SAND2019-6179PE

Modeling the Decomposition Behavior of Carbon Fiber Epoxy Composites

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SFPE London Student Chapter

June 10, 2019

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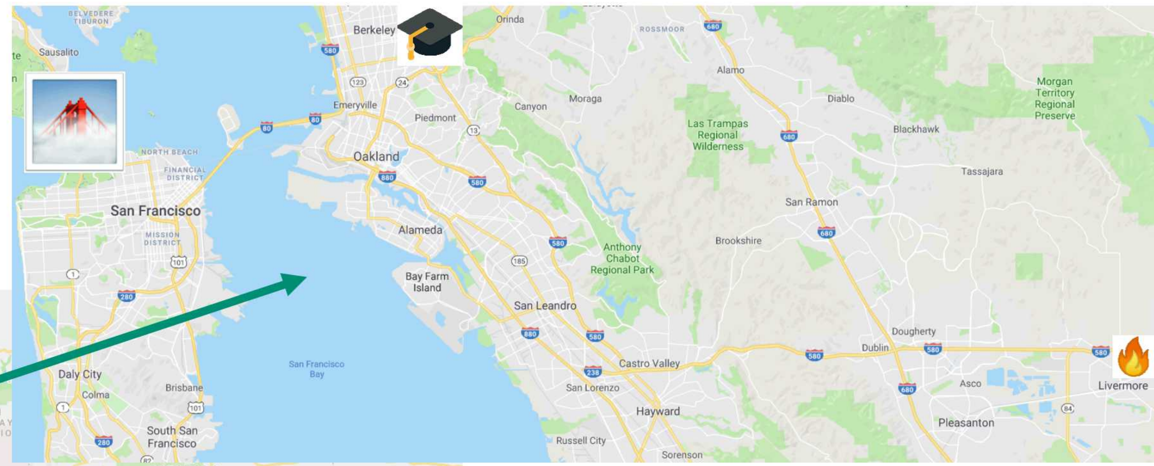
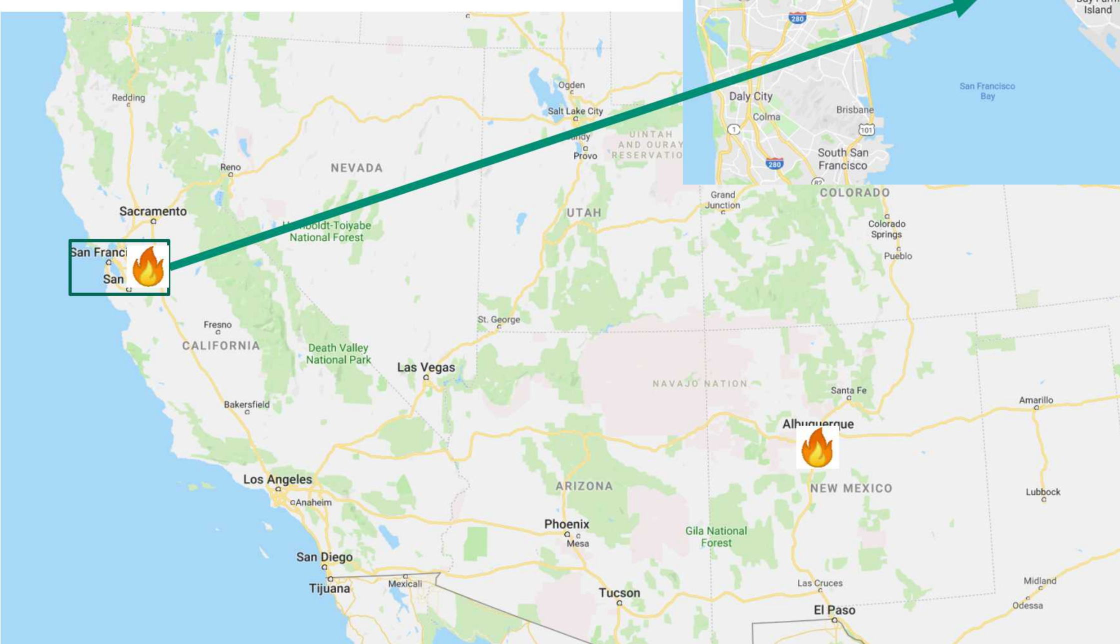
Federally funded research and development center (FFRDC)

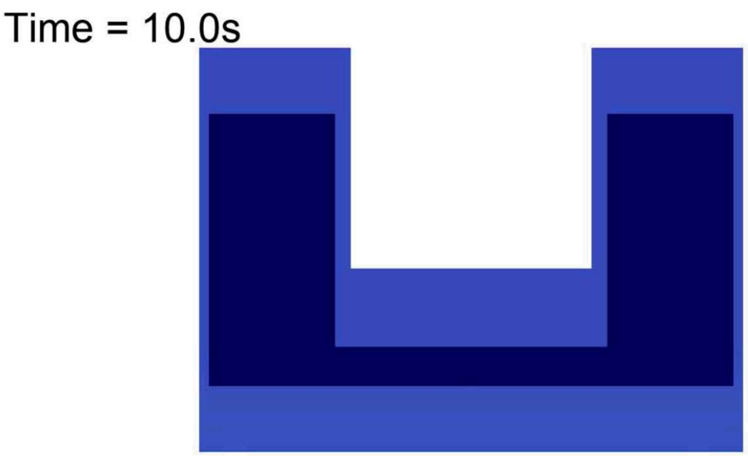


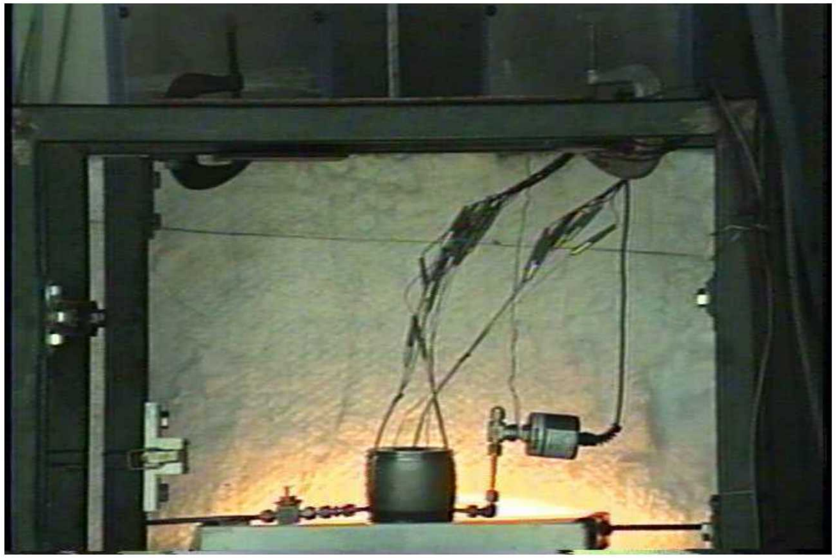


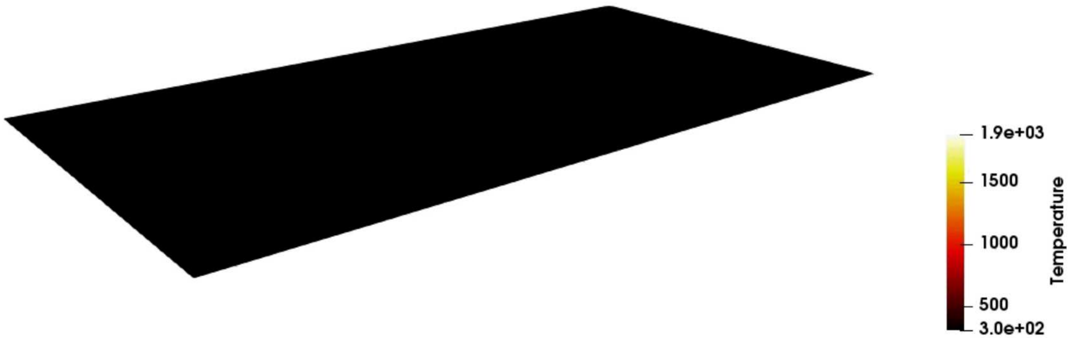
Two main locations:

- Albuquerque, NM
- Livermore, CA

My Work at Sandia







LNG - 10 m SNL 2005 LNG - 21 m SNL 2009 LNG - 83 m SNL 2009

Today's Talk on Composites

Motivation for Studying Fiber Reinforced Polymers in Fires

- These materials are different than traditional engineering materials
- This talk will focus on Carbon Fiber Epoxy Composites

Computational Model

- Description of the computational strategy
- Mechanism creation from TGA for a carbon fiber epoxy composite
- Parameters explored in uncertainty estimation

Model Validation and Uncertainty Estimation

- Comparison of prediction to experiments
- Sensitivity of input parameters to temperature and mass loss predication

Co-Authors

Victor Brunini, Andrew Kurzawski, John Hewson

- Sandia National Laboratories

Juan Hidalgo

- School of Civil Engineering, The University of Queensland

Rory Hadden, Stephen Welch

- School of Engineering, The University of Edinburgh

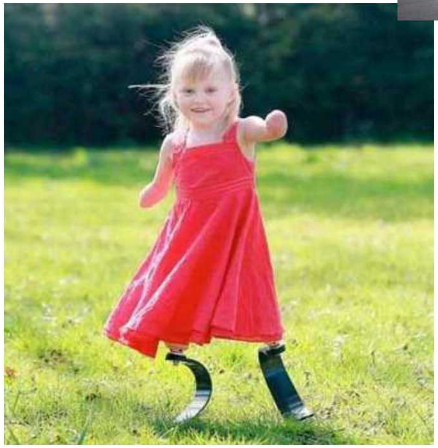
J. P. Hidalgo, R. Hadden, S. Welch, and P. Pironi, "Effect of Thickness on the Ignition Behavior of Carbon Fibre Composite Materials used in High Pressure Vessels," *Eighth Int. Semin. Fire Explos. Hazards*, pp. 353–363, 2016.

J. P. Hidalgo, P. Pironi, R. M. Hadden, and S. Welch, "A framework for evaluating the thermal behaviour of carbon fibre composite materials," *Eur. Symp. Fire Saf. Sci.*, pp. 195–200, 2015.

J. P. Hidalgo, R. Hadden, S. Welch, and P. Pironi, "Experimental Study of the Burning Behavior of a Commercial Carbon Fibre Composite Material used in High Pressure Vessels," in *ECCM17 - 17th European Conference of Composite Materials*, 2016, p. 8.

Motivation for Studying Carbon Fiber Epoxy Composites in Fires

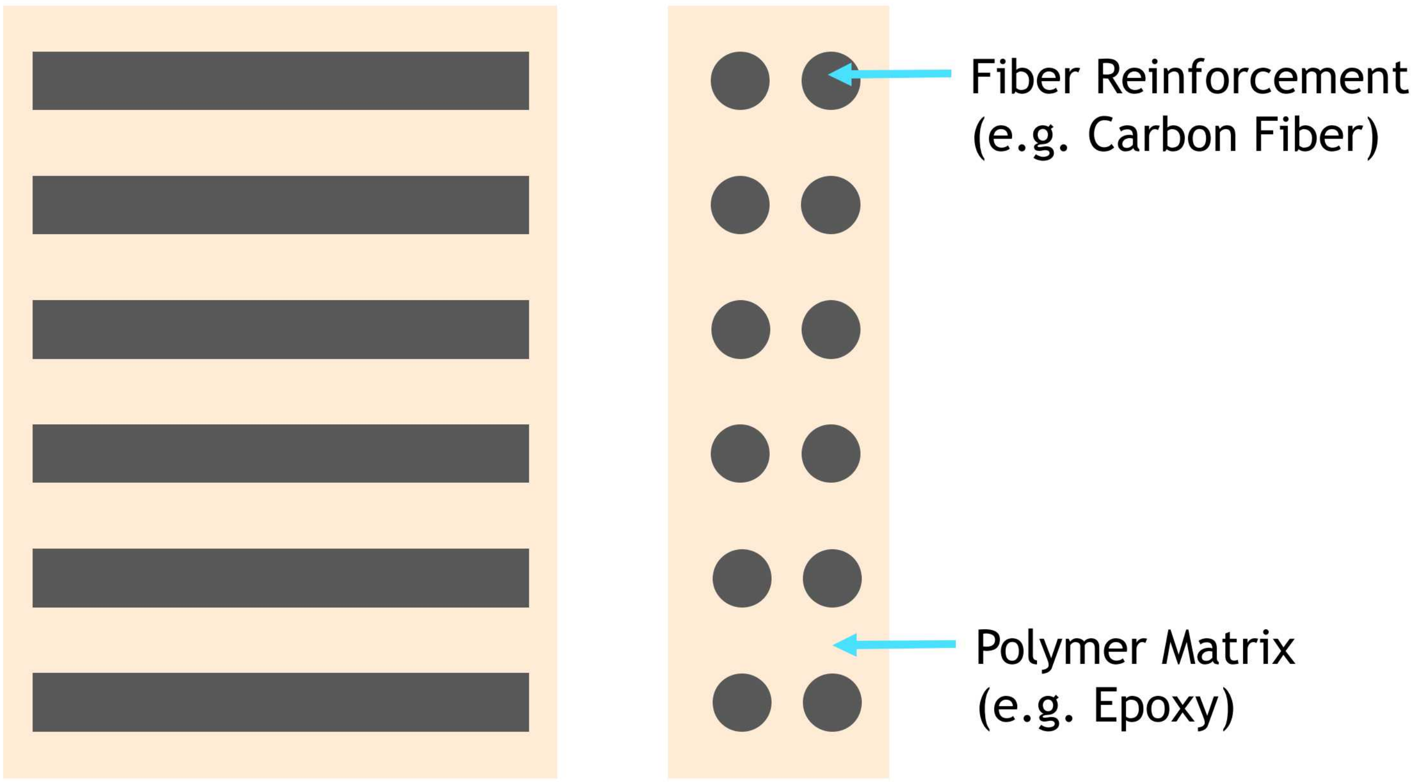
Fiber Reinforced Polymers



An increasing number of engineered systems that require high strength and low weight use fiber reinforce polymers

- Aerospace, automotive, sporting goods, electronics, transportation, prosthetics…

What is a Fiber Reinforced Polymer?



Fibers provide strength and rigidity to the polymer, while the polymer provides structure to the fibers.

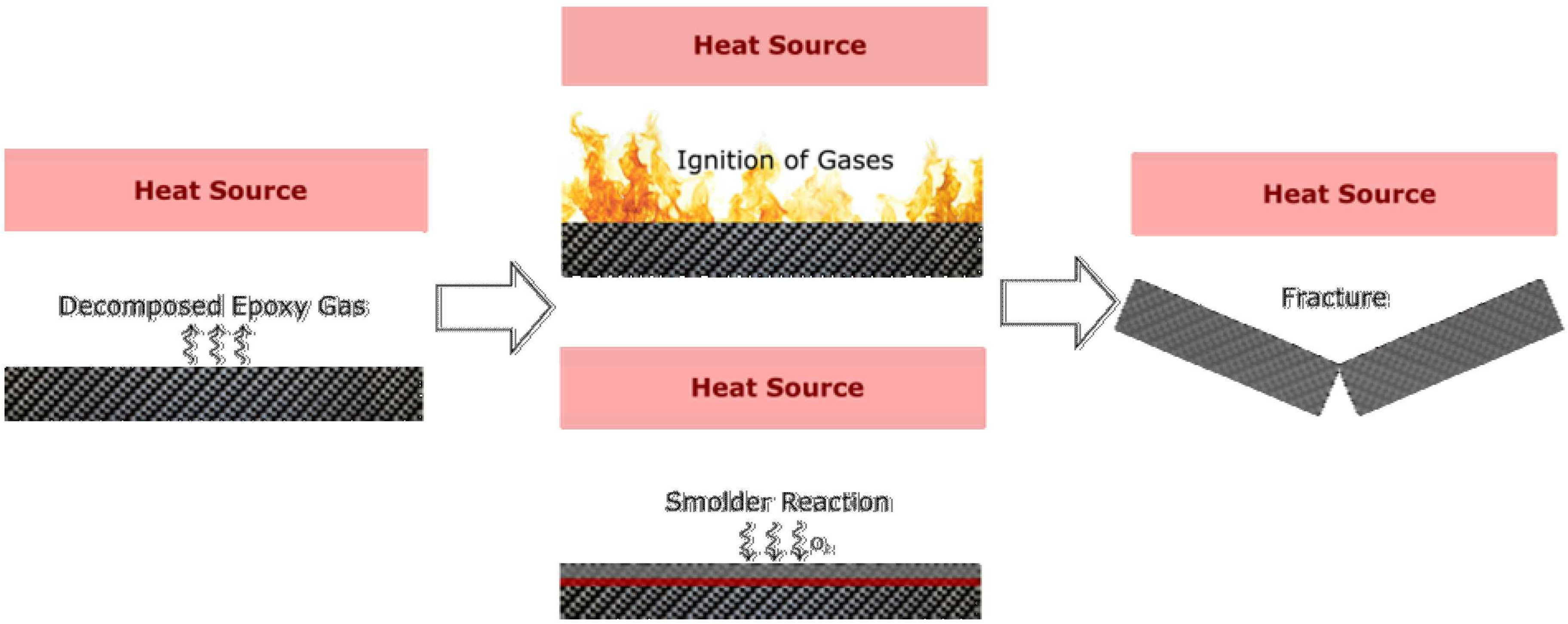
Carbon fiber epoxy composites are an example of a fiber reinforced polymer

The Trouble with Fiber Reinforced Polymers

The replacement of metals with fiber reinforced polymers cause concerns in fire environments.

The polymers and fibers can be fuel for the fire, were as traditional building materials are inert.

The Trouble with Fiber Reinforced Polymers



Subject to heating (e.g. fire), the epoxy decomposes into a vapor and residue. The gases can ignite, and the carbon fiber can oxidize. This will weaken the structure of the composite.

Objective of this Work

Create and validate a computational model of pyrolyzing and smoldering carbon fiber epoxy composite using cone calorimeter data.

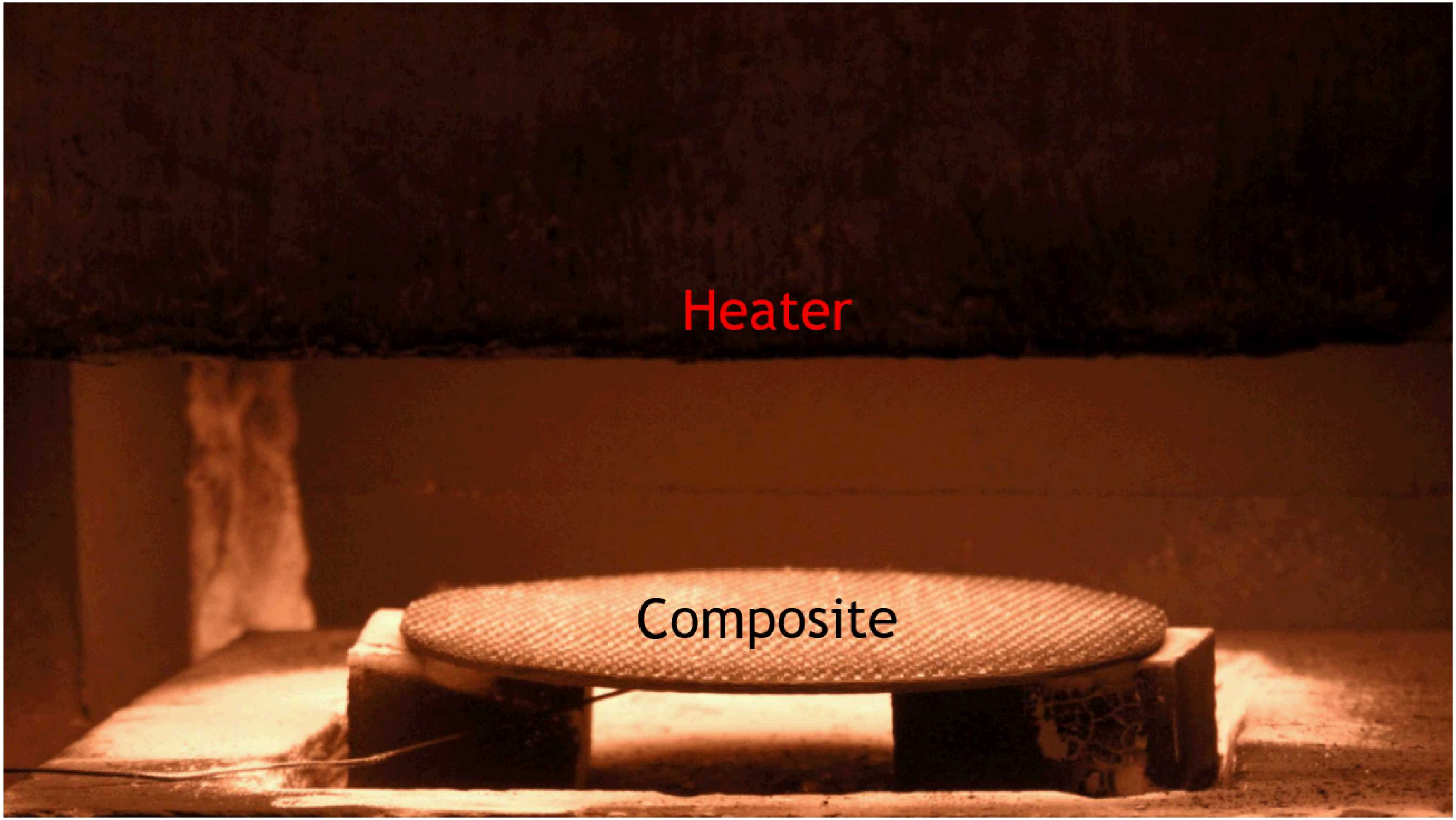
Compare temperature and mass loss data

Evaluate uncertainty and sensitivity of temperature and mass loss to variation of input parameters

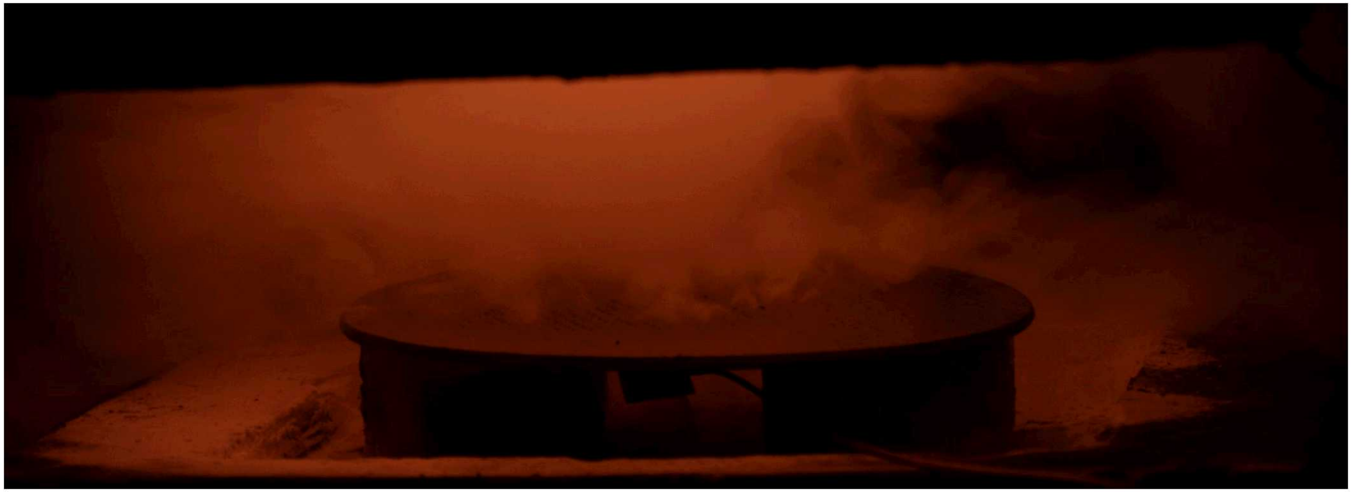

Computational Model Creation

Decomposing Carbon Fiber Epoxy Composite

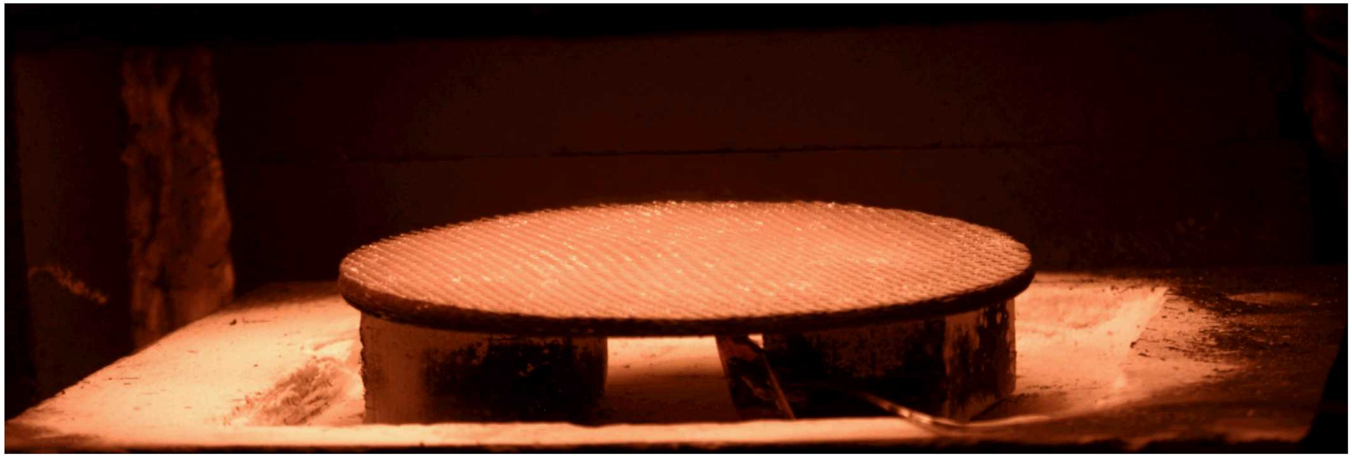
55 minute test compressed into 30 seconds



Decomposing Carbon Fiber Epoxy Composite



Pyrolysis



Oxidation

How are we going to model this?

Governing Equations

Reaction Parameters

Material Properties

Governing Equations

Solid Phase / Gas Phase

Continuity

Solid Phase:

$$\frac{\partial \rho_b}{\partial t} = -\dot{\omega}'''_{fk}$$

Gas Phase:

$$\frac{\partial(\bar{\psi}\rho_g)}{\partial t} + \frac{\partial(\rho_g u_{j,g})}{\partial x_j} = \dot{\omega}'''_{fk}$$

Species Continuity

Solid Phase:

$$\frac{\partial(\rho_b Y_k)}{\partial t} = \dot{\omega}'''_{fk} - \dot{\omega}'''_{dk}$$

Gas Phase:

$$\frac{\partial\left(\bar{\psi}\rho_g Y_{k.g}\right)}{\partial t} + \frac{\partial\left(\rho_g u_{j,g} Y_{k.g}\right)}{\partial x_j} = -\frac{\partial q^{Y,g}_{k,j}}{\partial x_j} + \left(\dot{\omega}'''_{s,fk} - \dot{\omega}'''_{s,dk}\right) + \left(\dot{\omega}'''_{g,fk} - \dot{\omega}'''_{g,dk}\right)$$

Enthalpy

Solid Phase:

$$\frac{\partial\left(\bar{\rho} c_p \bar{T}\right)}{\partial t} = -\frac{\partial q^h_j}{\partial x_j} + h_{cv}\left(T_g - \bar{T}\right) + \sum_k \left(\dot{\omega}'''_{s,fk} - \dot{\omega}'''_{s,dk}\right) h_{k.g}$$

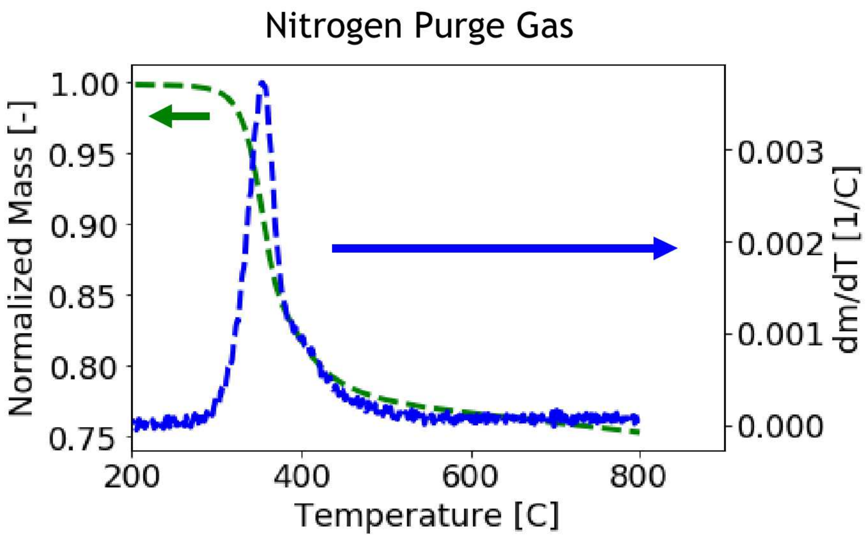
Gas Phase:

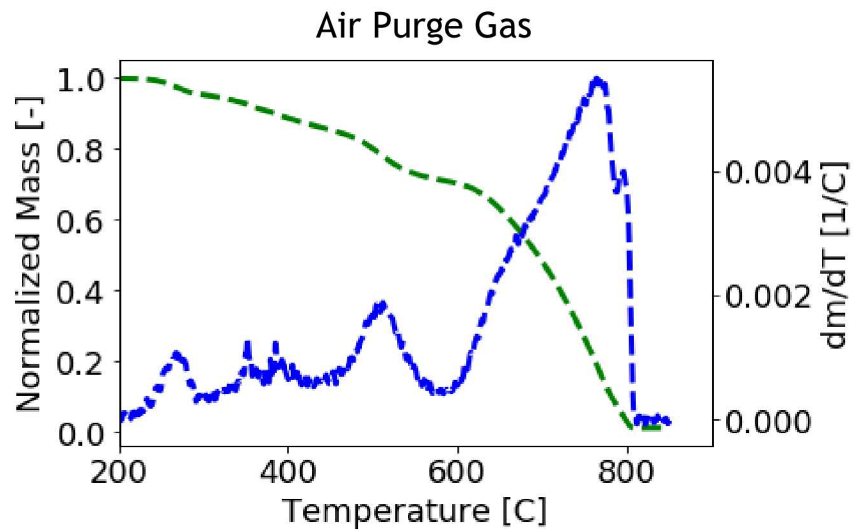
$$\frac{\partial\left(\bar{\psi}\rho_g h_g\right)}{\partial t} + \frac{\partial\left(\rho_g u_{j,g} h_g\right)}{\partial x_j} = -\frac{\partial q^{h,g}_{k,j}}{\partial x_j} + \frac{\partial\left(\bar{\psi} p_g\right)}{\partial t} + h_{cv}\left(\bar{T} - T_g\right) + \sum_k \left(\dot{\omega}'''_{s,fk} - \dot{\omega}'''_{s,dk}\right) h_{k.g}$$

Governing Equations

	Solid Phase		Gas Phase
Continuity	The mass lost in the solid must equal the mass gained in the gas	Reaction	The flow is governed by the pressure gradient and Darcy's law for flow through a porous medium The source of mass is the reaction
Species Continuity	The mass lost in the solid must equal the mass gained in the gas for each species	Reaction	The flow of each species is governed by the pressure, velocity, and diffusivity The source of mass in each species is the reaction
Enthalpy	Energy moves through the system through conduction Sources are convection and the reaction	Convection	Energy moves through the flow and diffusion Sources are convection and the reaction

Pyrolysis and Smoldering Mechanism





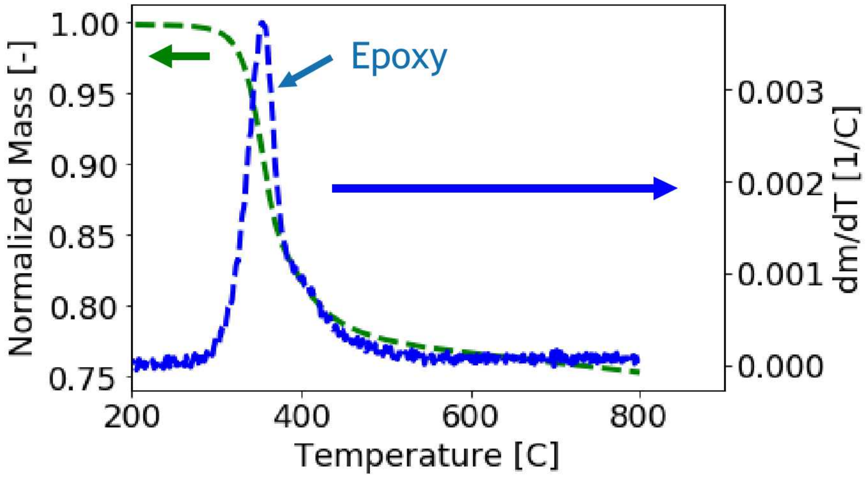
TGA conducted at 5 C/min

Nitrogen and air purge gas

Temperature and mass recorded

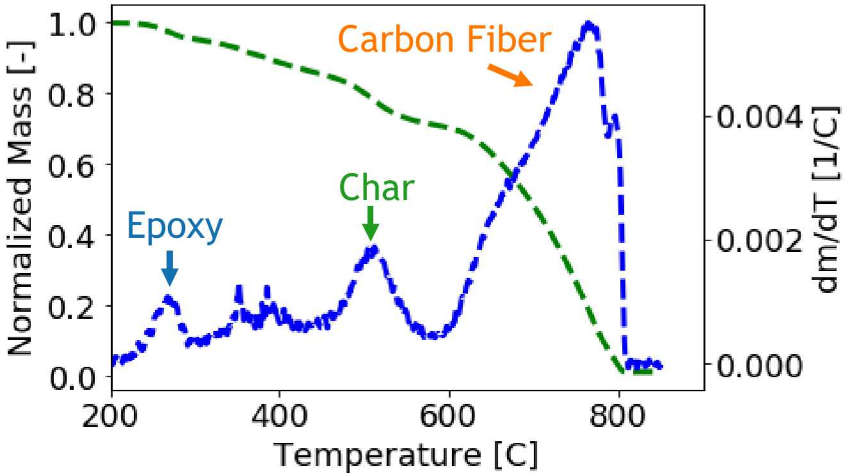
Pyrolysis and Smoldering Mechanism

Nitrogen Purge Gas



$$Epoxy \rightarrow Char + fuel$$

Air Purge Gas

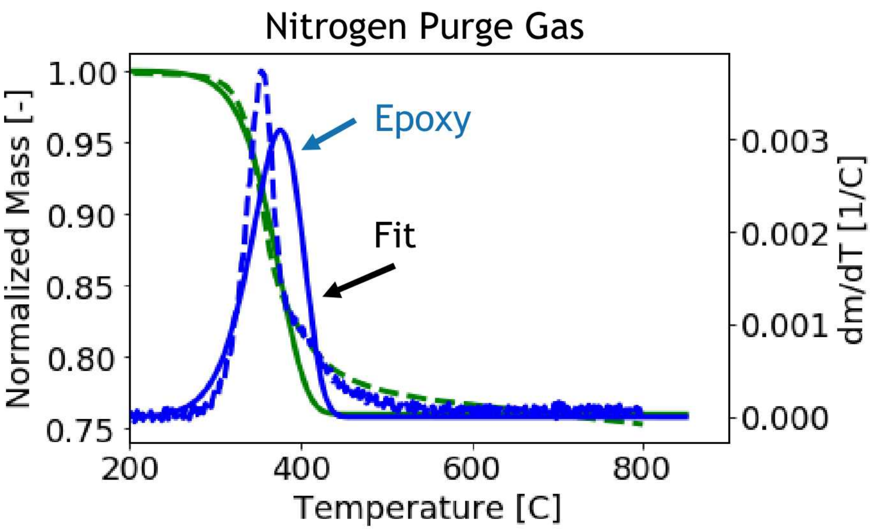


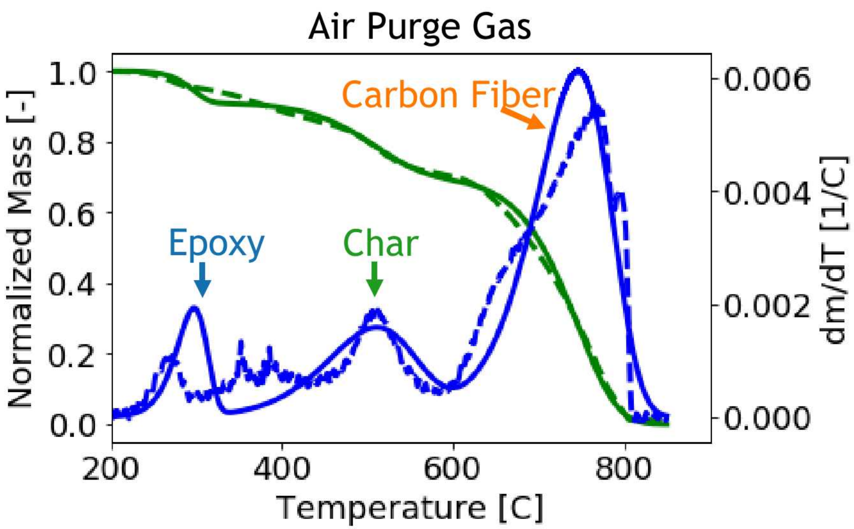
$$Epoxy + O_2 \rightarrow Char + fuel$$

$$Char + O_2 \rightarrow Residue + gas$$

$$Carbon\ Fiber + O_2 \rightarrow Residue + gas$$

Pyrolysis and Smoldering Mechanism





$$Epoxy \rightarrow Char + fuel$$

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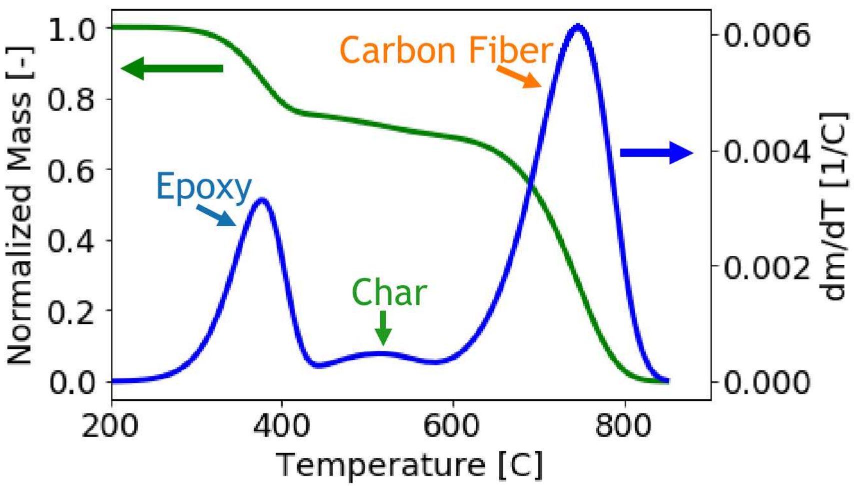
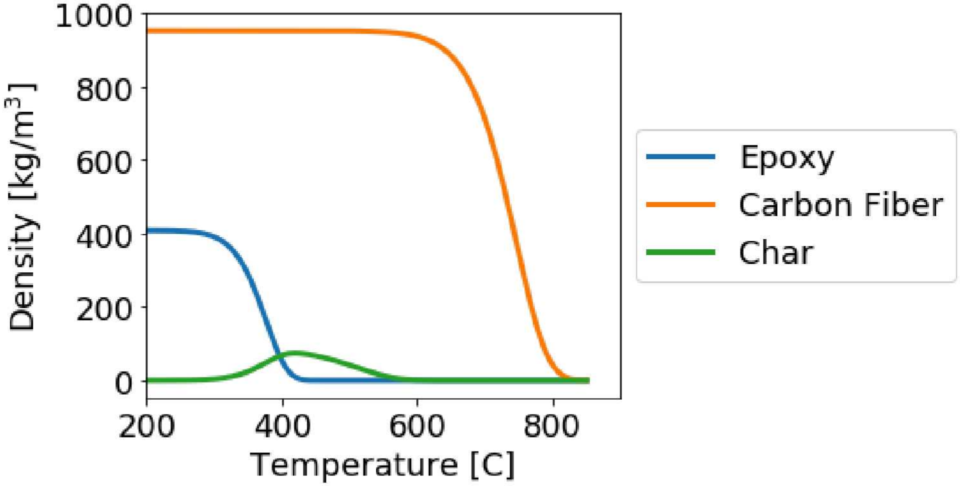
Pyrolysis and Smoldering Mechanism





$$Epoxy \rightarrow Char + fuel$$

~~$Epoxy + O_2 \rightarrow Char + fuel$~~

$$Char + O_2 \rightarrow Residue + gas$$

$$Carbon\ Fiber + O_2 \rightarrow Residue + gas$$

Material Properties

Each Composite Phase

(Epoxy, Char, Carbon Fiber)

- Conductivity
- Specific Heat
- Density
- Permeability
- Radiative Conductivity
- Emissivity

Each Gas Phase

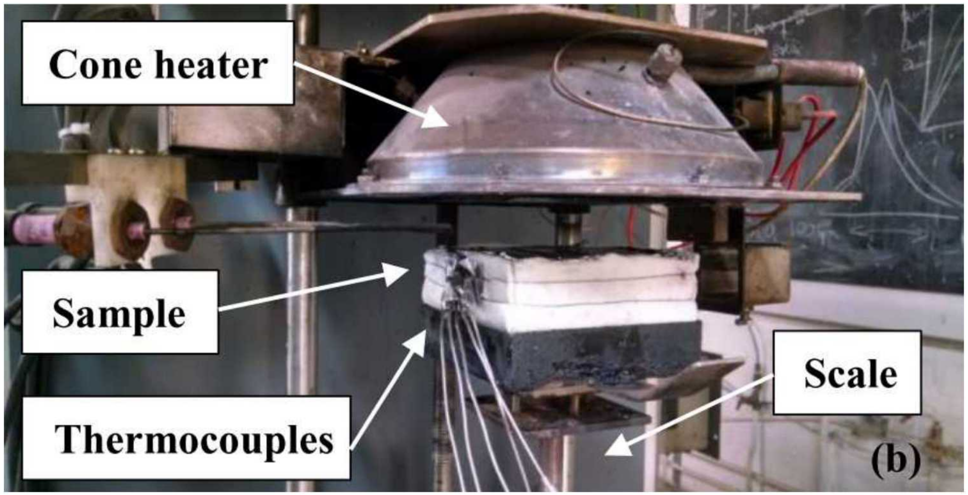
(CH_4, CO, CO_2 O_2, N_2)

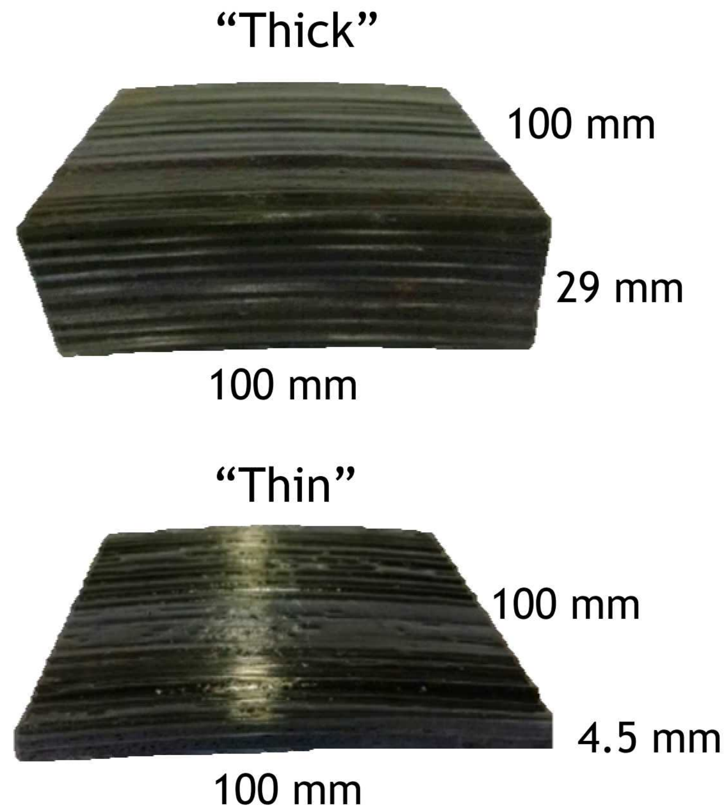
- Specific Heat
- Molecular Weight
- Mass Diffusivity

Properties are a function of temperature, reaction, or both

Properties come from measurement, literature, and calibration

Experiments to Model





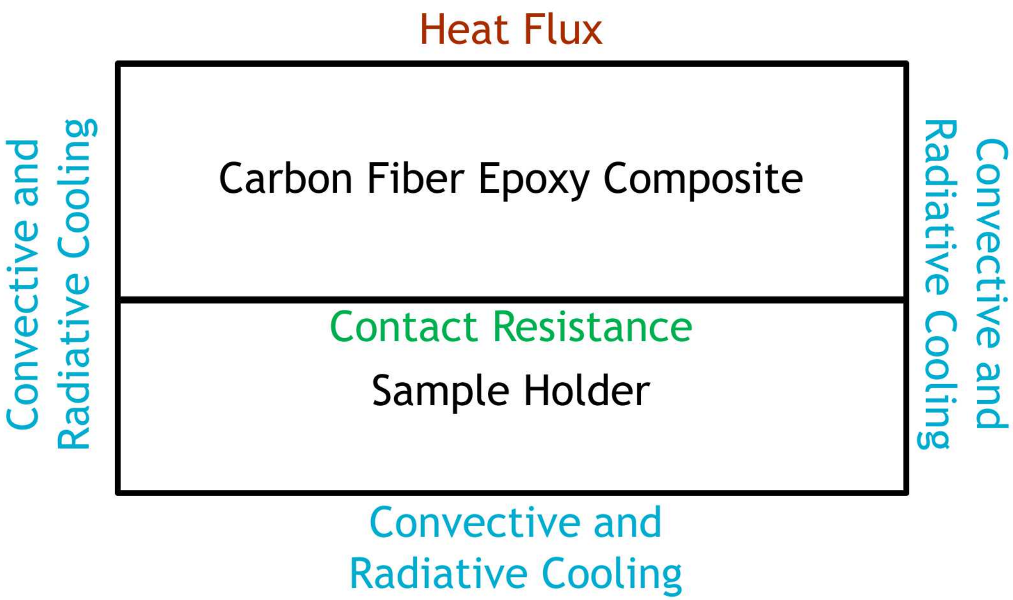
Two sample thicknesses: 4.5 mm and 29 mm

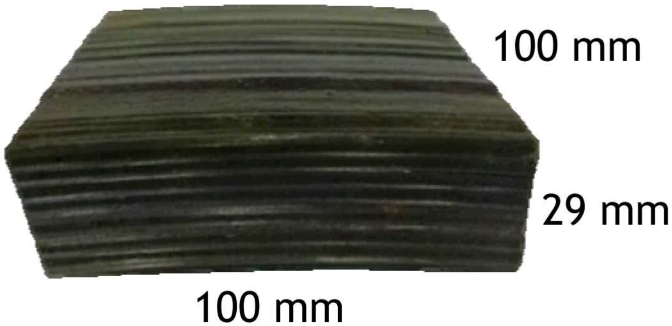
Two sample holder materials: Aluminum and Ceramic

Heat flux: 30 kW/m^2 – 80 kW/m^2

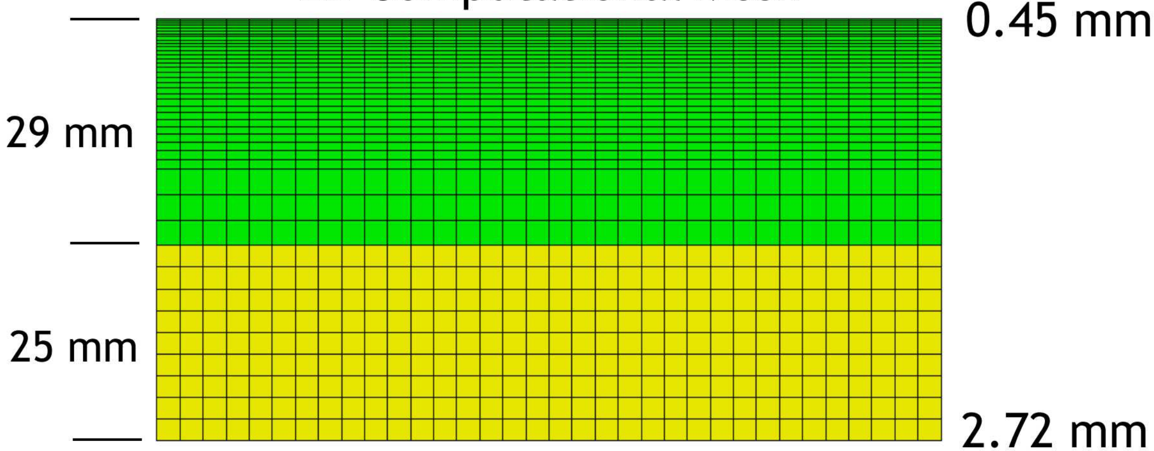
Temperature and mass loss recorded

Translating the Experiment into a Model - Thick

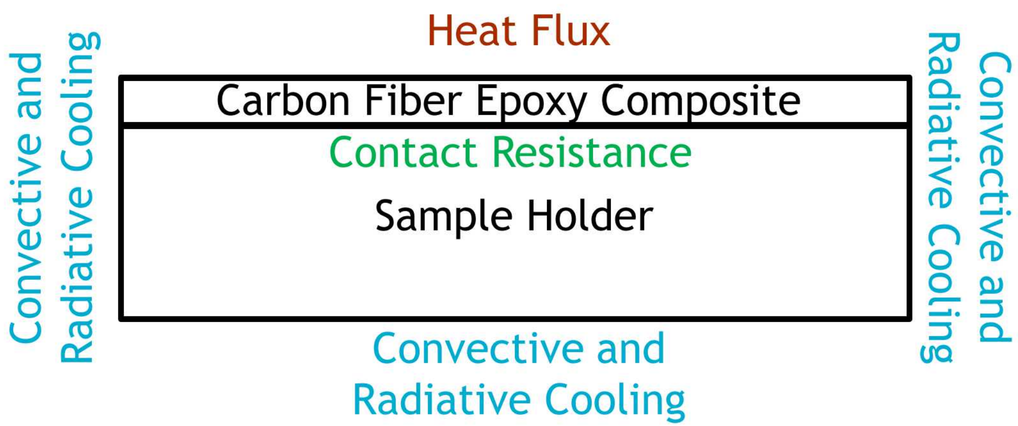


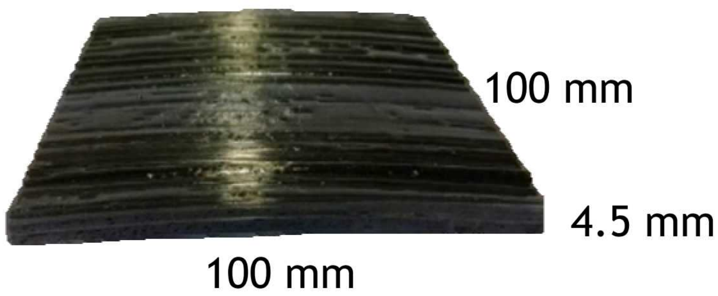


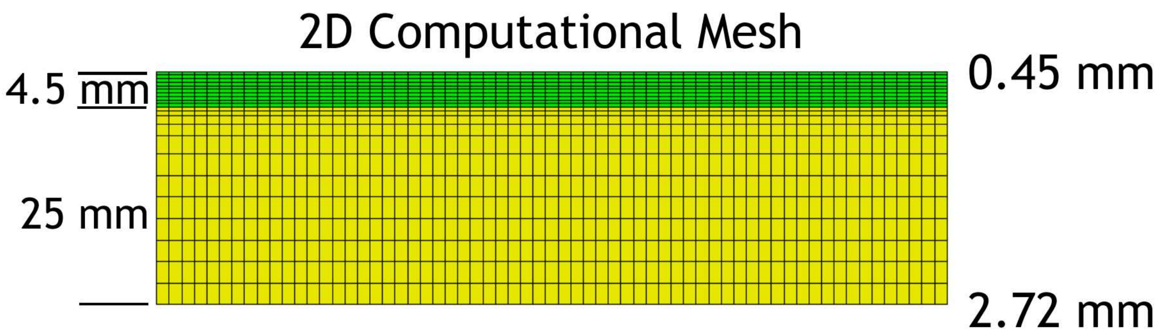
2D Computational Mesh



Translating the Experiment into a Model - Thin

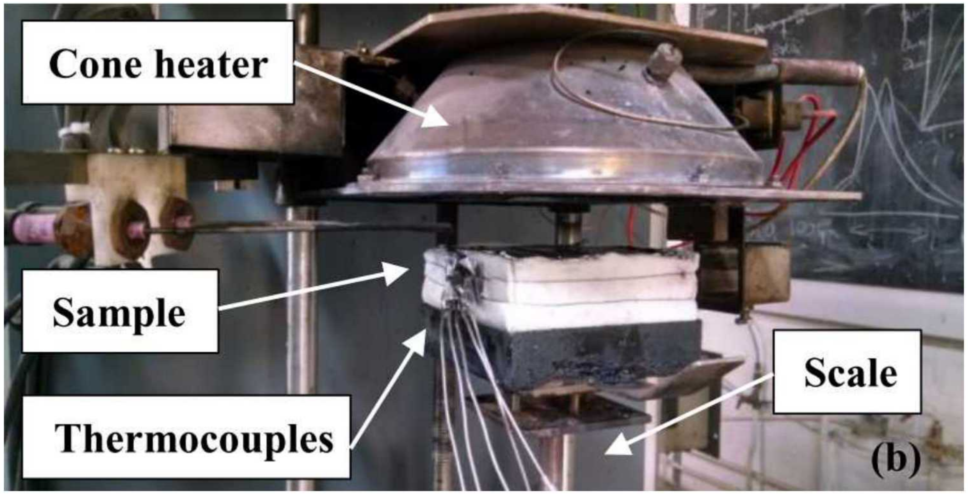






Model Validation, Uncertainty, and Sensitivity

29 mm “Thick” Sample – 30 kW/m²



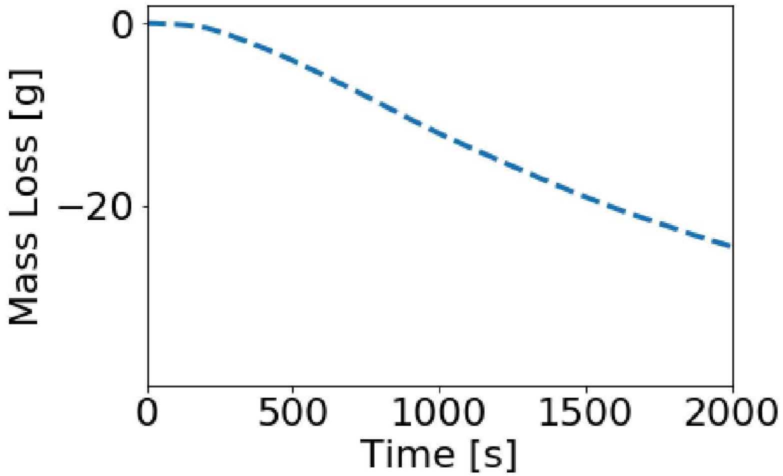
Sample dimensions: 100 x 100 x 29 mm

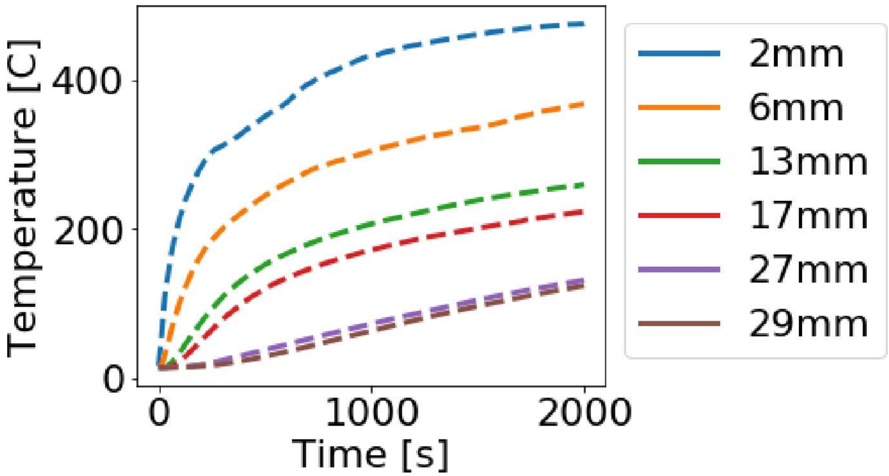
Sample holder material: Aluminum

Heat flux: 30 kW/m^2

Temperature and mass loss recorded

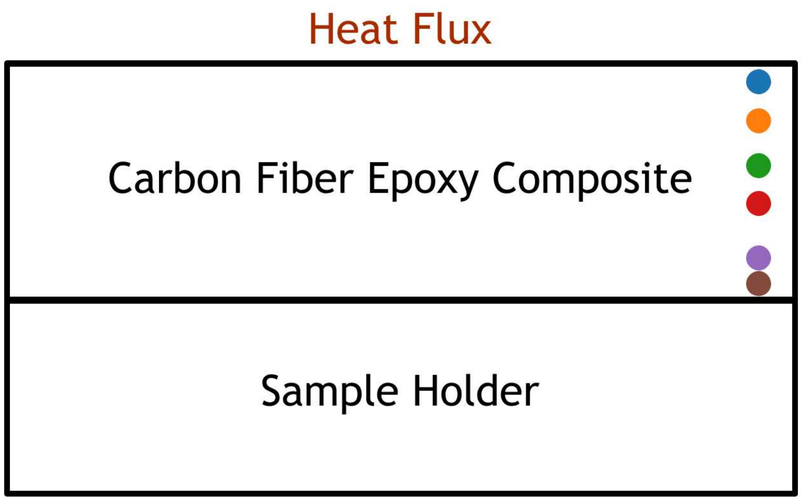
29 mm “Thick” Sample – 30 kW/m²



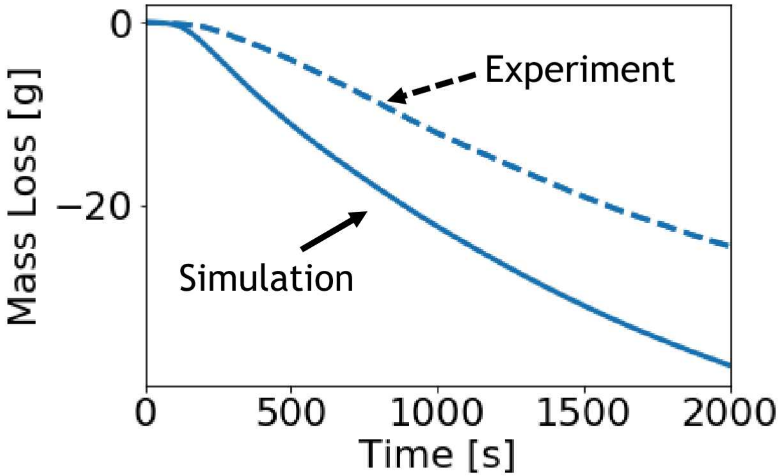


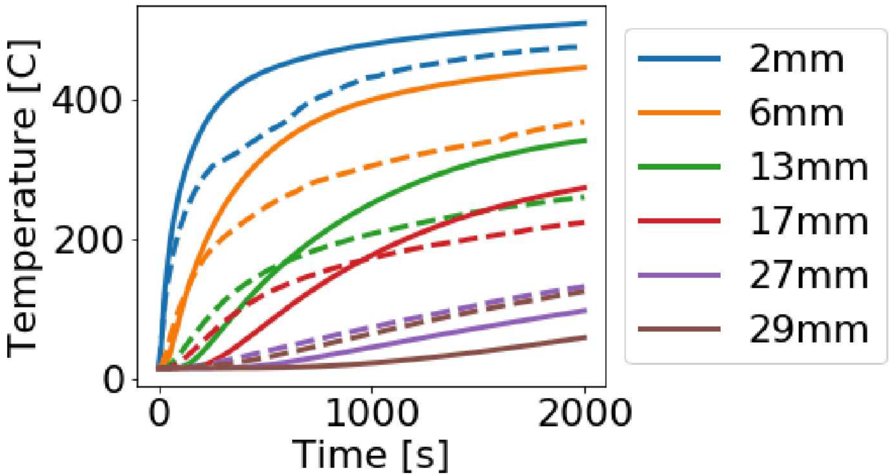
20 g (5%) of the sample are lost over the half hour test

200 C temperature gradient over the sample



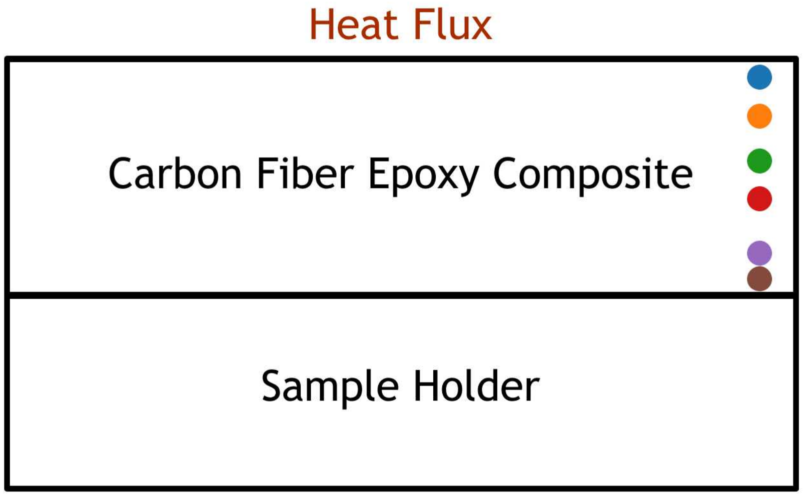
29 mm “Thick” Sample – 30 kW/m^2





Mass loss: good qualitative agreement

Temperature: Over predicting in the middle of the sample



Model Parameters for Uncertainty Evaluation

27 Parameters

Each Composite Phase:

- Conductivity (k)
- Volumetric Heat Capacity (ρc_p)
- Permeability (K)
- Radiative Conductivity (k_e)
- Emissivity (ϵ)
- Initial Carbon Fiber ($\%CF$)

Each Reaction:

- Pre-Exponential Factor (A)
- Activation Energy (E_a)
- Stoichiometric coefficient (ν)
- Heat Release (H)

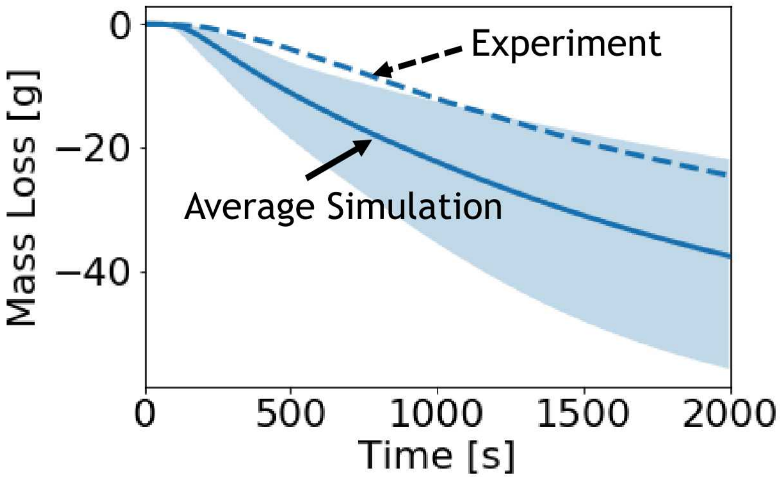
Each Holder Material:

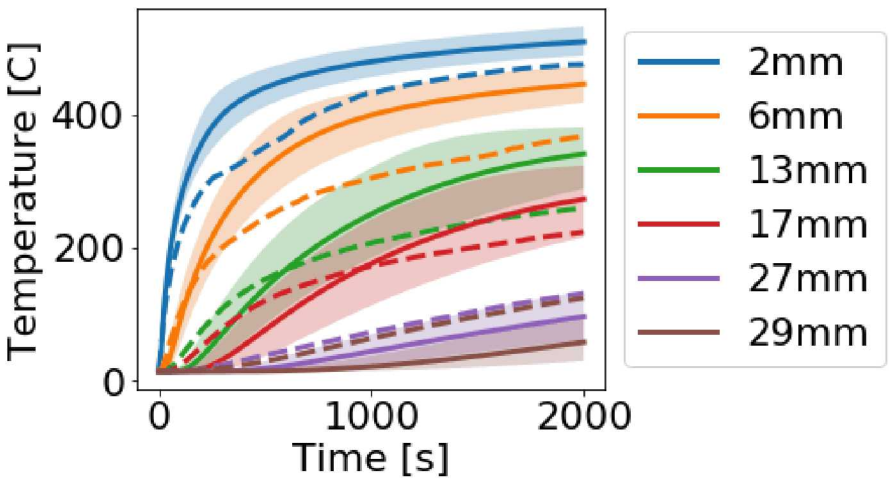
- Conductivity (k)
- Volumetric Heat Capacity (ρc_p)
- Emissivity (ϵ)

Boundary Conditions:

- Heat Flux (q)
- Convective Heat Transfer (h_{cv})
- Contact Resistance (R_c)

29 mm "Thick" Sample – 30 kW/m²





270 simulation in the ensemble

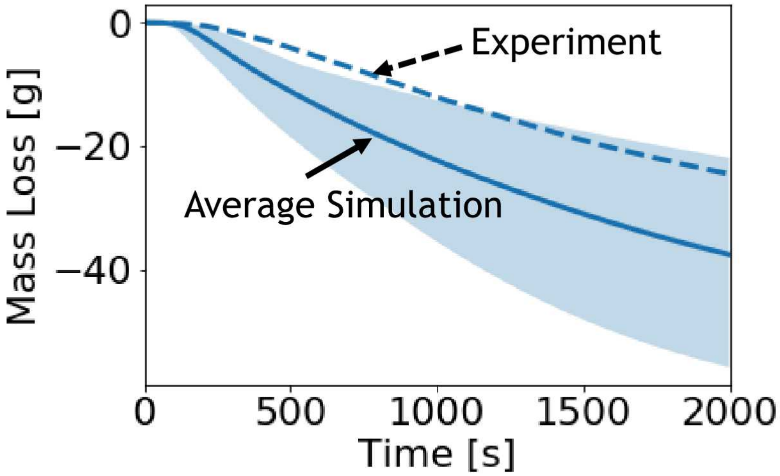
Average Simulation presented with min/max bounds

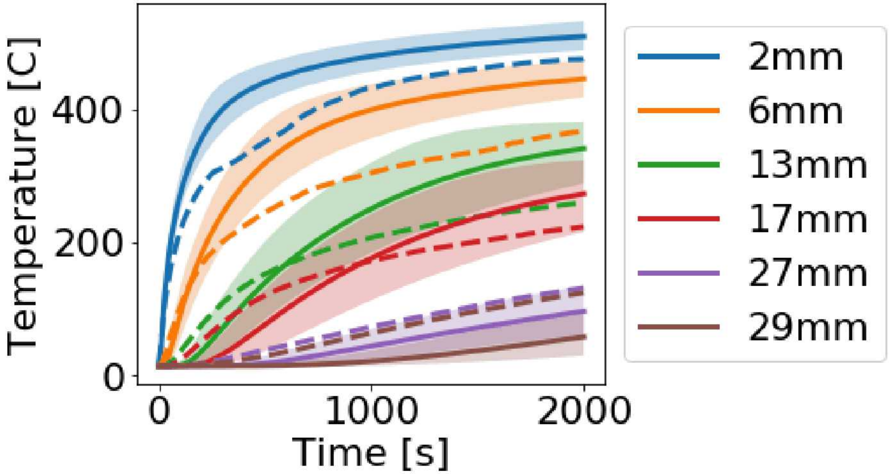
TC locations measured from top of the sample

Mass loss: Captures the experimental data, but bounds are large

Temperature: Largest uncertainty is in the middle of the sample

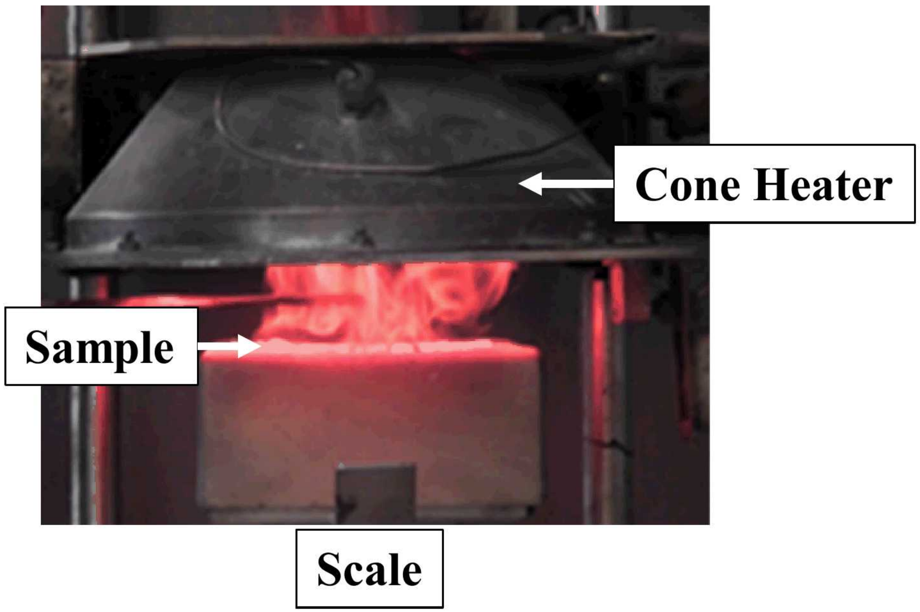
29 mm “Thick” Sample – 30 kW/m^2

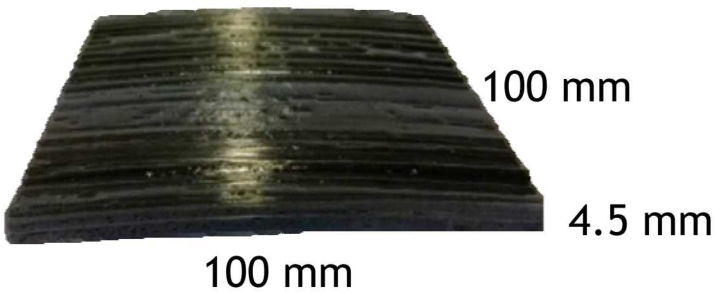




Rank	2mm	6mm	13mm	17mm	27mm	29mm	Mass Loss
1	Composite ρc_p	Composite ρc_p	Composite ρc_p	Composite ρc_p	Carbon fiber k	Carbon fiber k	$\%CF$
2	Composite ϵ	Carbon fiber k	Carbon fiber k	Carbon fiber k	Composite ρc_p	Composite ρc_p	Composite ρc_p
3	$\%CF$	Composite ϵ	Composite k_{rad}	Composite k_{rad}	Epoxy k	Epoxy k	Carbon fiber k

29 mm “Thin” Sample – 30-80 kW/m²





Sample thicknesses: 4.5 mm

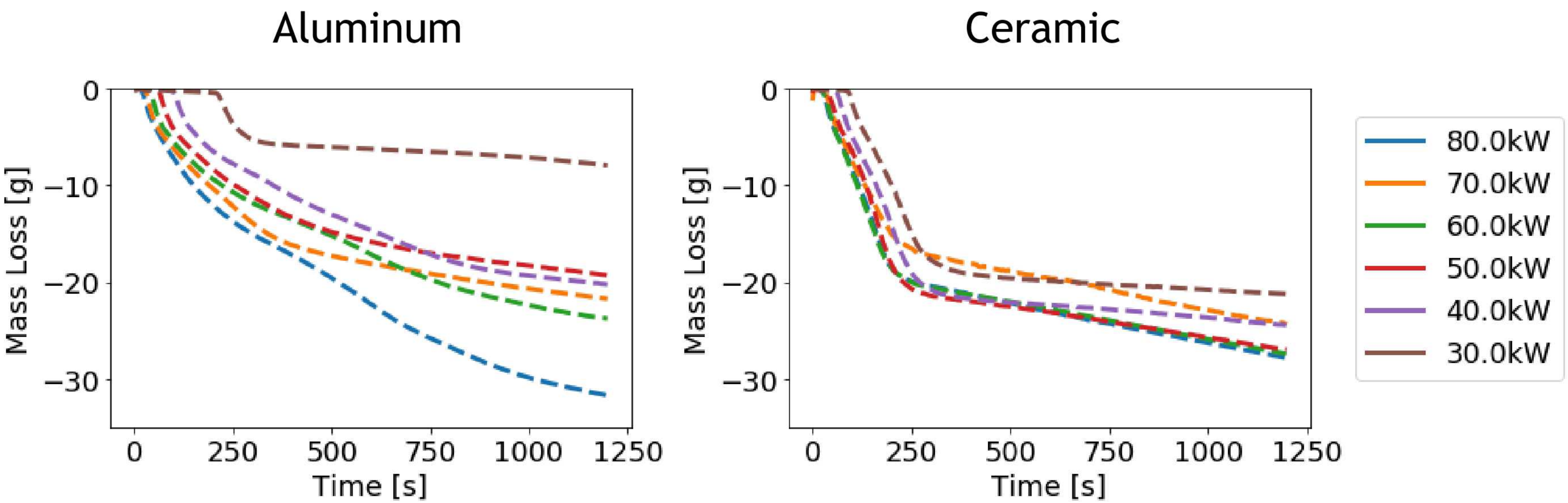
Two sample holder materials: Aluminum and Ceramic

Heat flux: 30 - 80 kW/m^2

Mass loss recorded

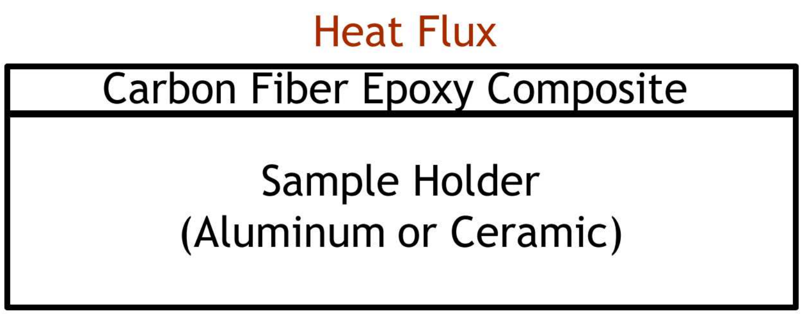
Flaming Ignition: Yes

4.5 mm "Thin" Sample – Experimental Results

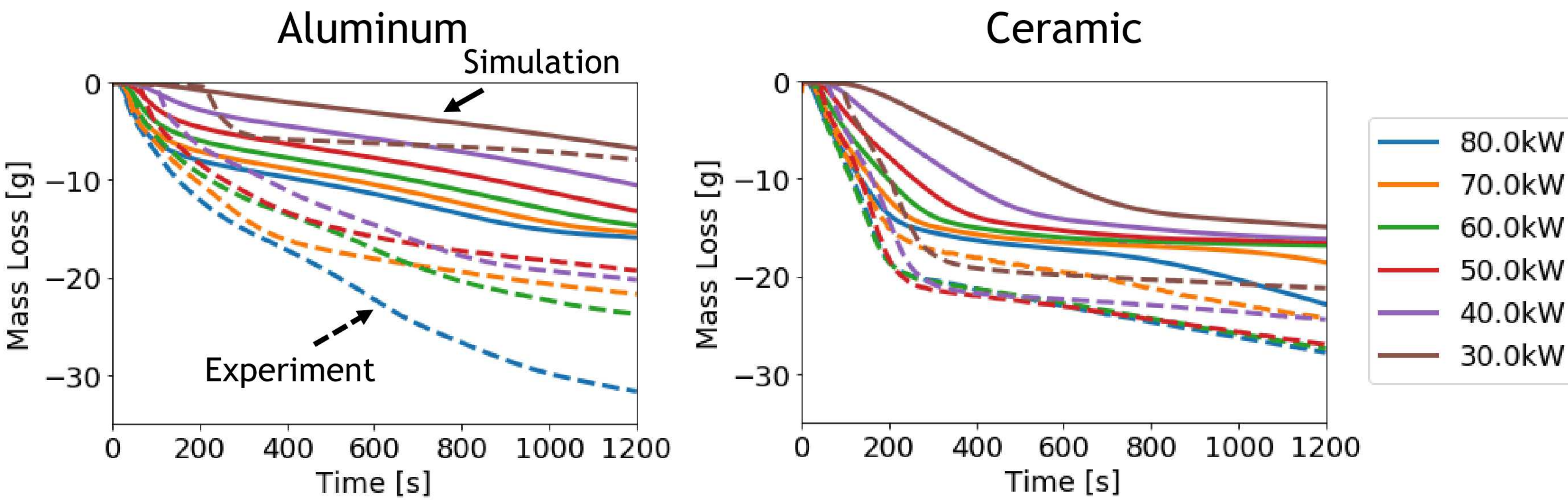


61 grams initial mass. Up to half is lost over the 20 minute test.

The aluminum has a slower mass loss rate, and is more dependent on heat flux



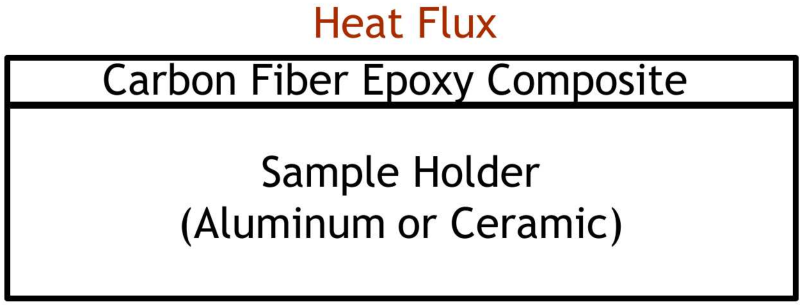
4.5 mm “Thin” Sample – 30-80 kW/m^2



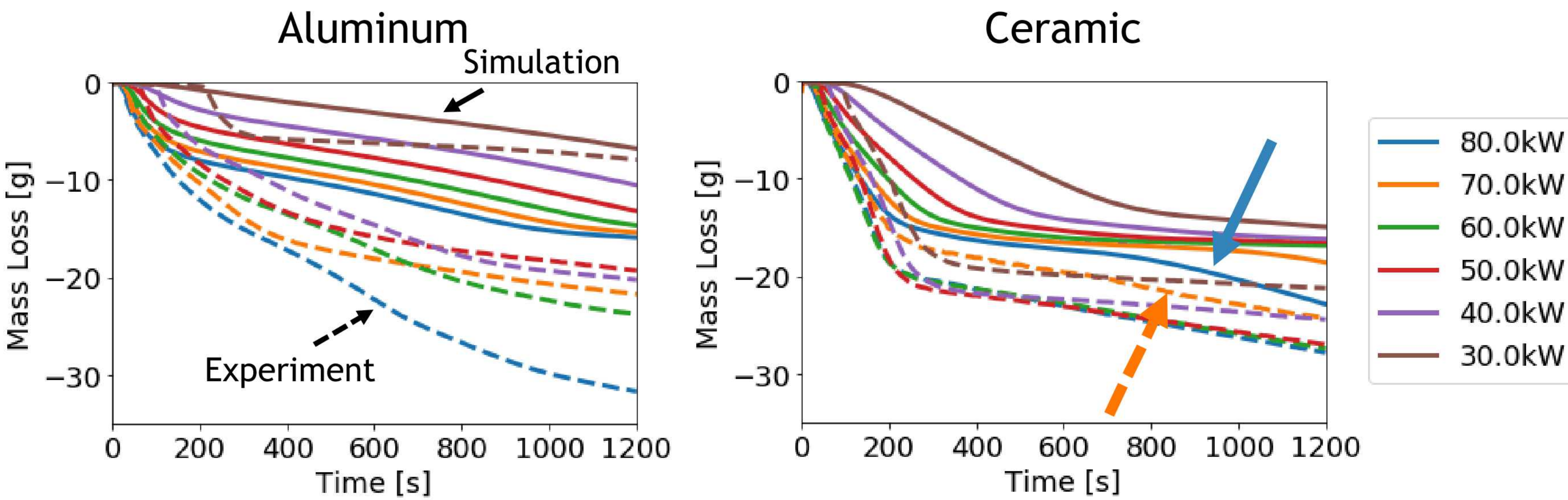
Under predict the mass loss (the aluminum more than the ceramic)

Predict correct trend that in mass loss rate and dependence on heat flux

Flaming ignition is an issue



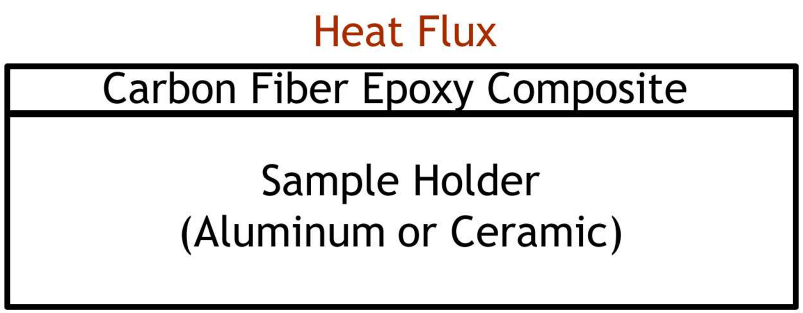
4.5 mm “Thin” Sample – 30-80 kW/m^2



Under predict the mass loss (the aluminum more than the ceramic)

Predict correct trend that in mass loss rate and dependence on heat flux

Flaming ignition is an (unmodeled) issue



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Boundary Conditions:

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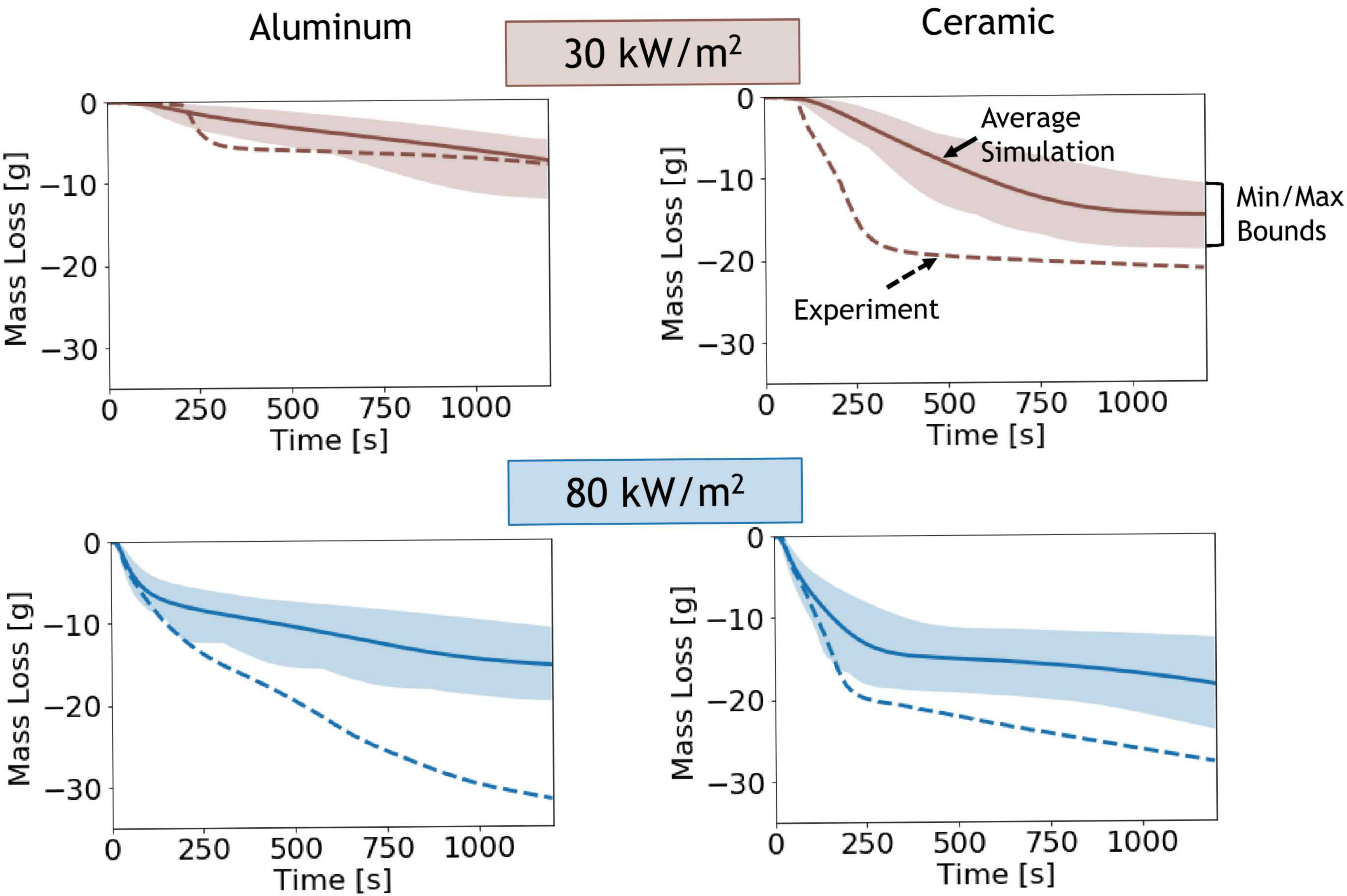
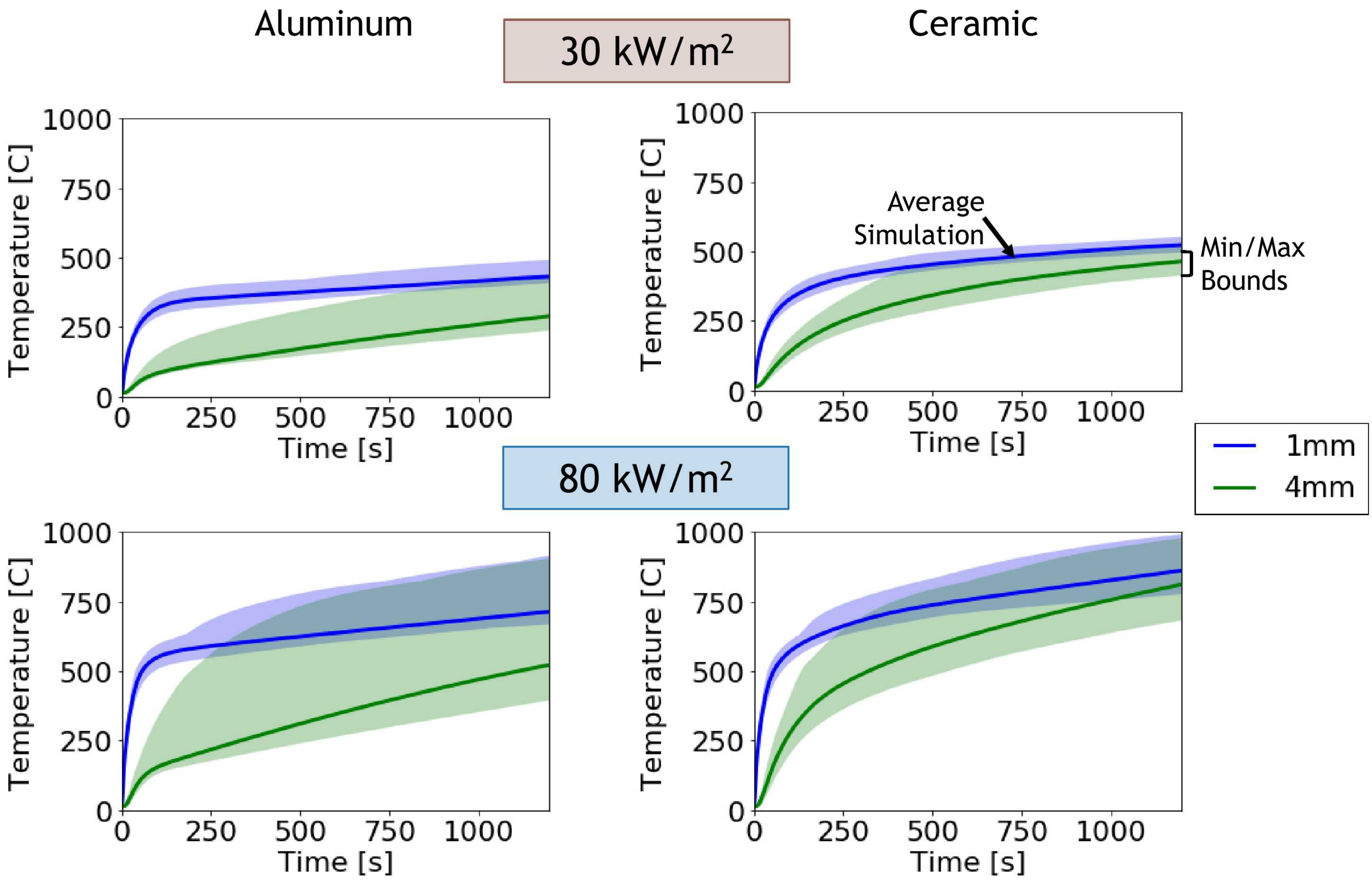
- Contact Resistance (R_c)

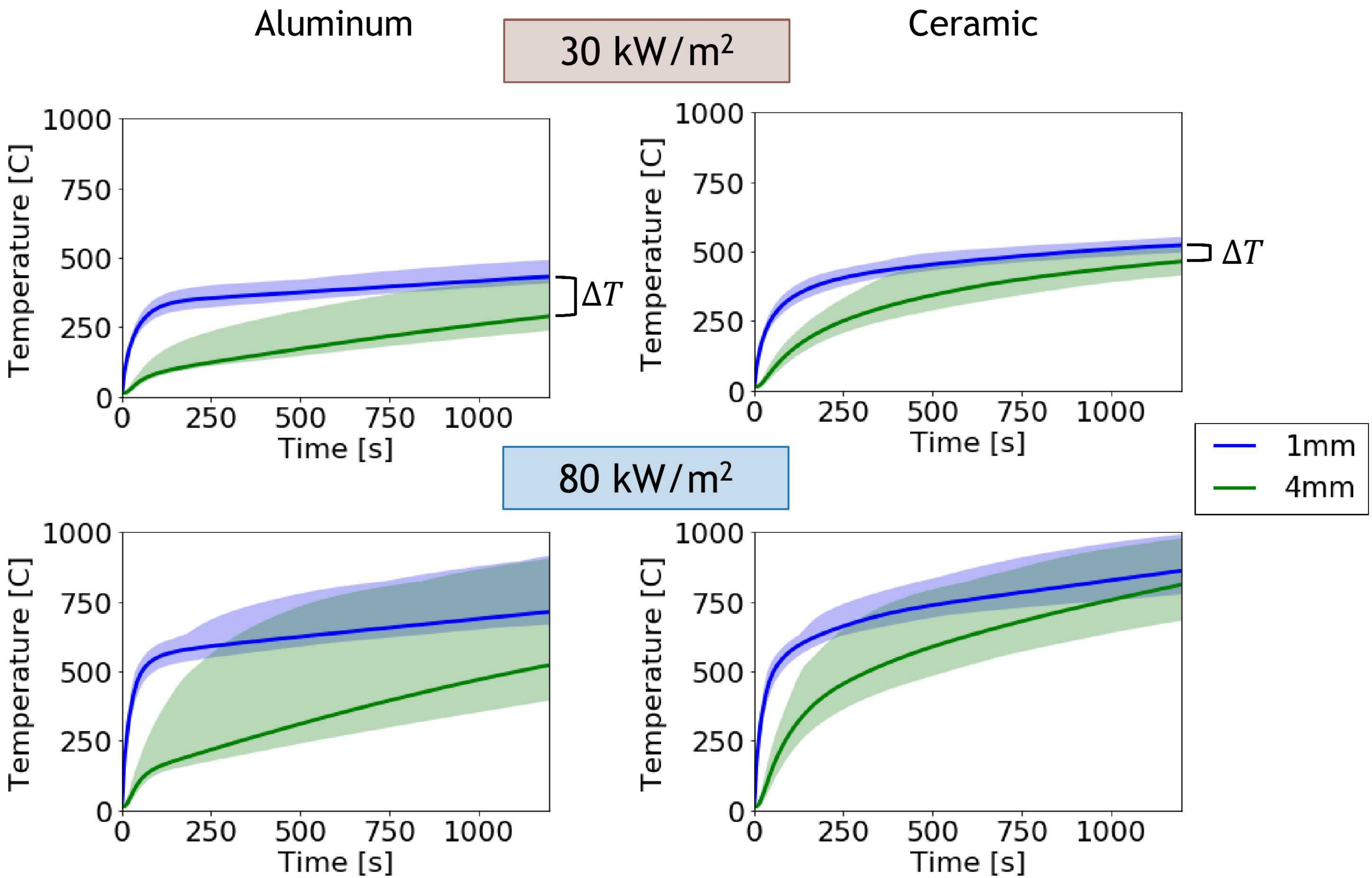
4.5 mm “Thin” Sample – 30 & 80 kW/m²



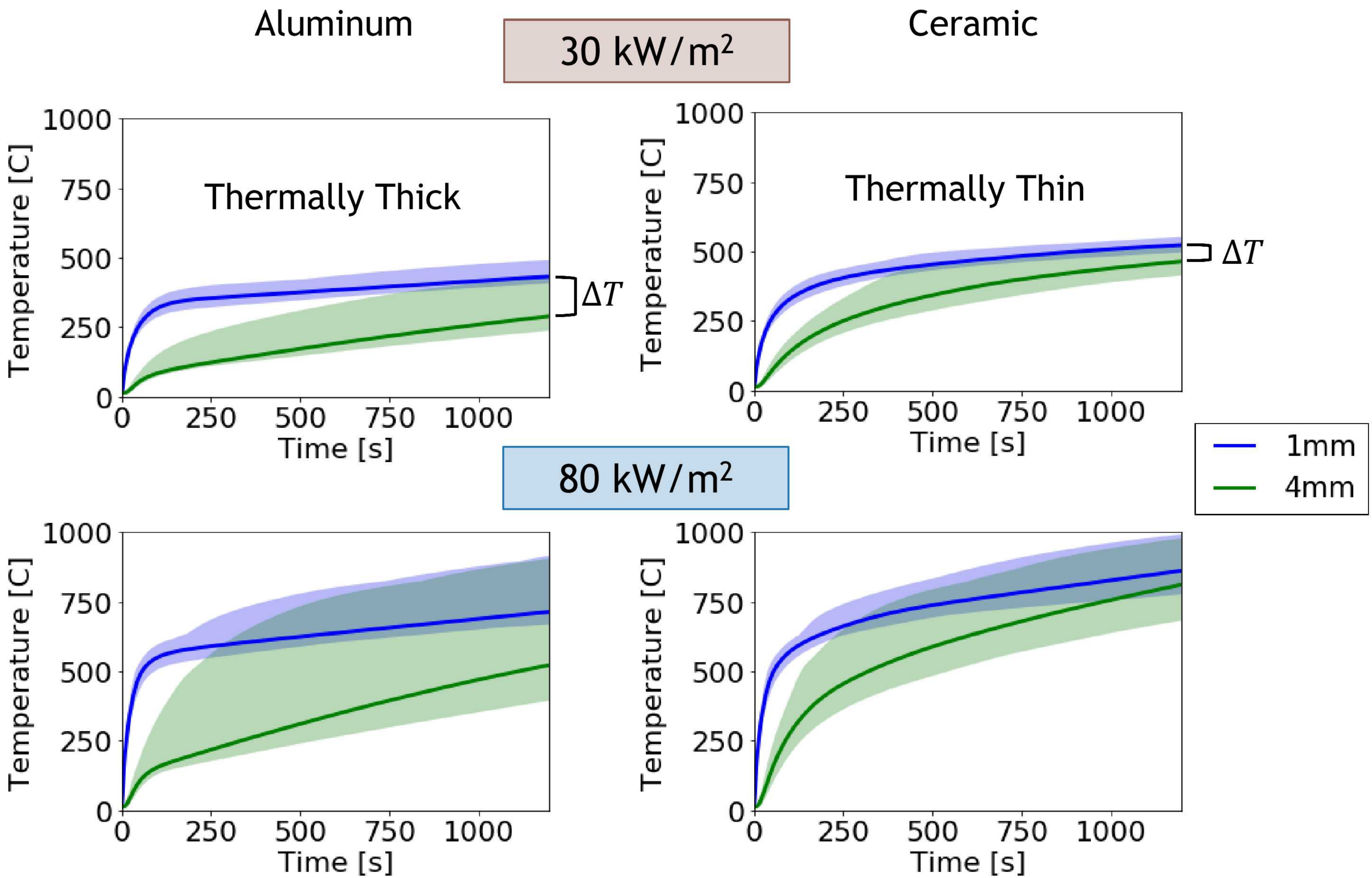
4.5 mm "Thin" Sample – 30 & 80 kW/m²



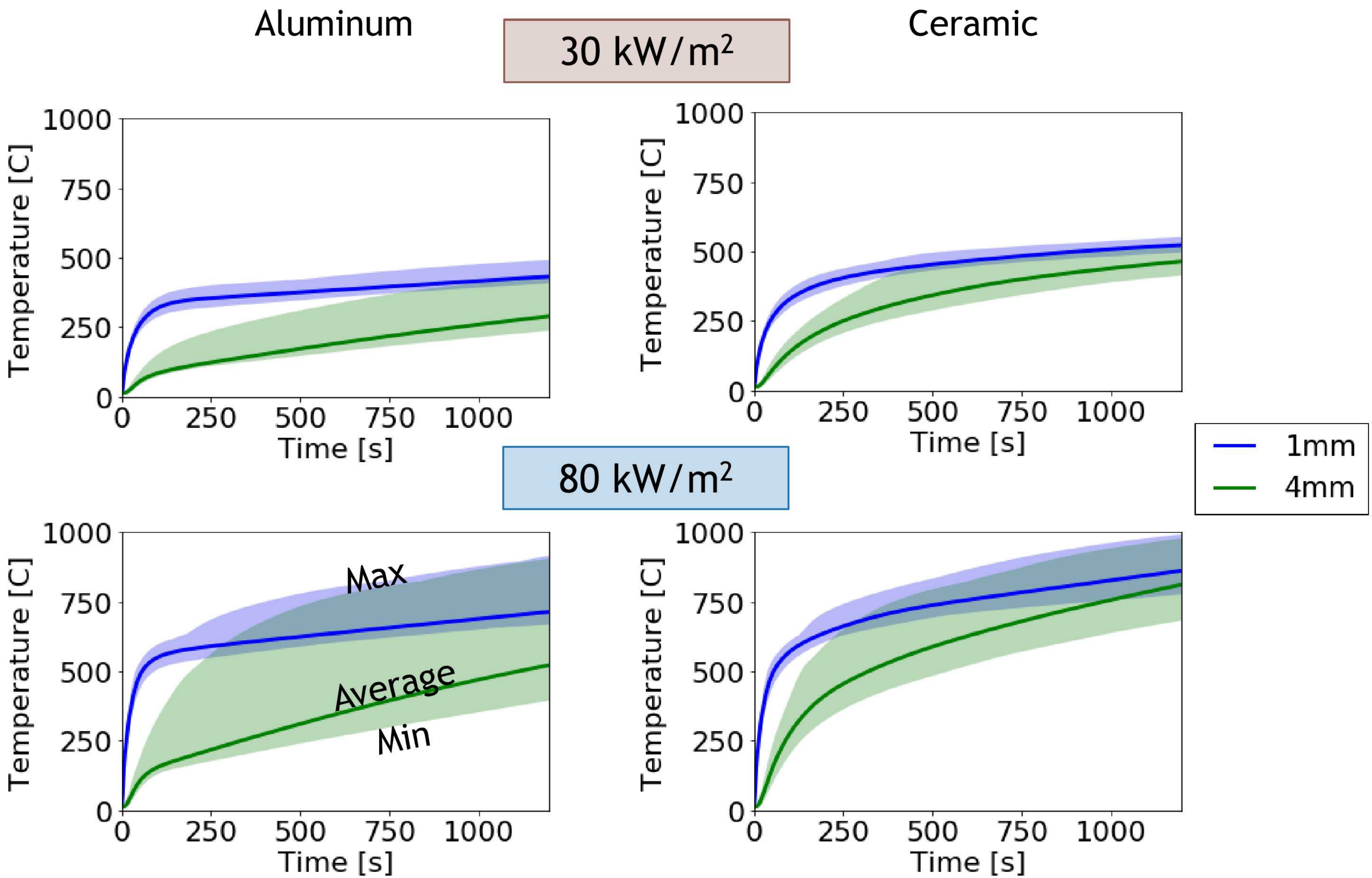
4.5 mm "Thin" Sample – 30 & 80 kW/m^2



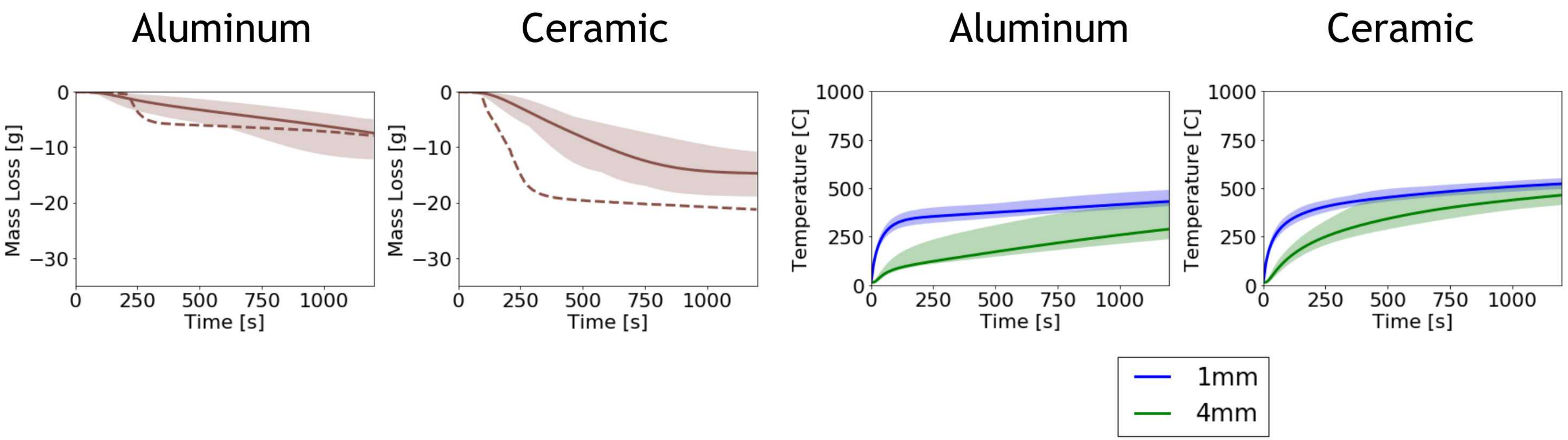
4.5 mm "Thin" Sample – 30 & 80 kW/m²



4.5 mm “Thin” Sample – 30 & 80 kW/m²



4.5 mm "Thin" Sample – 30 kW/m²

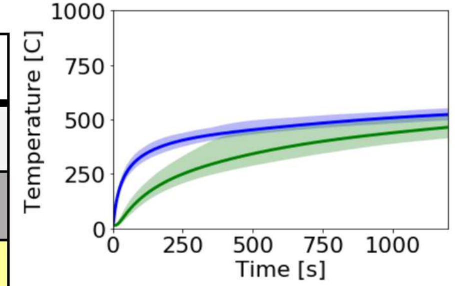


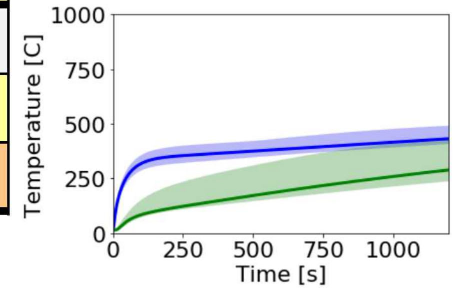
	1mm	2mm	3mm	4mm	Mass Loss
Aluminum	Carbon fiber k	$R_{contact}$	$R_{contact}$	Carbon fiber k	$\%CF$
	Composite ϵ	Carbon fiber k	Carbon fiber k	$R_{contact}$	Carbon fiber k
	$R_{contact}$	Aluminum ρc_p	Aluminum ρc_p	Aluminum ρc_p	$R_{contact}$
Ceramic	Composite ϵ	Composite ρc_p	Carbon fiber k	Carbon fiber k	$\%CF$
	Composite ρc_p	Carbon fiber k	Composite ρc_p	Composite ρc_p	$R_{contact}$
	Carbon fiber k	Composite ϵ	Composite ϵ	Ceramic ρc_p	ν

4.5 mm "Thin" Sample – 30 kW/m²

30 kW/m²

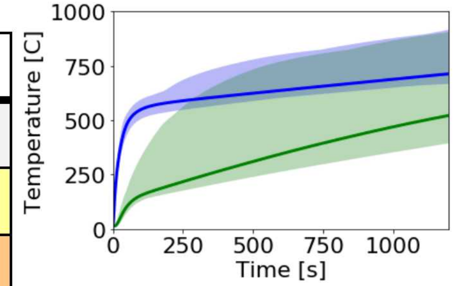
		1mm	2mm	3mm	4mm	Mass Loss
Aluminum		Carbon fiber k	$R_{contact}$	$R_{contact}$	Carbon fiber k	$\%CF$
		Composite ϵ	Carbon fiber k	Carbon fiber k	$R_{contact}$	Carbon fiber k
		$R_{contact}$	Aluminum ρc_p	Aluminum ρc_p	Aluminum ρc_p	$R_{contact}$
Ceramic		Composite ϵ	Composite ρc_p	Carbon fiber k	Carbon fiber k	$\%CF$
		Composite ρc_p	Carbon fiber k	Composite ρc_p	Composite ρc_p	$R_{contact}$
		Carbon fiber k	Composite ϵ	Composite ϵ	Ceramic ρc_p	ν

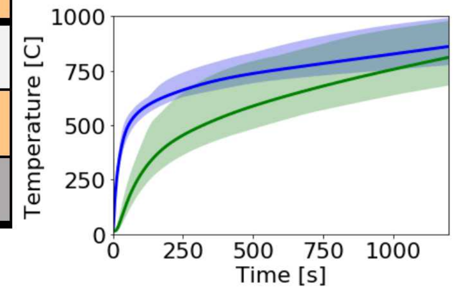




80 kW/m²

		1mm	2mm	3mm	4mm	Mass Loss
Aluminum		$R_{contact}$	$R_{contact}$	$R_{contact}$	$R_{contact}$	$\%CF$
		Composite ϵ	Composite ϵ	Carbon fiber k	Carbon fiber k	$R_{contact}$
		Carbon fiber k	Carbon fiber k	Composite k_{rad}	Aluminum ρc_p	ν
Ceramic		Composite ϵ	Composite ϵ	Carbon fiber k	Carbon fiber k	$\%CF$
		$R_{contact}$	$R_{contact}$	$R_{contact}$	$R_{contact}$	ν
		Composite ρc_p	Carbon fiber k	Composite ϵ	Composite ϵ	Carbon fiber k





Summary and Future Work

Summary

Computational Model

- 2D FEM Model, smoldering and pyrolysis, gas and condensed phase
- Mechanism created from TGA using both nitrogen and air data

Model Validation and Uncertainty Estimation

- Two sample thincknesses
- 27 input parameters varied to improve understanding of uncertainty
- Better agreement for thicker sample
- Increased importance of the sample holder and contact resistance for the thinner sample

Future Work

Improve material characterization, particularly conductivity, specific heat, and ratio of carbon fiber to epoxy

Model gas phase combustion to improve prediction for the thin samples

Couple solid phase model to gas phase model

Thank You To…

Guillermo for extending the invitation

Francesca for organizing

Questions?

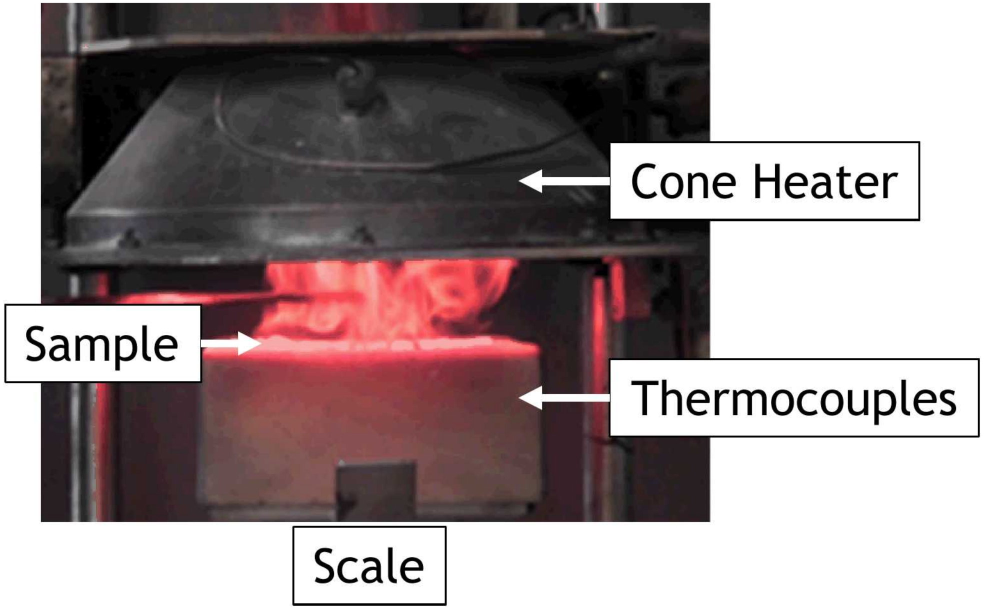
Model Parameters

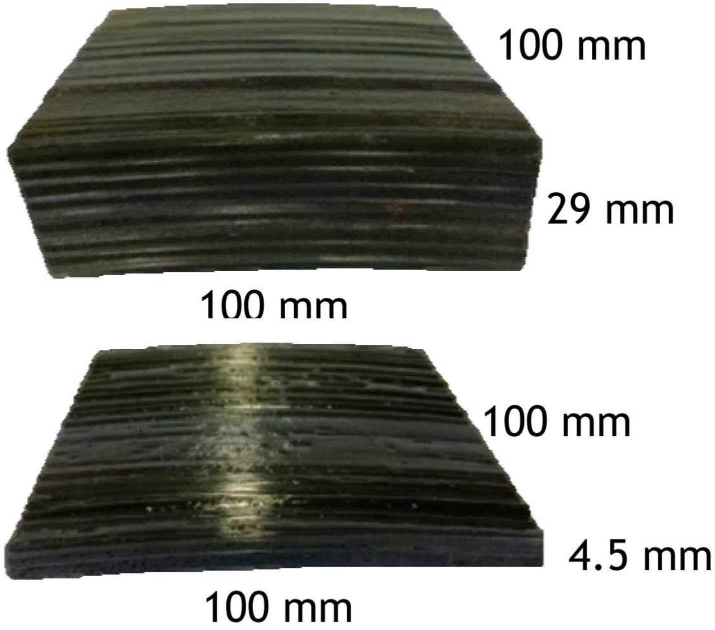
Parameter	**Value / Correlation**	**Uncertainty**	**Units**
Conductivity (k)			W/(mK)
Epoxy	0.145	±35%	
Carbon Fiber	$0.335\ln(T) - 1.8257$	±35%	
Char	0.029	±70%	
Residue	0.00725	±70%	
Density (ρ)			kg/m^3
Epoxy	408	±20%	
Carbon Fiber	952	±20%	
Char	650	±20%	
Residue	2000	±20%	
Specific Heat (c_p)			J/(kgK)
Epoxy	866	±20%	
Carbon Fiber	$4.0997\text{ T} - 369.12$	±20%	
Char	936	±20%	
Residue	866	±20%	
Permeability (K)			m^2
Epoxy	2.42e-15	-90% +900%	
Carbon Fiber	2.42e-14	-90% +900%	
Char	2.83e-12	-90% +900%	
Residue	2.42e-11	-90% +900%	
Radiative Conductivity (k_e)	$16/(3 * 5000)\sigma T^3$	-60% +400%	W/(mK)
Emissivity (ϵ)	0.91	-10% + 8%	-
Initial Carbon Fiber ($\%CF$)	70	±10%	%

Model Parameters

	A		E_a		ν		H	
	[1/s]		*[J/kmol]*		[-]		*[kJ/kg]*	
Reaction 1a	3.33 e6	±10%	1.13 e8	±0%	0.2	±20%	0	±10 [kJ/kg]
Reaction 1b	1.33 e11	-	1.47 e8	-	0.7	-	0	-
Reaction 2	1895	±10%	9.15 e7	±0%	.0001	±0%	12730	±20%
Reaction 3	9.48 e6	±10%	1.90 e8	±0%	.0001	±0%	24770	±20%

Experiments





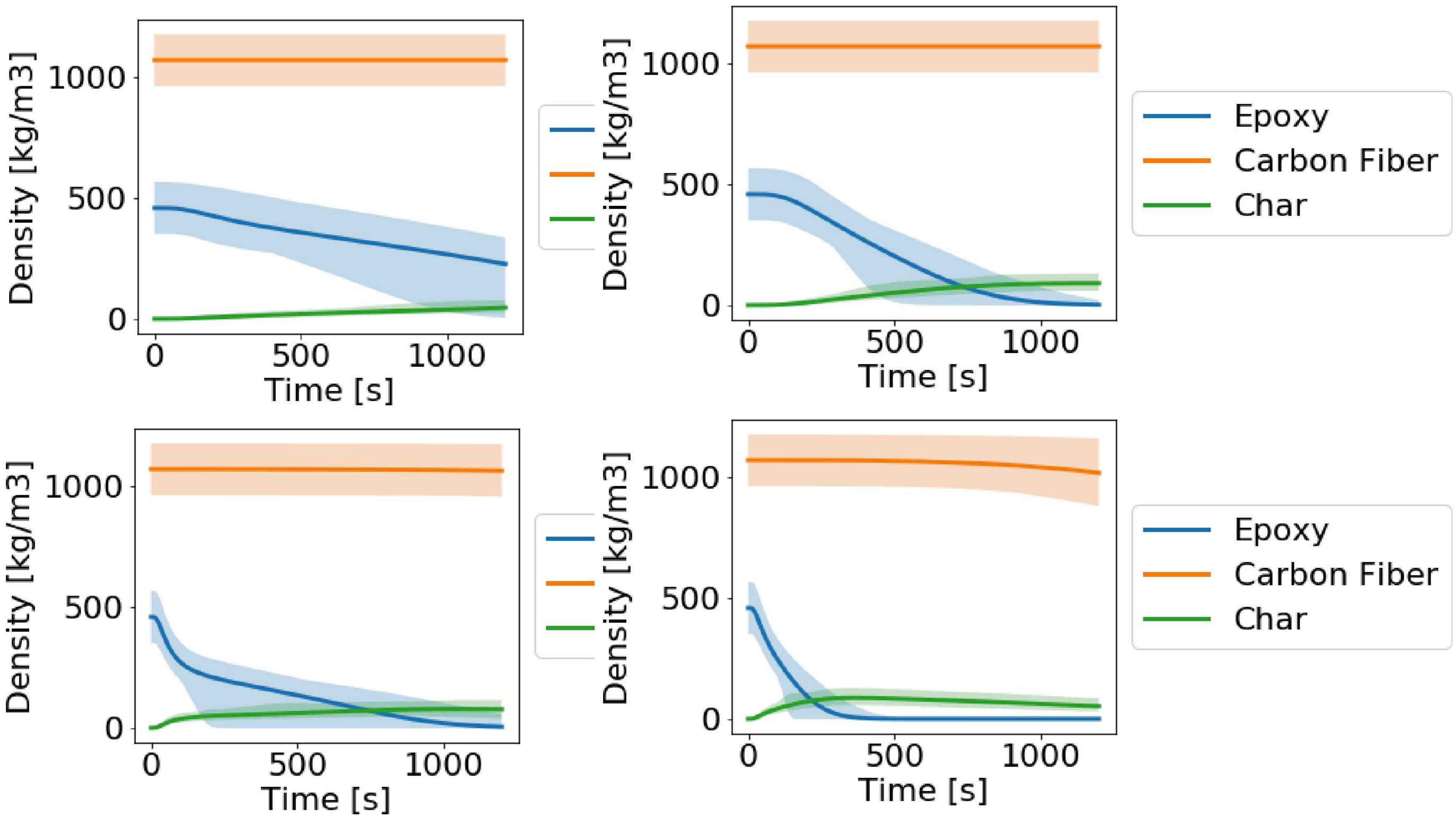
Two sample thicknesses: 4.5 mm and 29 mm

Two sample holder materials: Aluminum and Ceramic

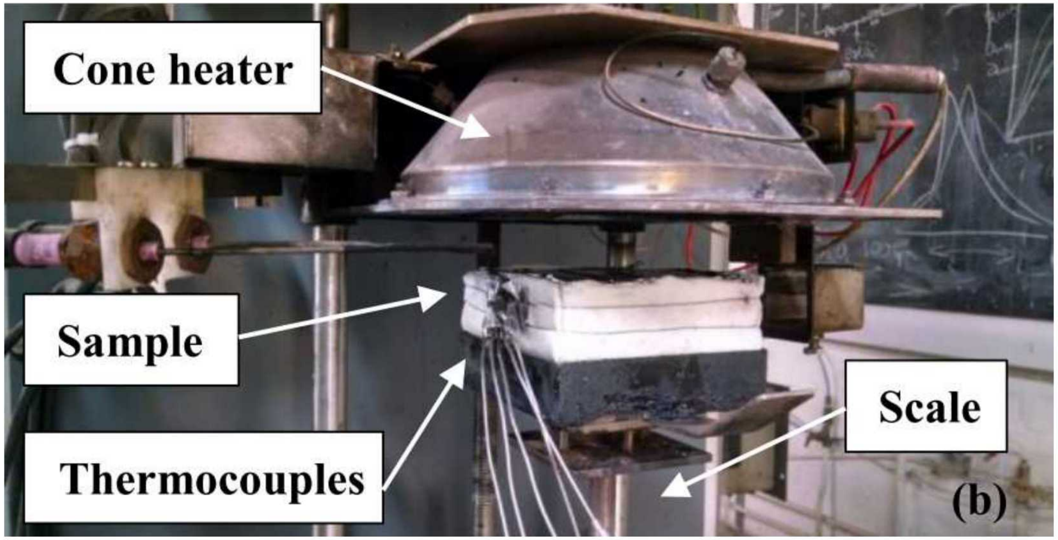
Two heat fluxes: 30 kW/m^2 and 80 kW/m^2

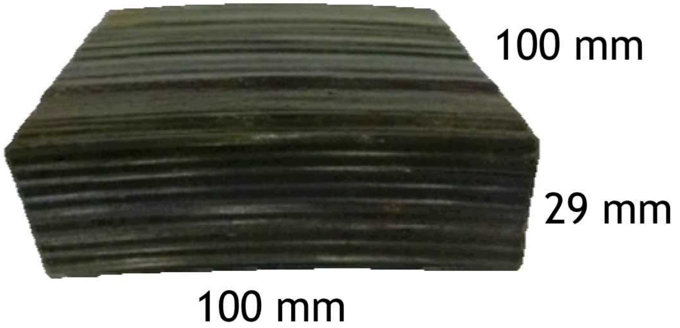
Temperature and mass loss recorded

4.5 mm “Thin” Sample – 30-80 kW/m^2



Experiment





Sample dimensions: 100 x 100 x 29 mm

Sample holder material: Aluminum

Heat flux: 30 kW/m^2

Temperature and mass loss recorded

Flaming Ignition: No