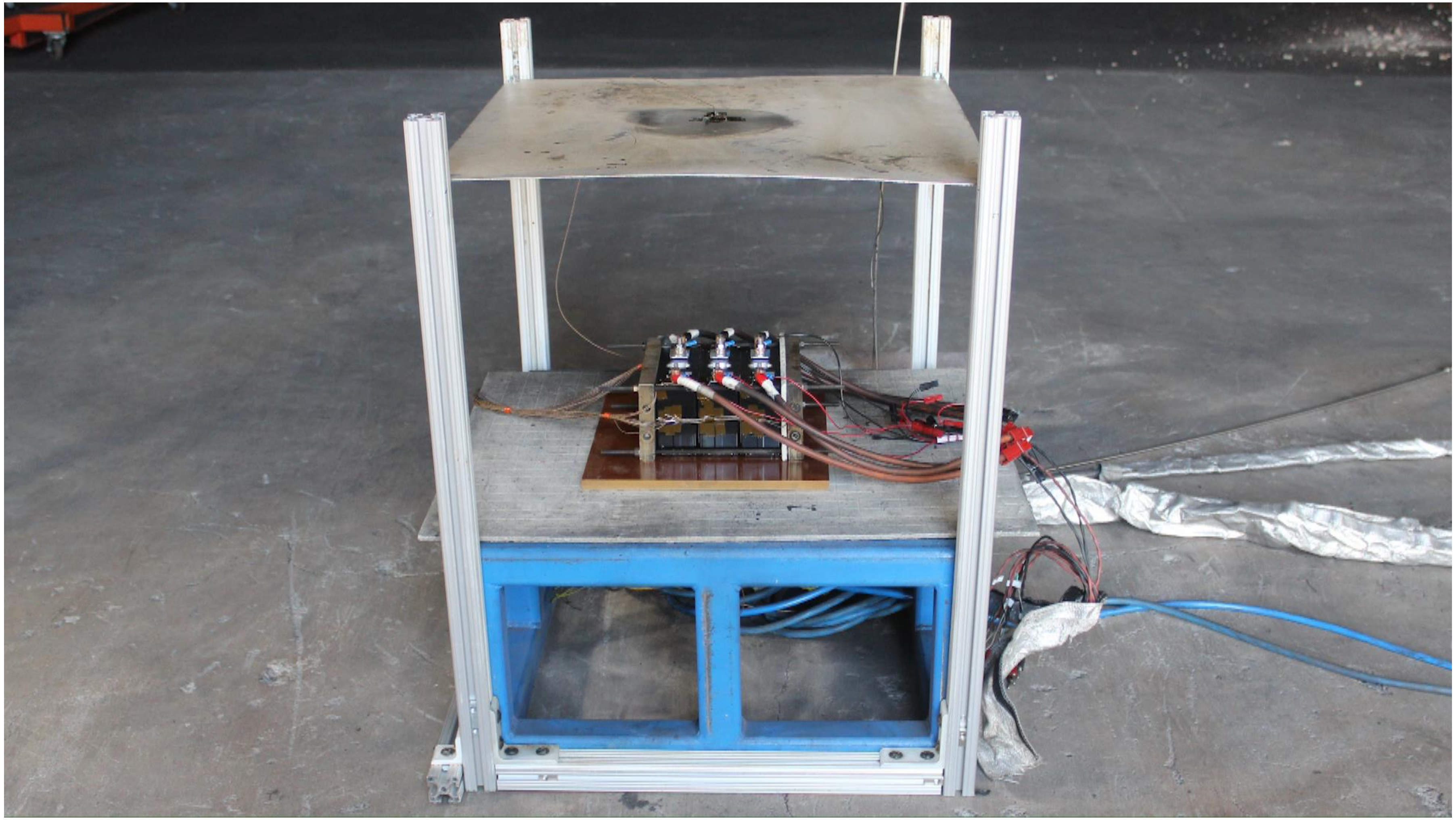
VENTING SCENARIO



Scoping experiments: plate with 1 – 3 thermocouples 12” above the cells

How do we go from temperature measurements to heat flux? **Solve the inverse problem!**

VENTING SCENARIO



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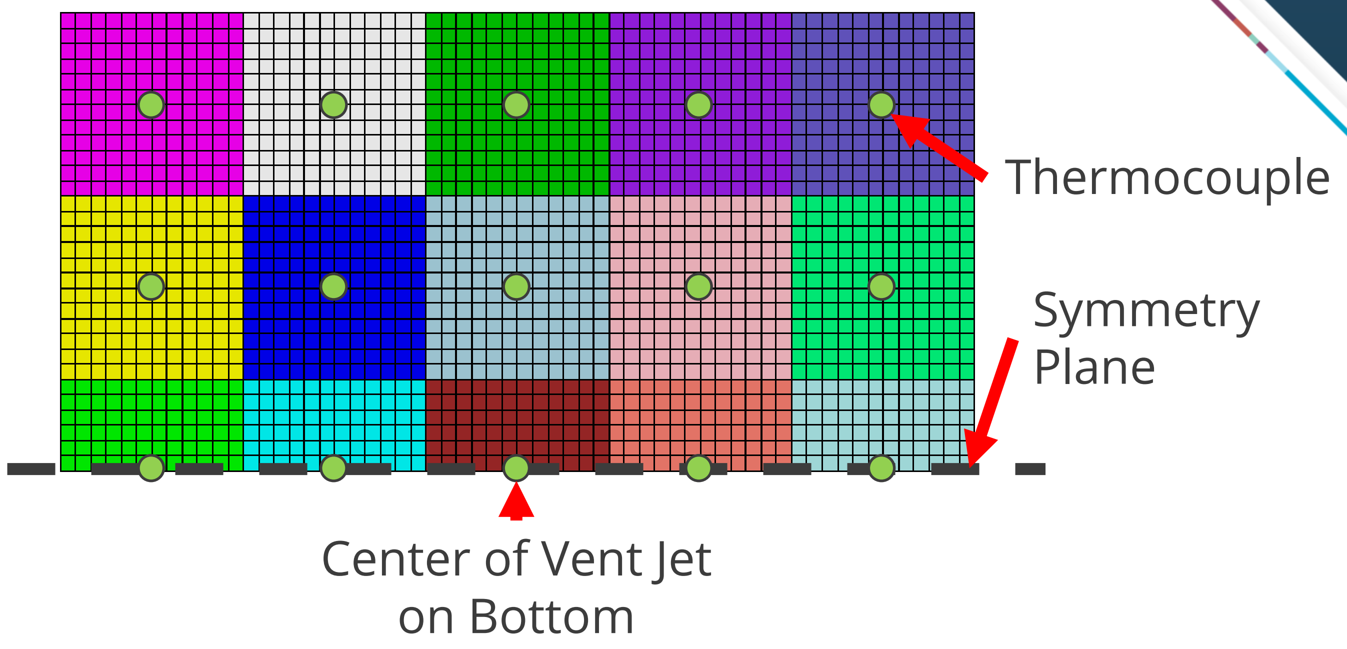
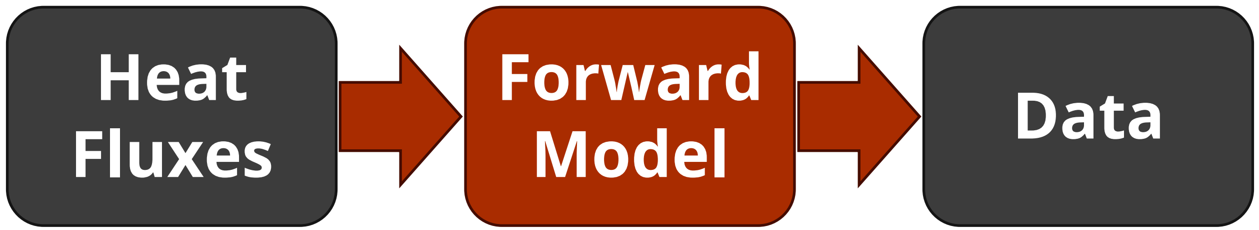
SIMULATION METHODS

- Model: 3D finite element heat transfer in SIERRA Aria
- Symmetric domain
  - 2' x 2' steel plate (variable thickness)
  - One symmetry plane
  - Thermocouples on the top (variable #)
  - Heat flux applied to the bottom
- Given thermocouple temperatures, solve the inverse problem for heat flux as a function of space and time.
- Inverse Aria uses adjoints for efficient optimization of unknown heat fluxes.

Simulation Domain: Top View





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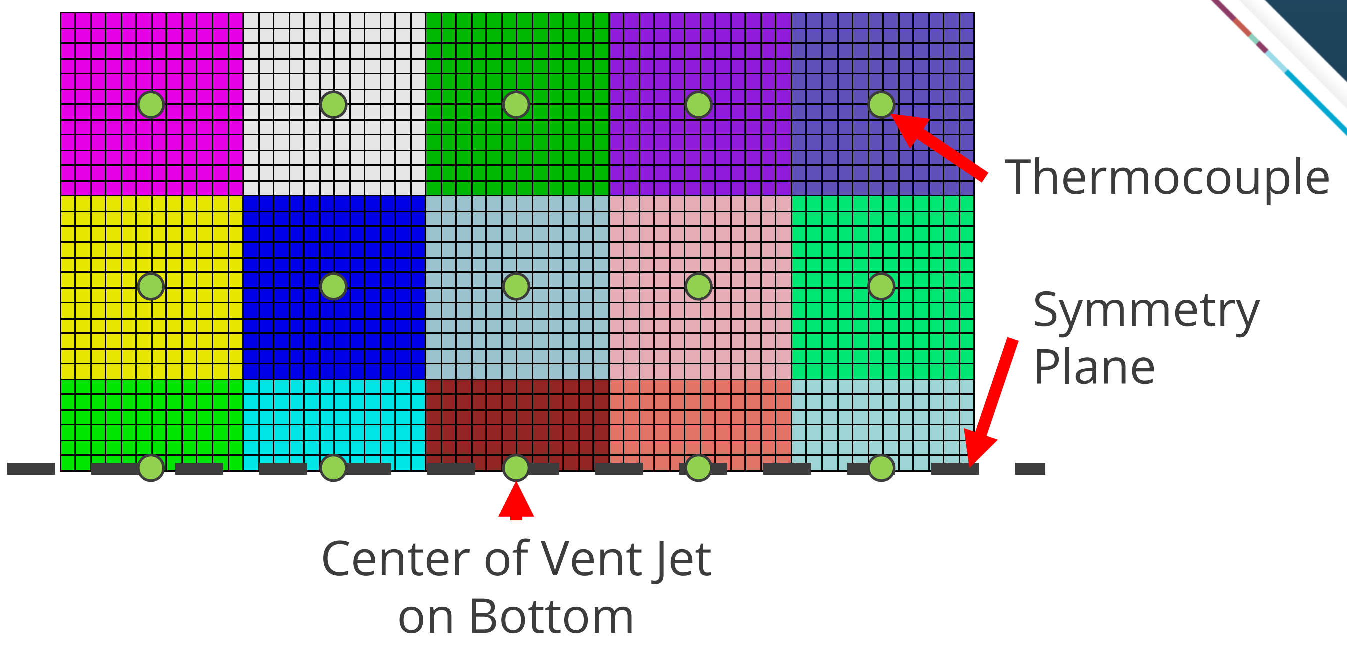
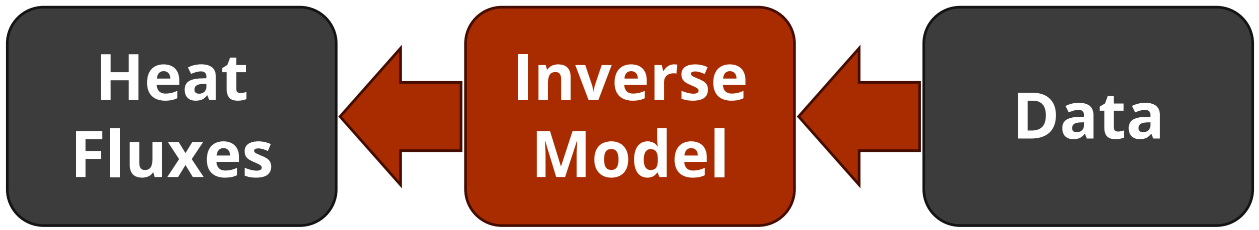
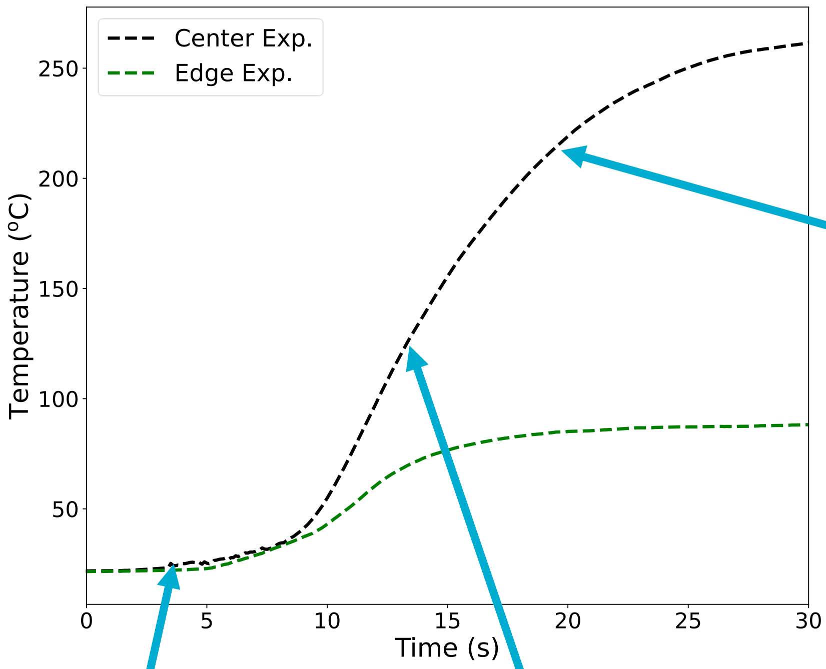




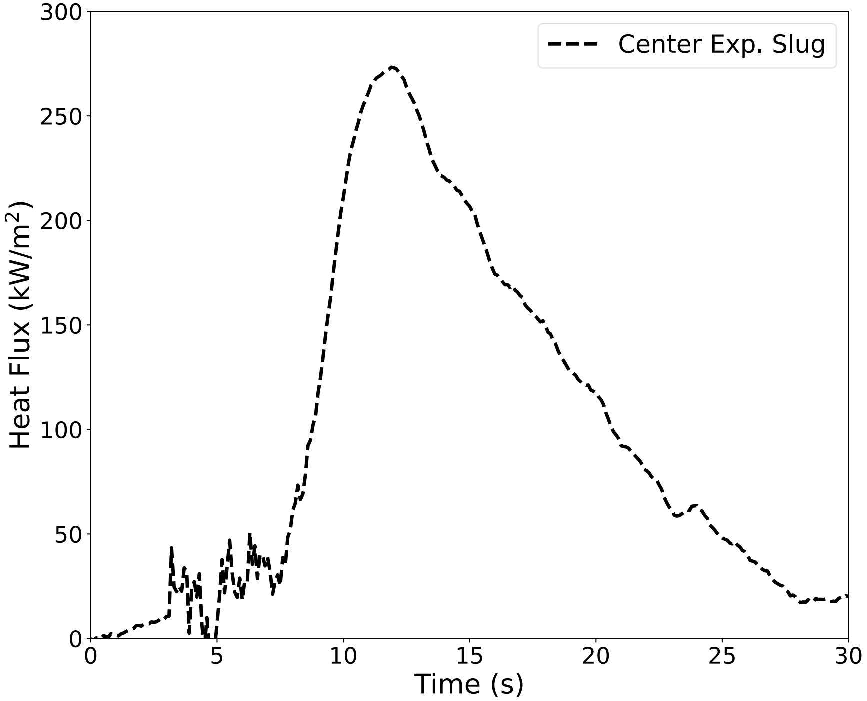
We need to generate synthetic data to test a range of scenarios.

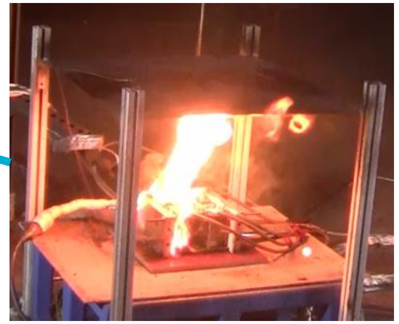
GENERATION OF APPROXIMATE HEAT FLUX PROFILE



Venting progression:

- Unburned gas and hot particles
- Fast flaming
- Slow flaming





Processed experimental TCs with a slug calorimeter approximation that ignores transverse losses:

$$q''_{Center\ Exp.\ Slug} = \rho c_p \delta \frac{dT_{Center\ Exp.}}{dt}$$

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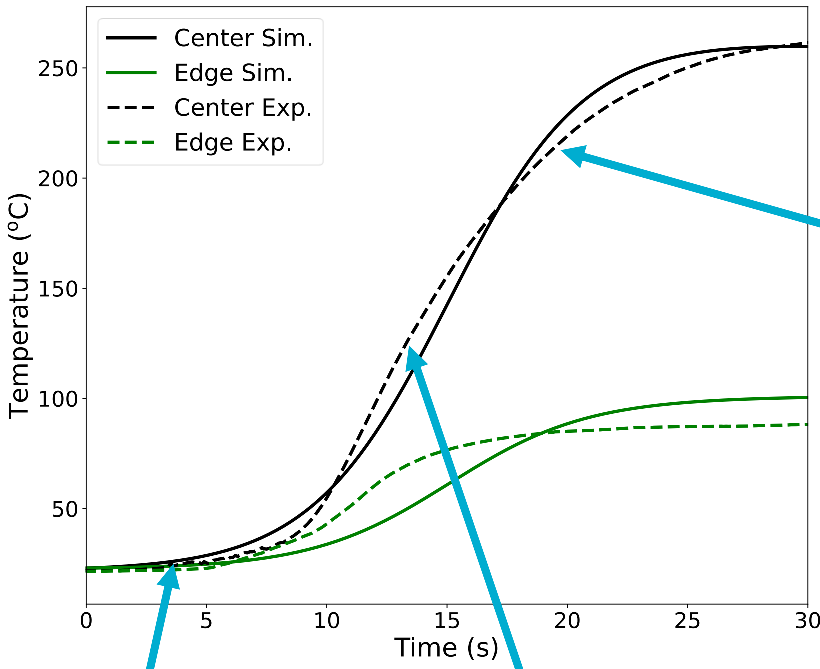

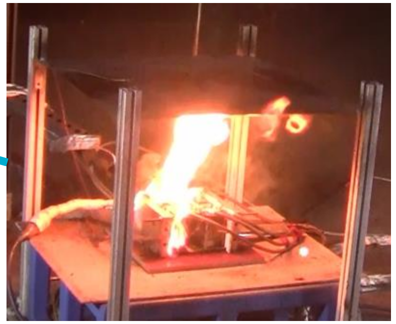

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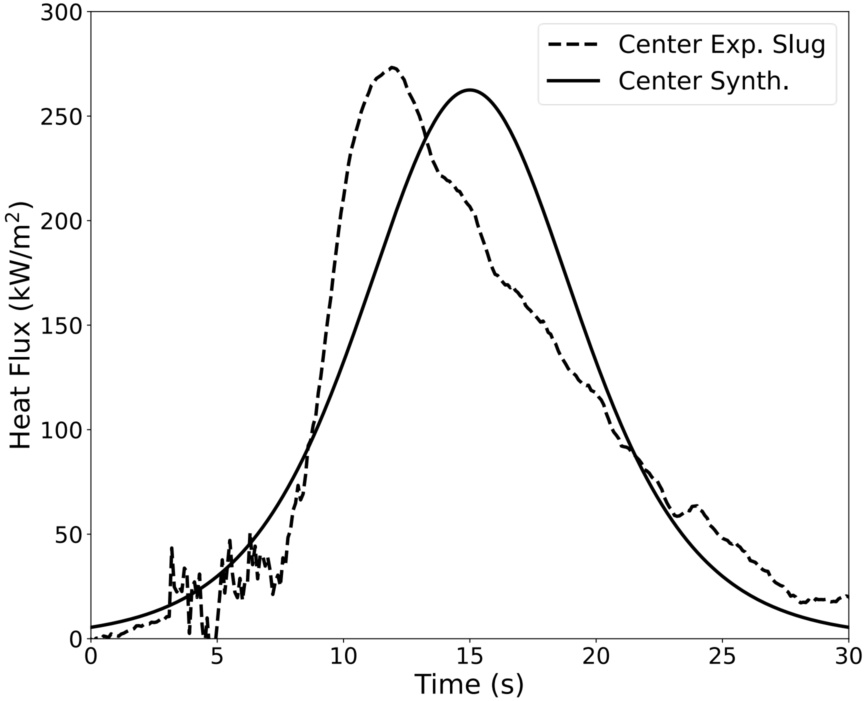

Generated approximate synthetic heat flux profile to explore the inverse problem

Gaussian flux centered on jet, peaks at 15 s

GENERATION OF APPROXIMATE HEAT FLUX PROFILE

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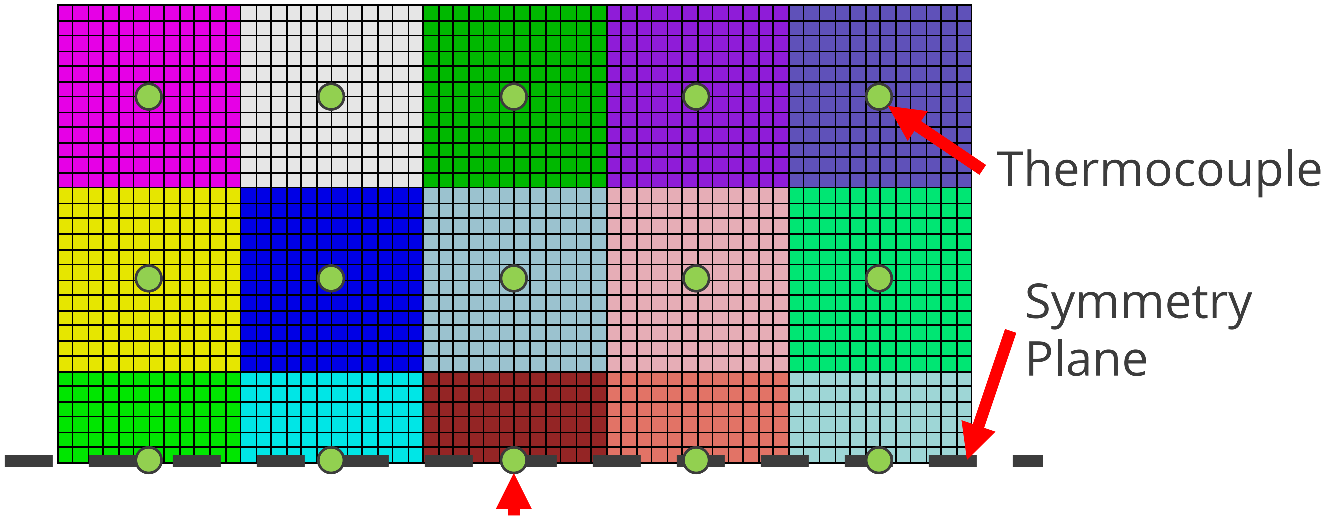

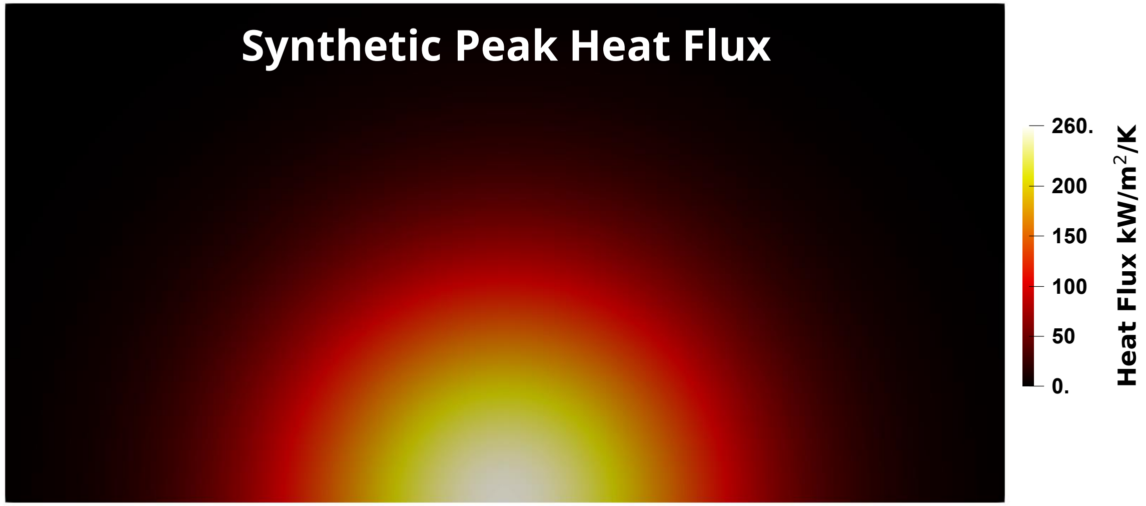

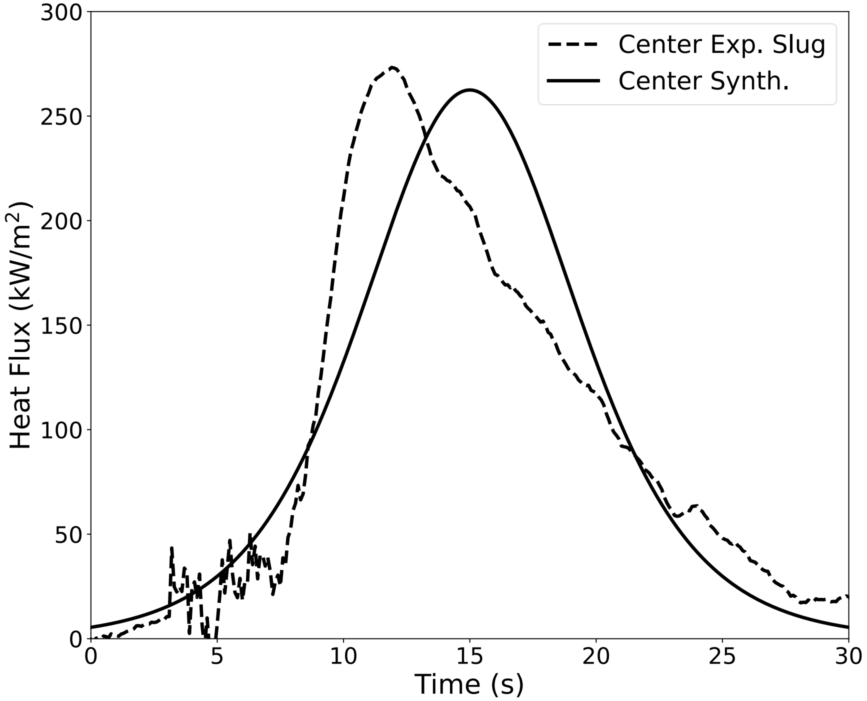

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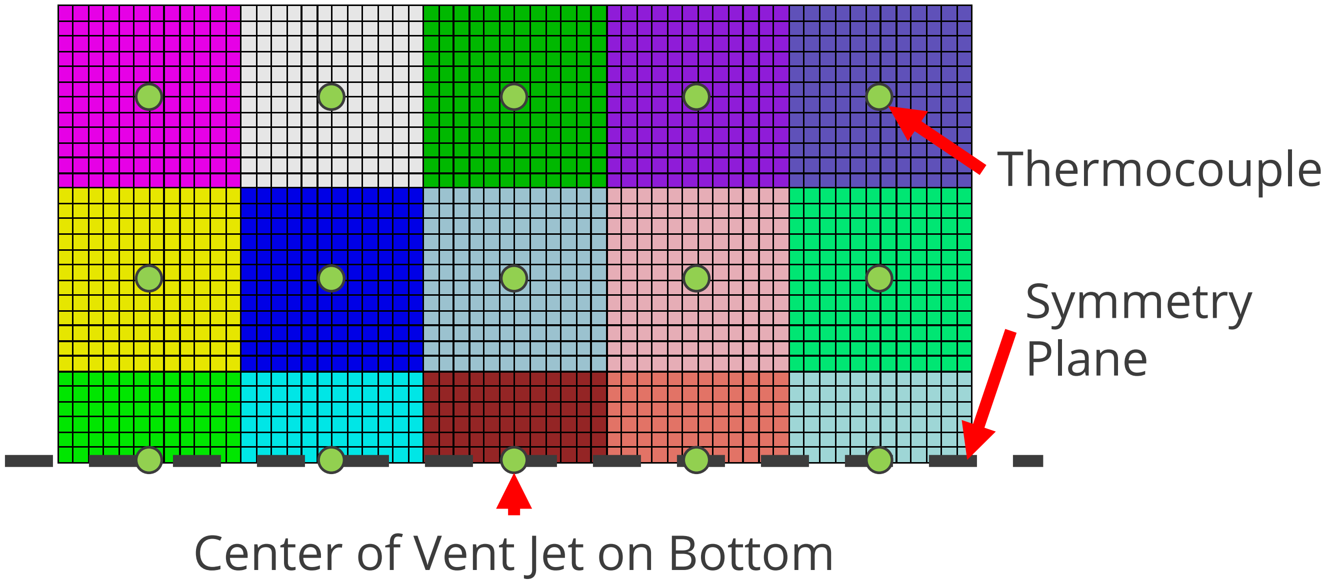
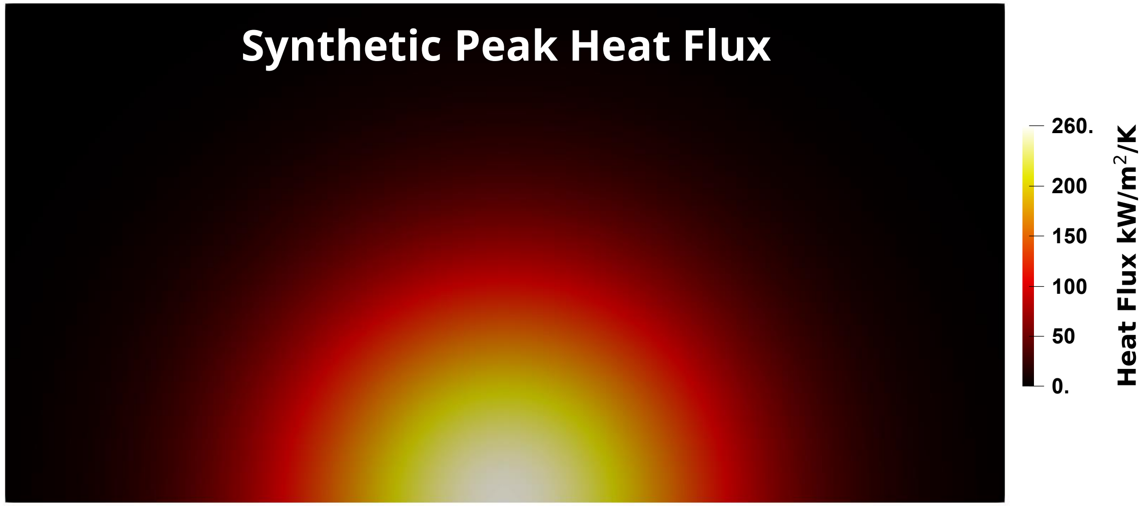
INVERSE HEAT FLUX PROBLEM

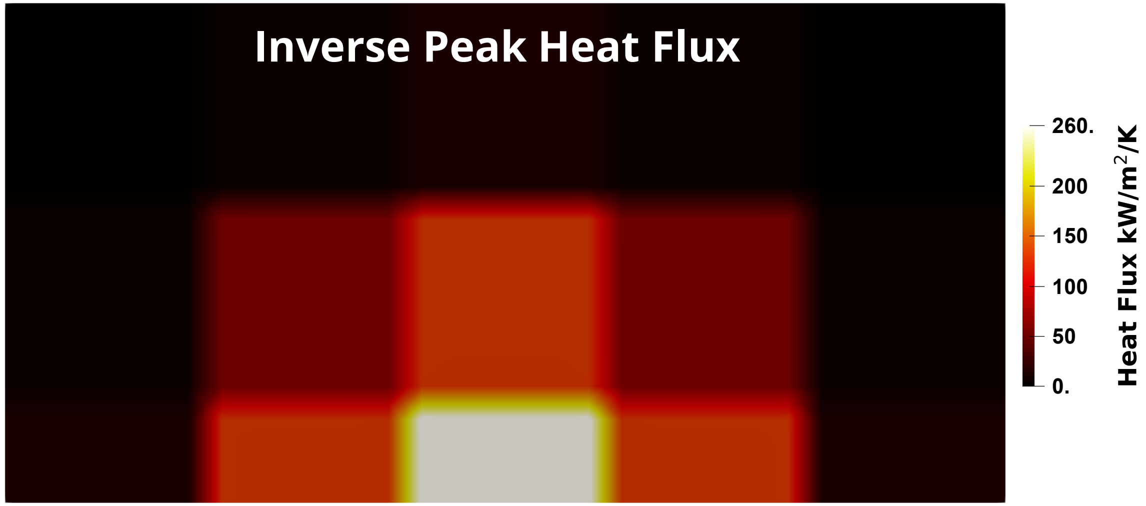
Simulation Domain: Top View



Inverse problem:

- Symmetric 3-D domain
- Each surface patch has spatially constant heat flux and a thermocouple centered on the patch
- Invert for transient piecewise linear heat flux at fixed intervals over 30 seconds at each patch

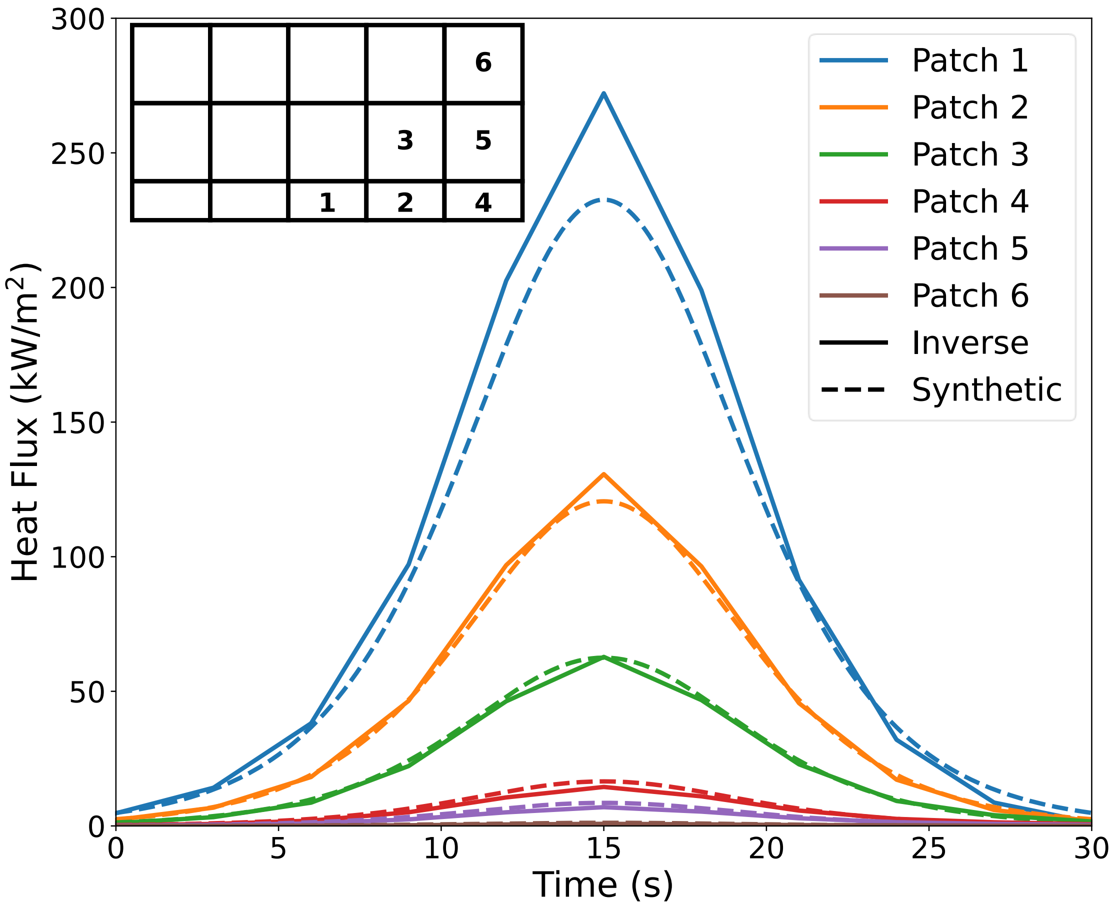




RESULTS: PLATE THICKNESS

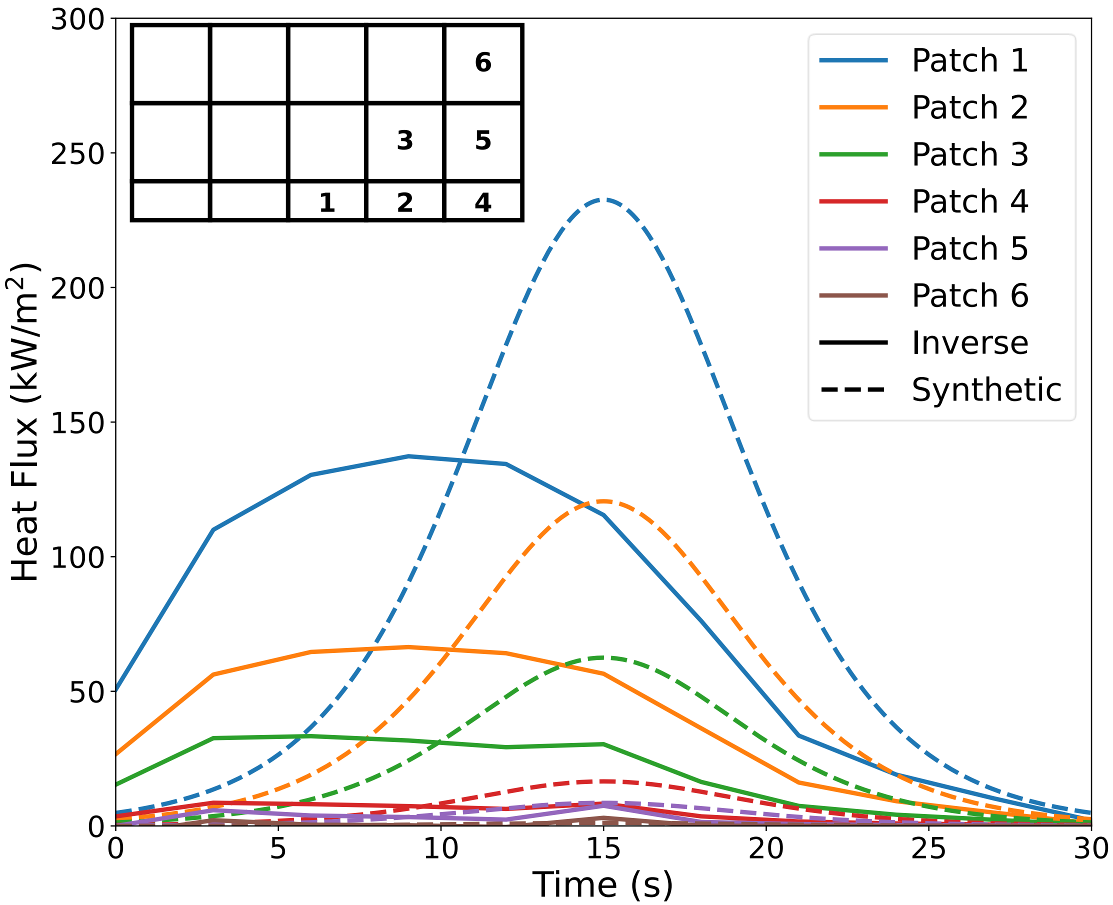
1/16" Plate

- Some over-prediction at the center



1/8" Plate

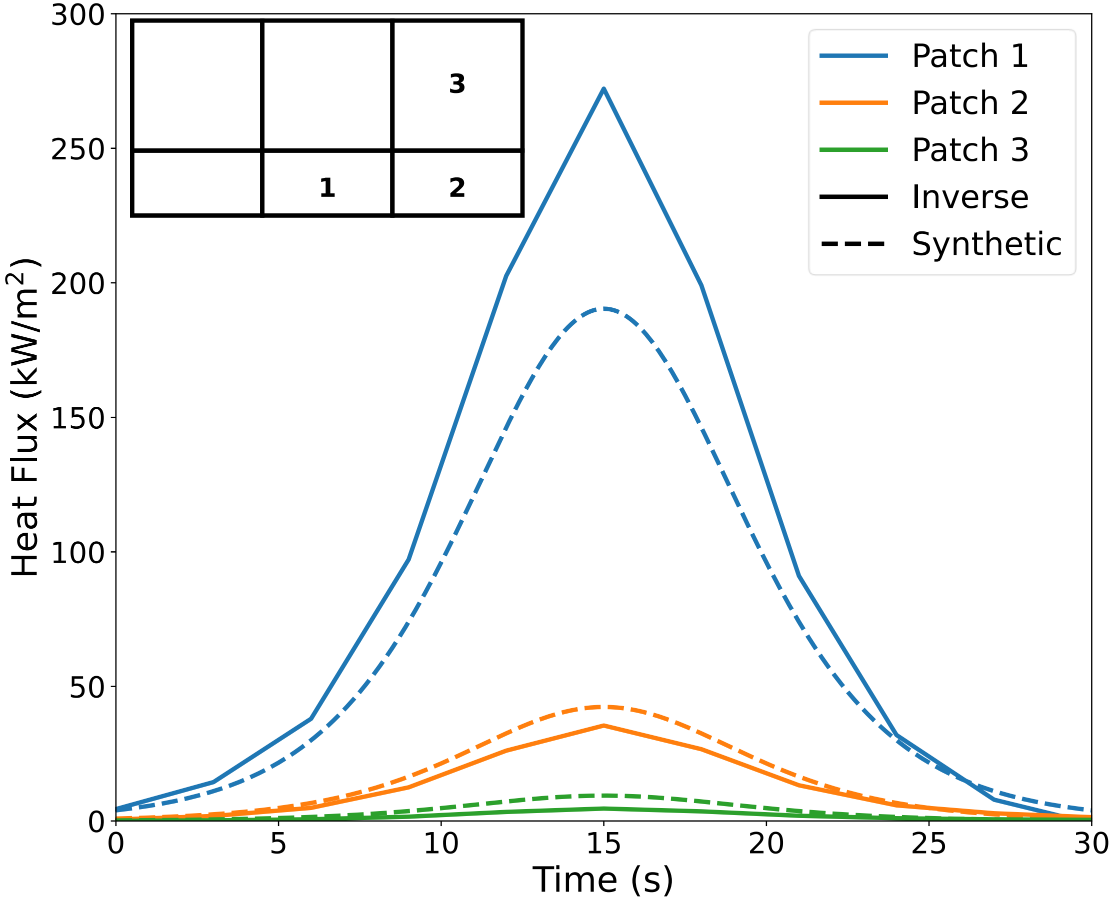
- Optimizer fails due to lack of sensitivity



RESULTS: THERMOCOUPLE DENSITY

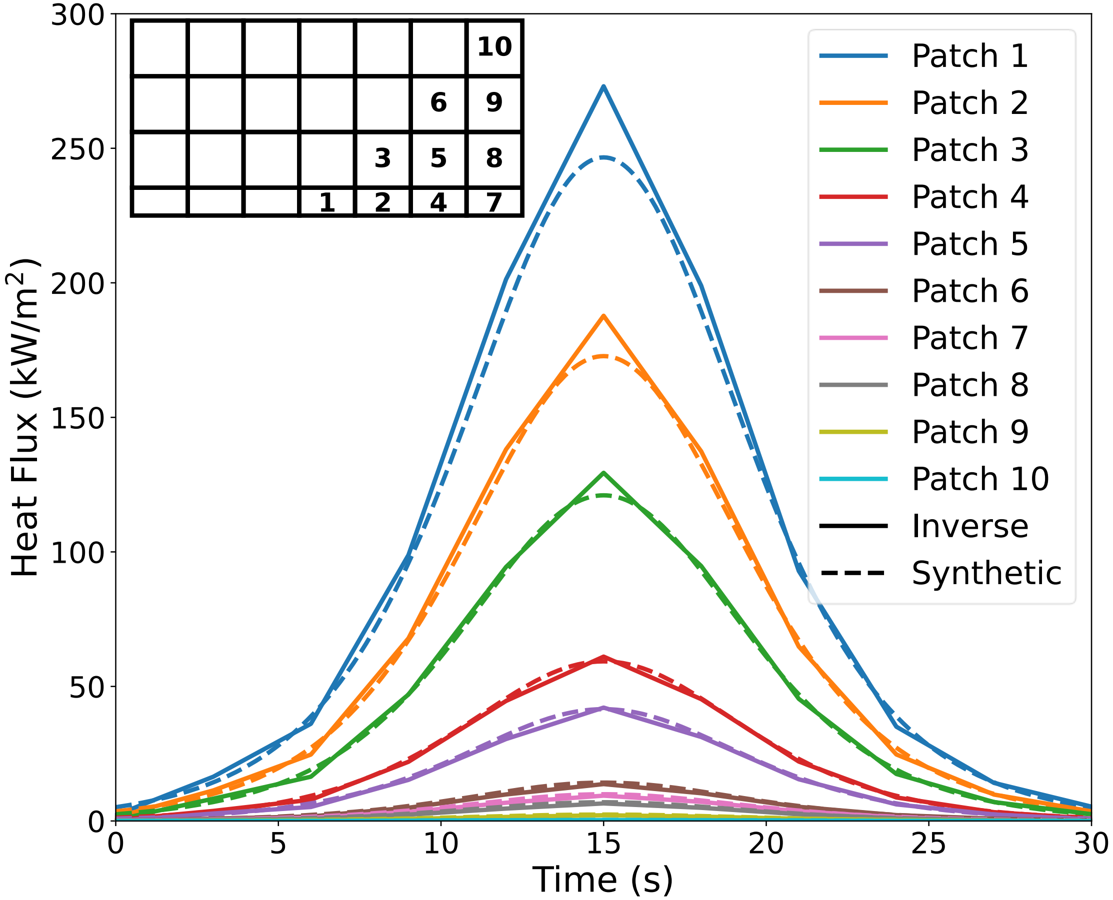
3 x 3 Grid

- Large over-prediction at the center
- Under-prediction away from the center



7 x 7 Grid

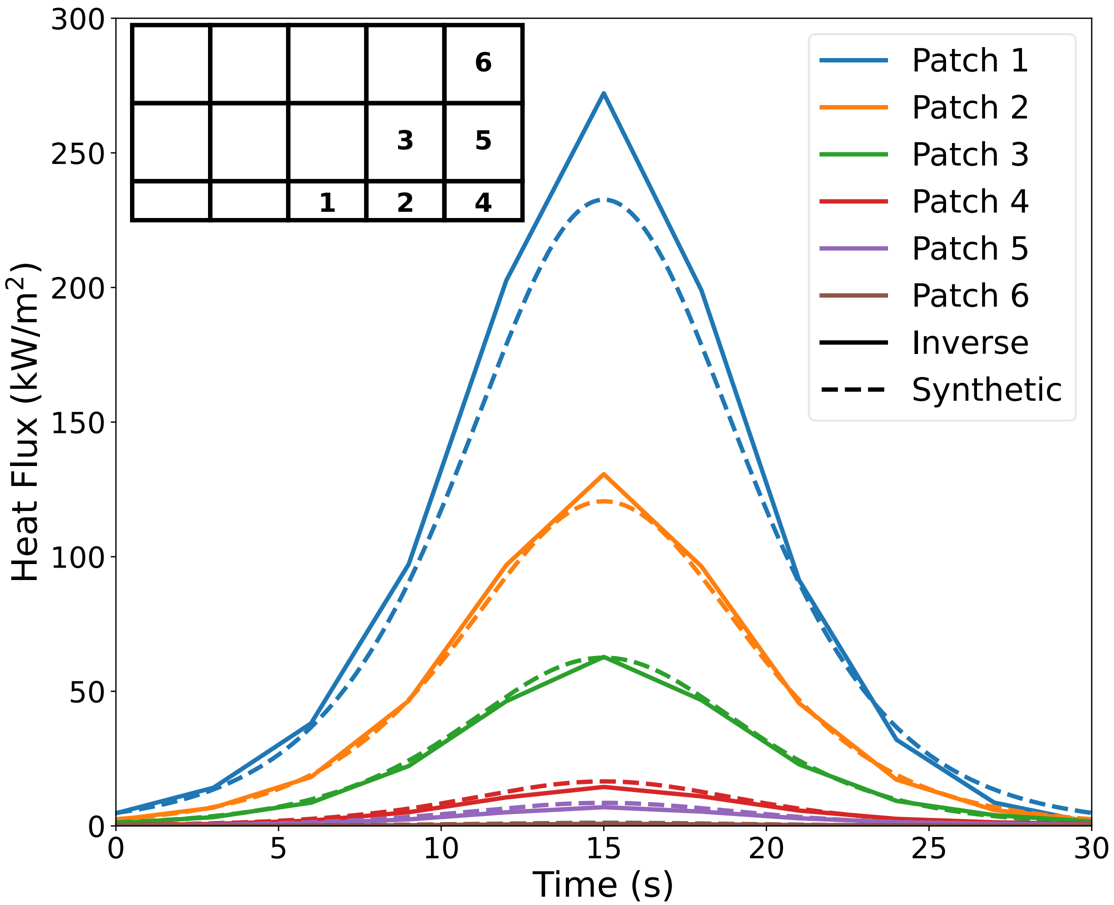
- Improved predictions with increased spatial resolution



RESULTS: PREDICTION BIAS

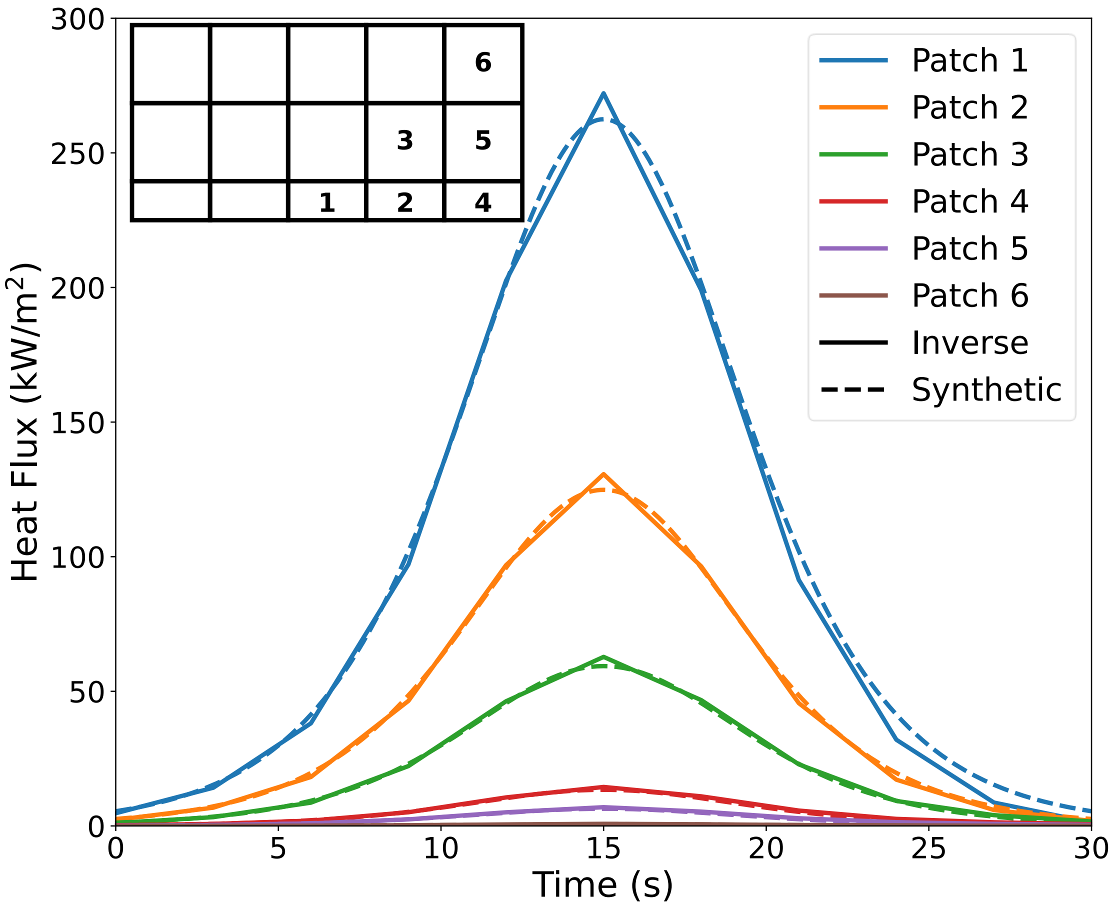
Average heat flux

- Some over-prediction at the center



Local heat flux at thermocouple

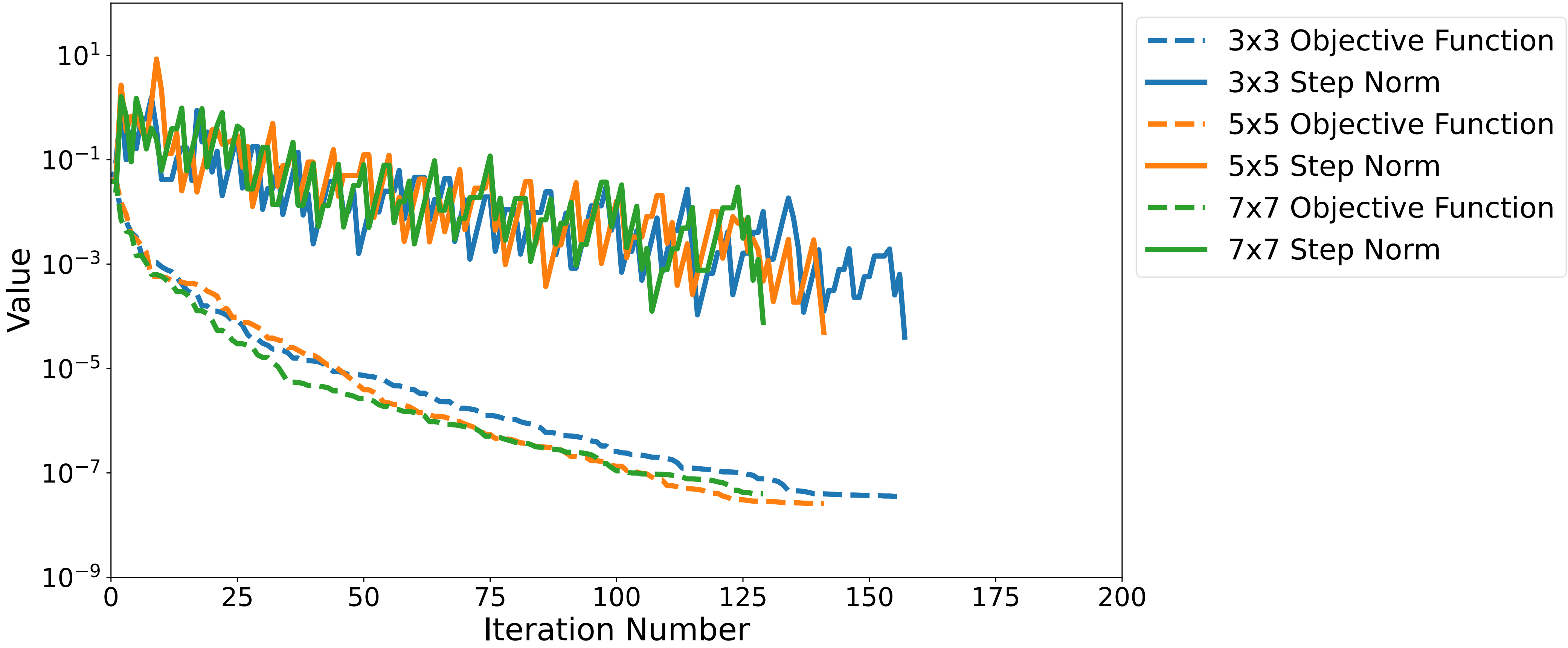
- Predictions biased towards local flux



RESULTS: COMPUTATIONAL COST

Cost: ~30 minutes to do the inverse problem on 4 processors

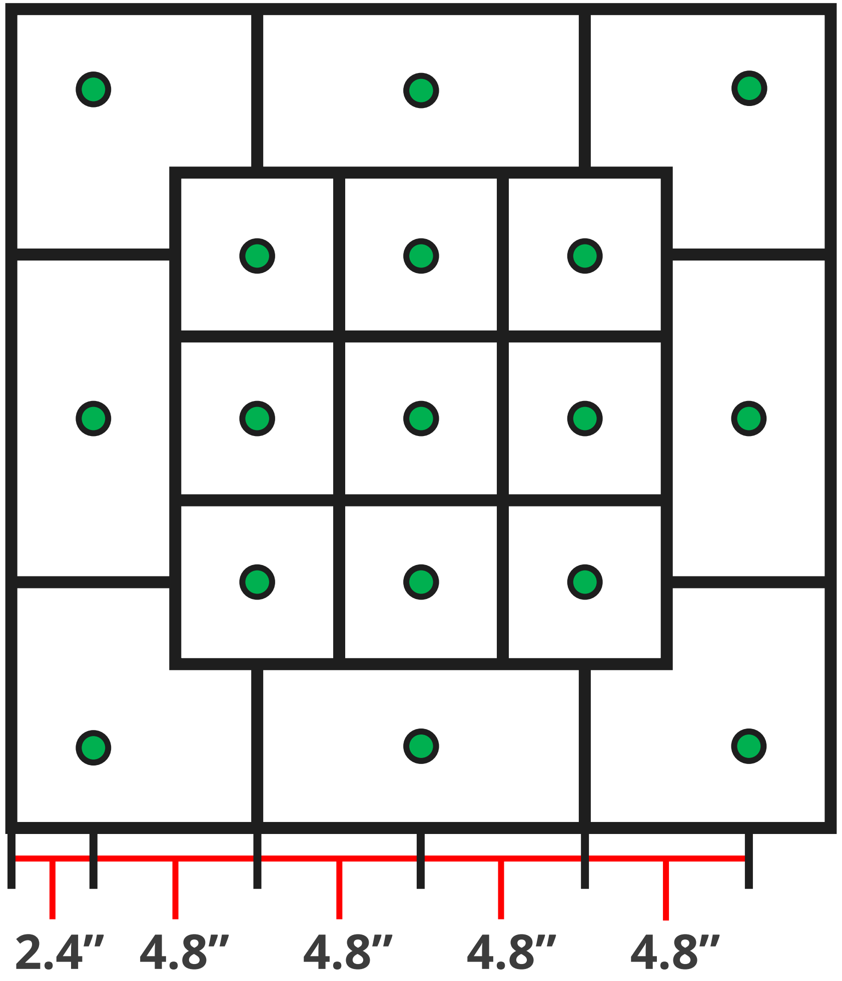
Higher number of patches converges faster

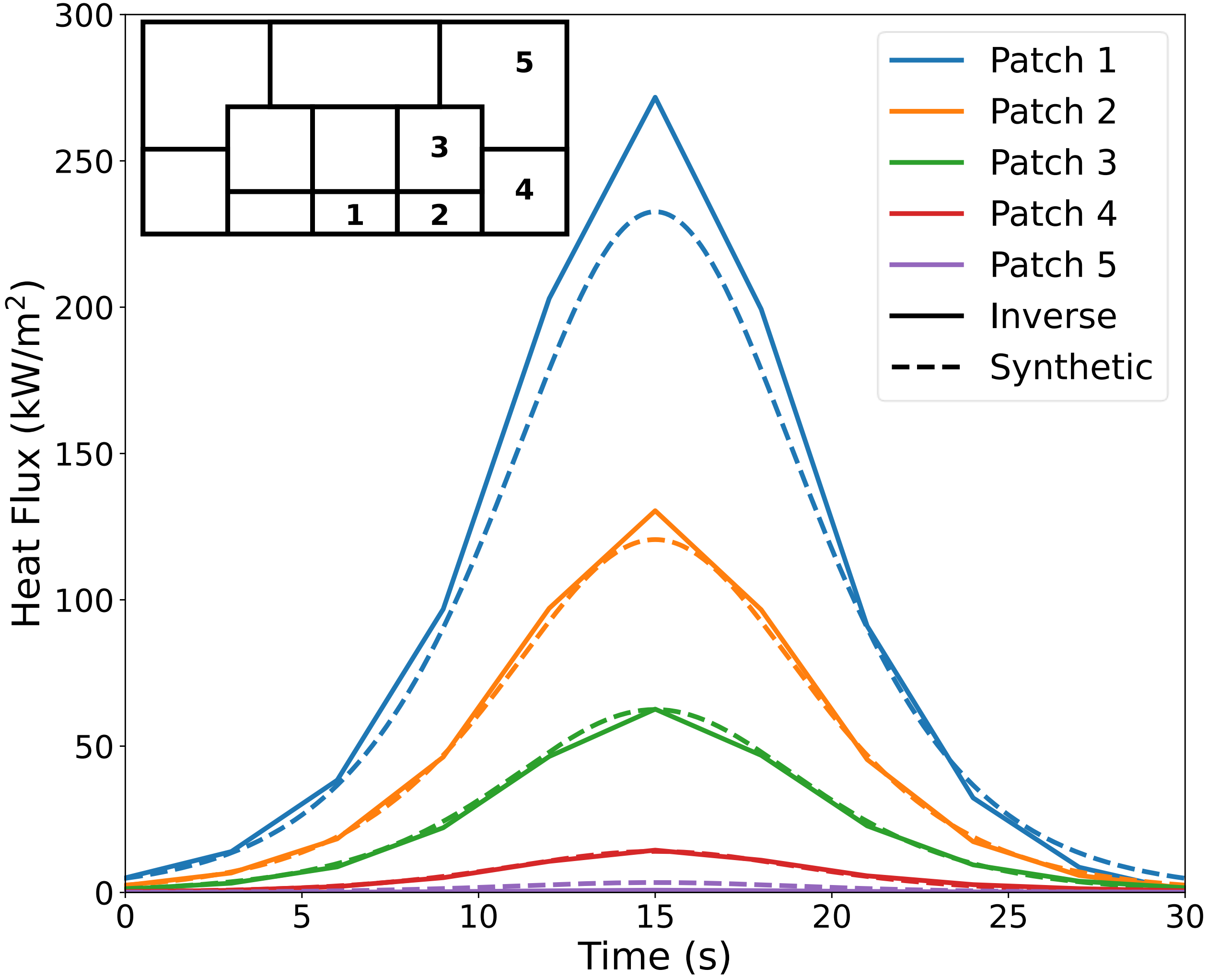


RESULTS: THERMOCOUPLE DENSITY

More thermocouples = more assembly time

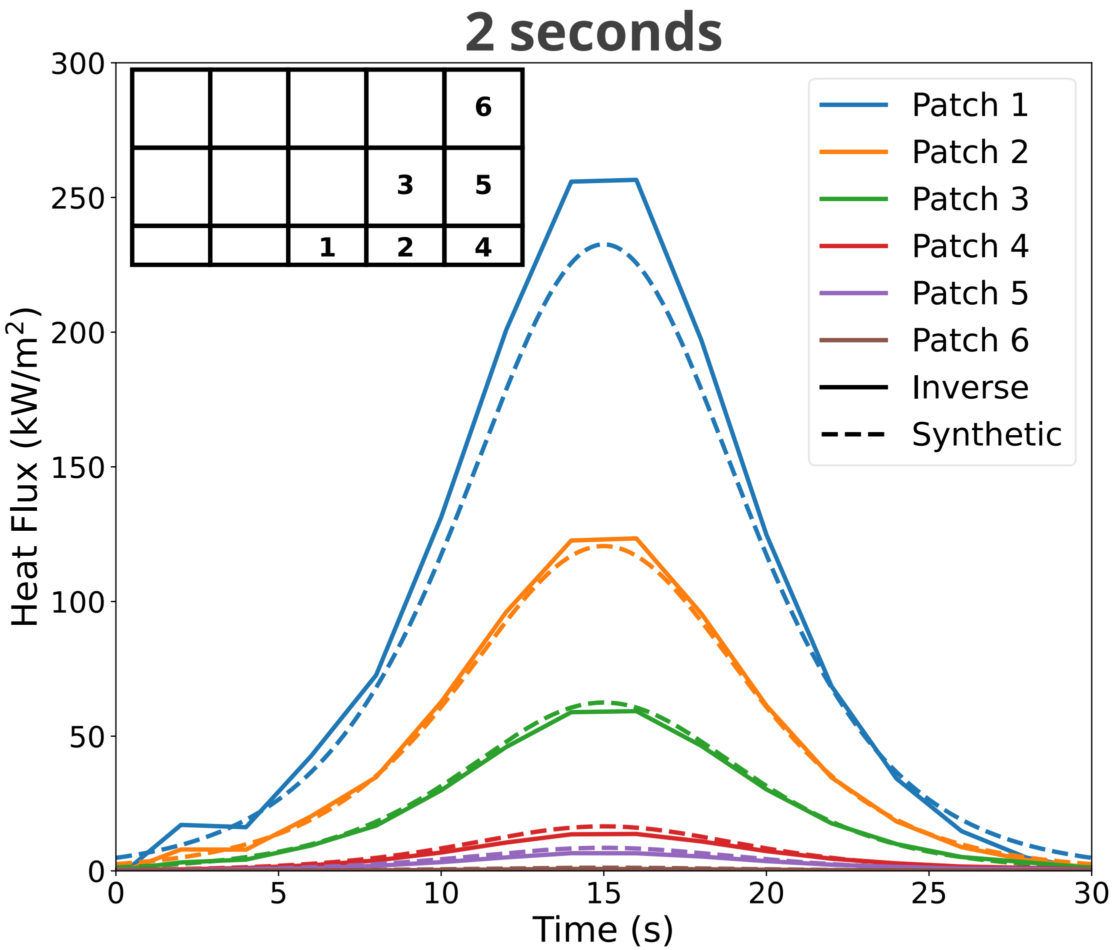
17 thermocouple grid

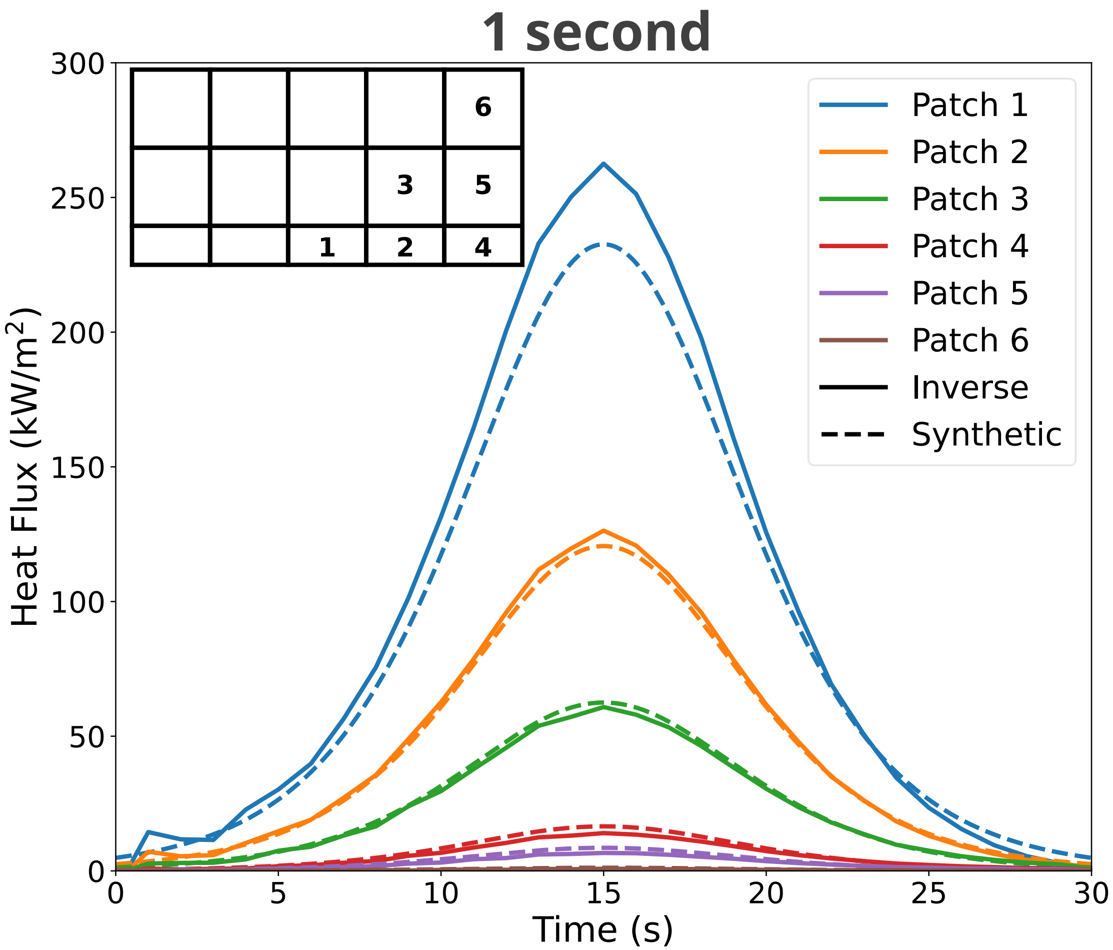




RESULTS: INVERSE TIME INTERVAL

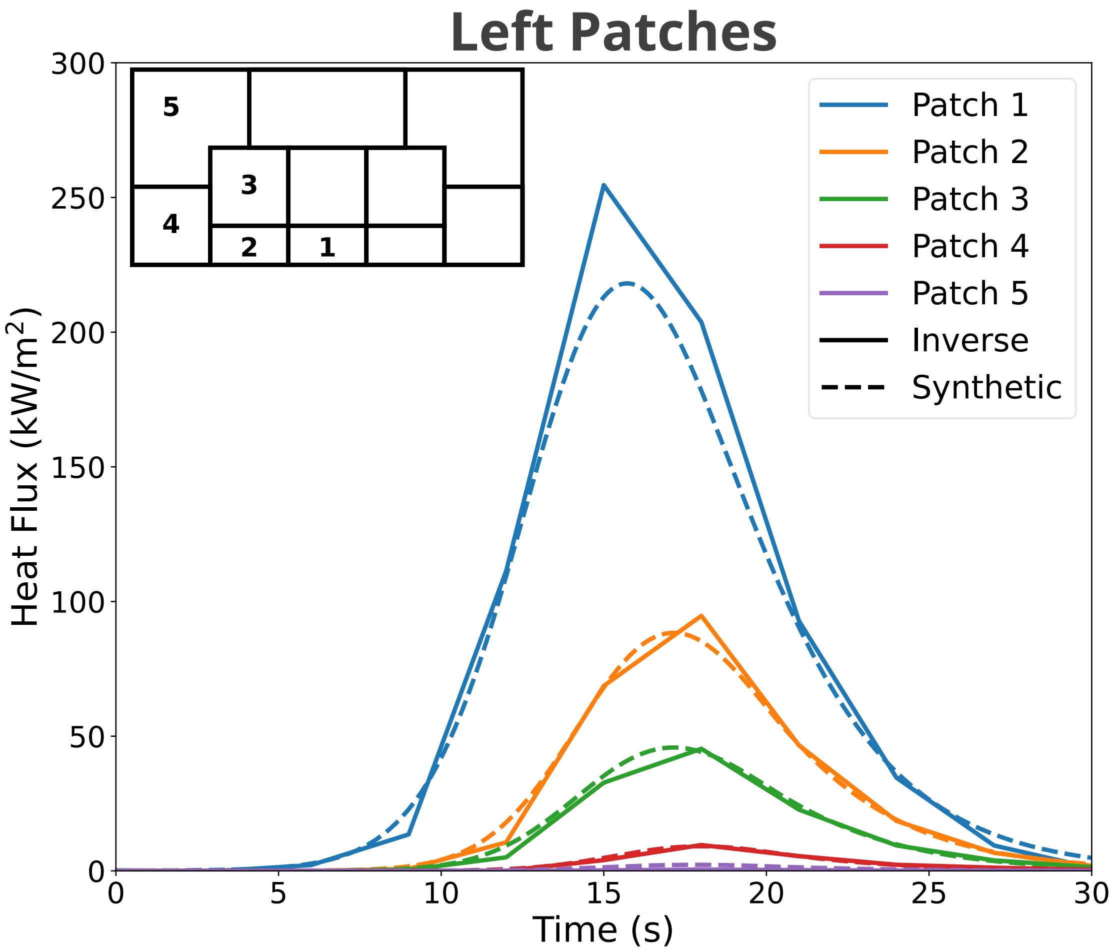
- Lower peak-over prediction compared to 3 seconds
- Insufficient sensitivity to early time heat fluxes

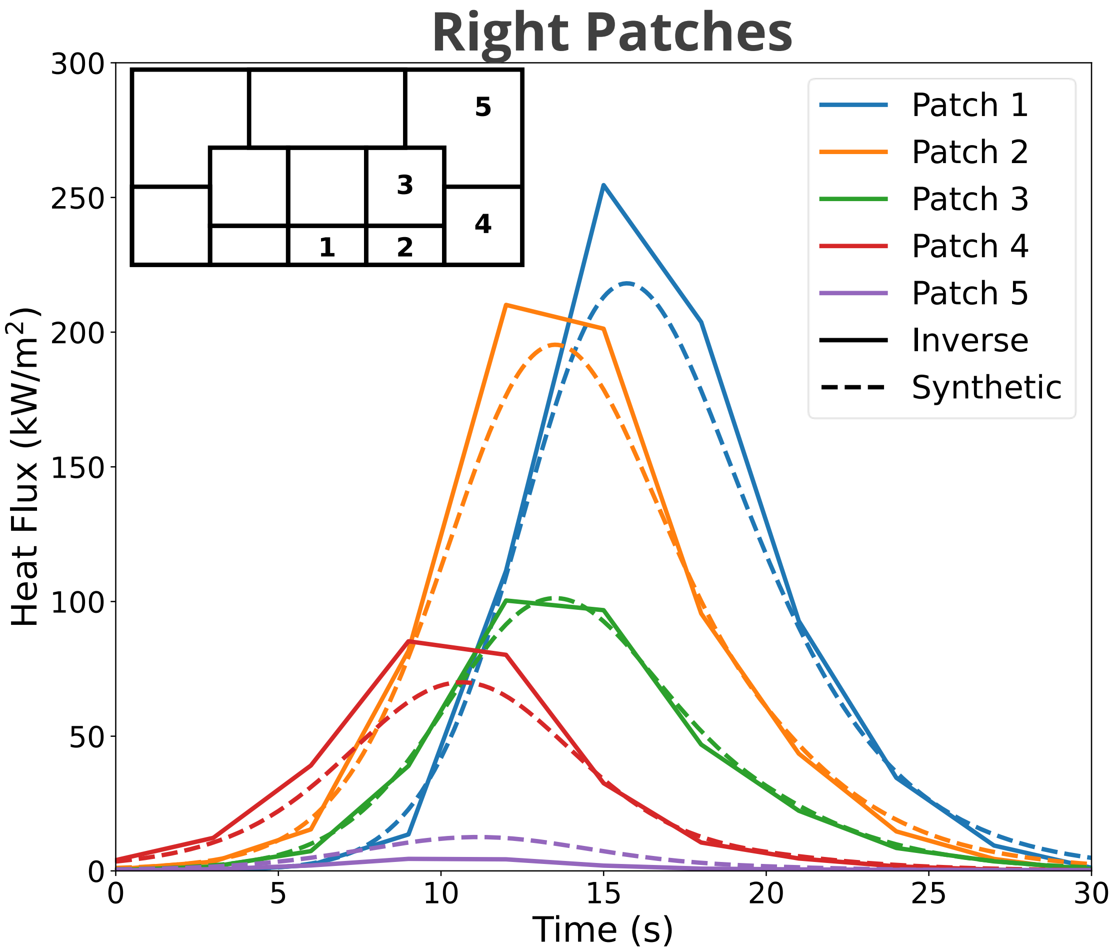




RESULTS: MOVING VENT

- Experimental observations showed the vent moving during thermal runaway
- Example: vent moves from the right edge to the center over 20 seconds





CONCLUSION

- Based on simulations, it should be possible to estimate heat fluxes from experimental temperature measurements using inverse techniques.
- A 1/16” plate with either the 5 x 5 or hybrid thermocouple grid is recommended.
- There is a bias towards over prediction at the center of the jet.
- A different spatial representation of the flux may improve predictions compared to the square patches.
- Future work will investigate a basis function approach to heat flux inversion.

ACKNOWLEDGEMENTS

Thanks to our collaborators at the National Institute of Technology Evaluation (NITE) NLAB in Japan for the joint testing that inspired to this simulation exercise.

Thanks to all of the members of the Battery Abuse Lab at Sandia National Laboratories for adding scoping measurements to a set of experiments and helping identify a rough estimate of the magnitude of the venting heat flux.

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