SAND2019-3067C

Validation and Uncertainty Estimation of Carbon Fiber Epoxy Composite Model

Sarah Scott[1], Victor Brunini[1], Andrew Kurzawski[1], John Hewson[1], Juan Hidalgo[2], Rory Hadden[3], Stephen Welch[3]

[1] Sandia National Laboratories
[2] School of Civil Engineering, The University of Queensland
[3] School of Engineering, The University of Edinburgh

11th U. S. National Combustion Meeting

March 24–27, 2019

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Outline

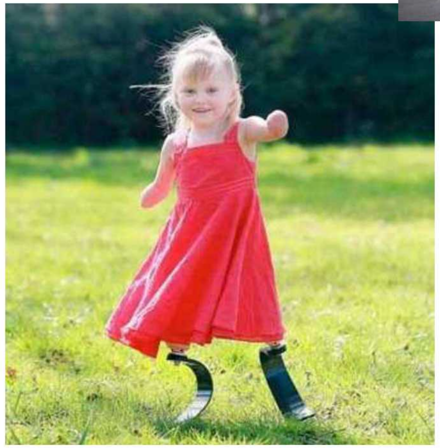
Motivation for Studying Fiber Reinforced Polymers in Fires
- These materials are different than traditional engineering materials
- This talk will focus on Carbon Fiber Epoxy Composites

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

Motivation for Studying Carbon Fiber Epoxy Composites in Fires

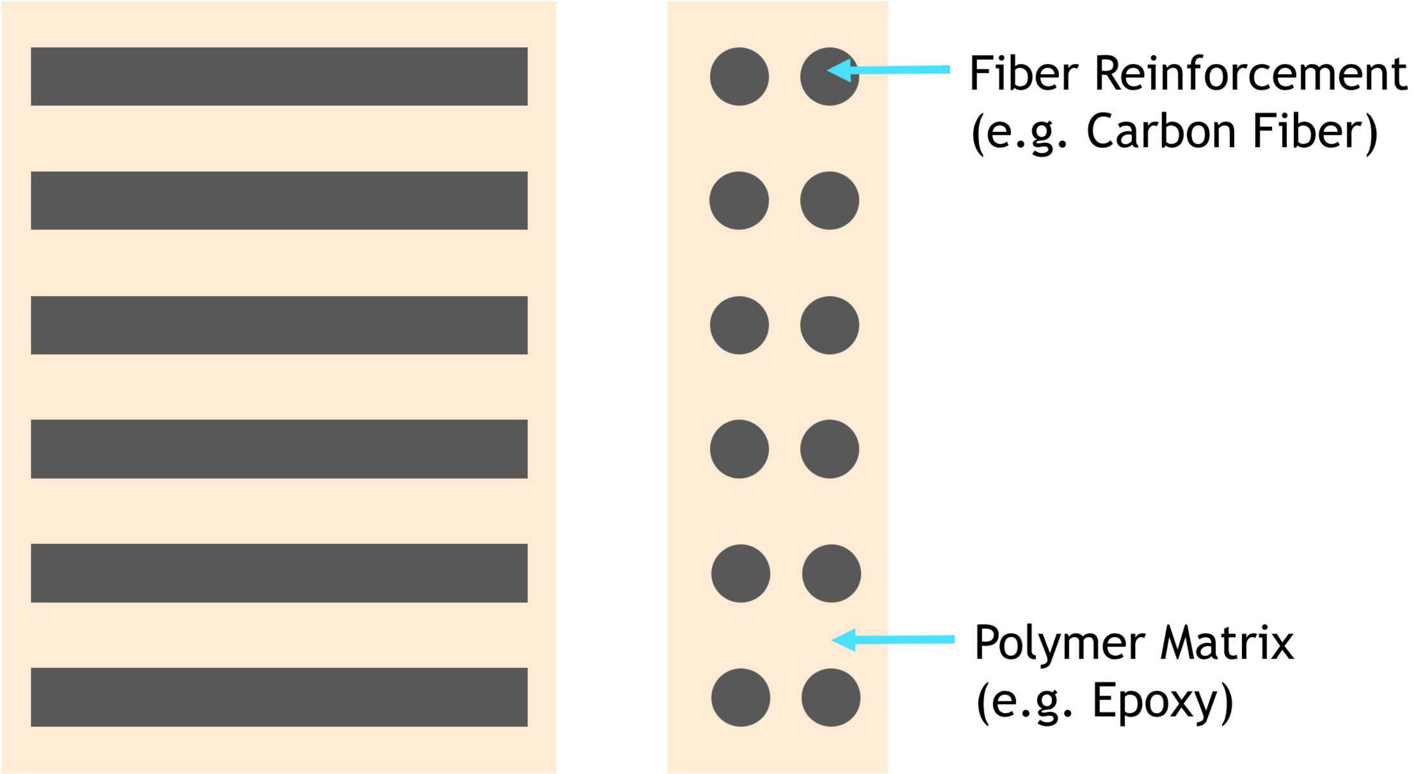
Fiber Reinforced Polymers



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.

Objective of this Work

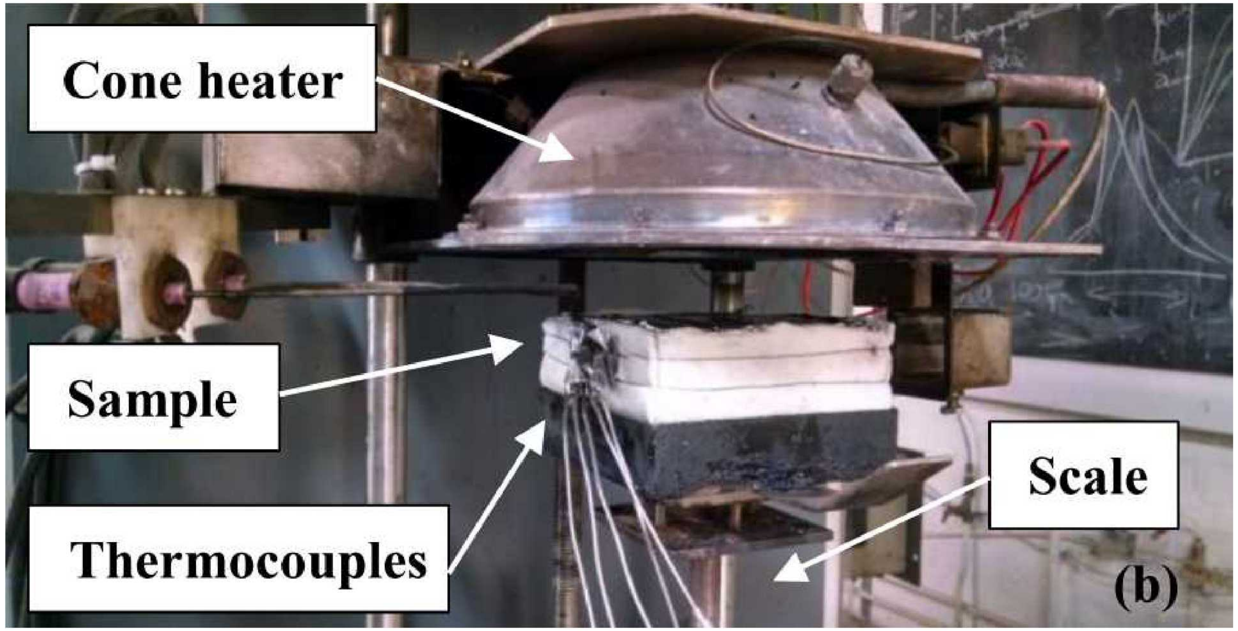
Validate a computational model of pyrolyzing and smoldering carbon fiber epoxy composite using cone calorimeter data.

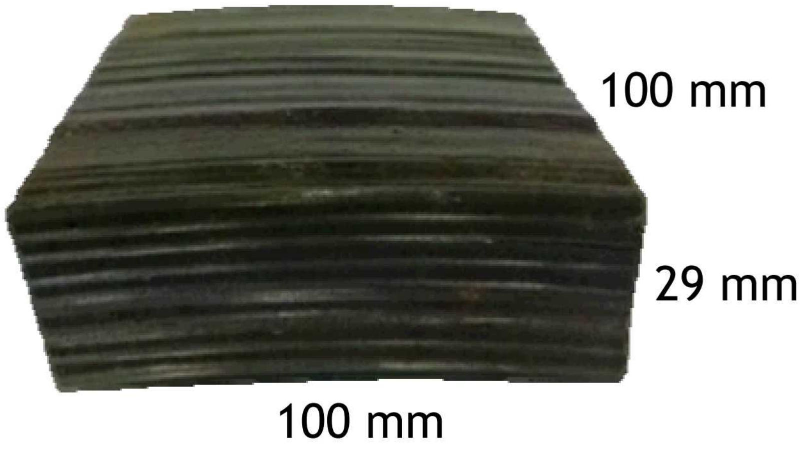
Compare temperature and mass loss data

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

Computational Model

Experiments





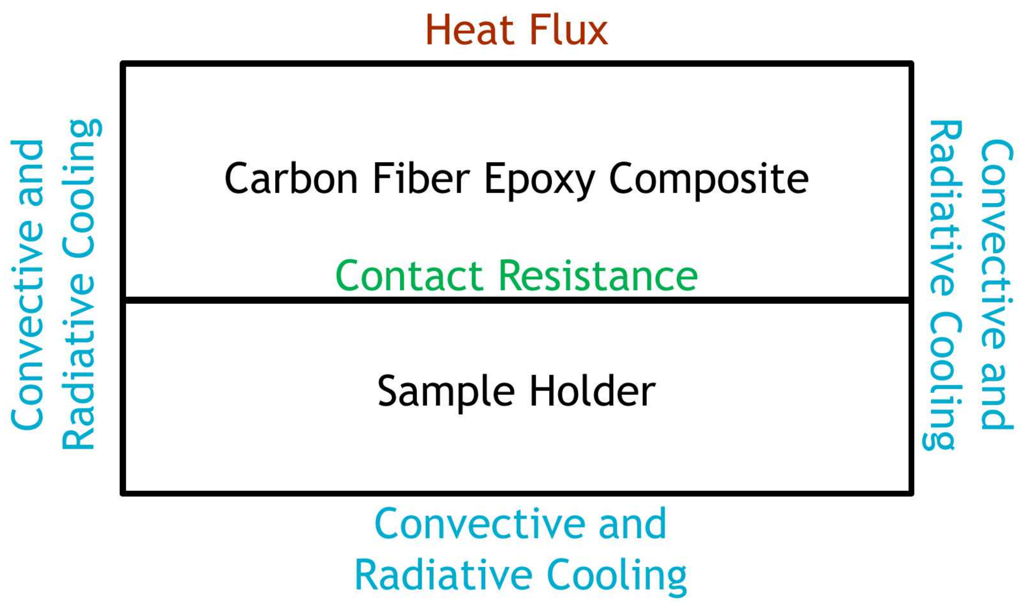
Sample thicknesses: 29 mm

Sample holder material: Aluminum

Heat flux: 30 kW/m^2

Temperature and mass loss recorded

Computational Model



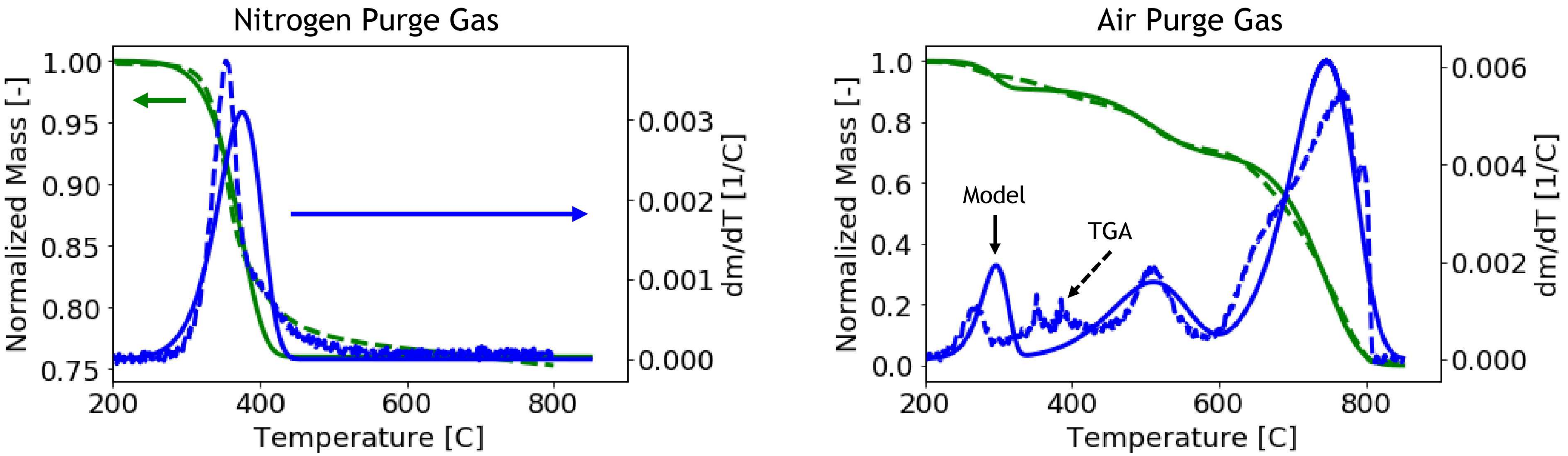
2D FEM Model in Sierra Thermal/Fluids

Pyrolysis and smoldering mechanisms

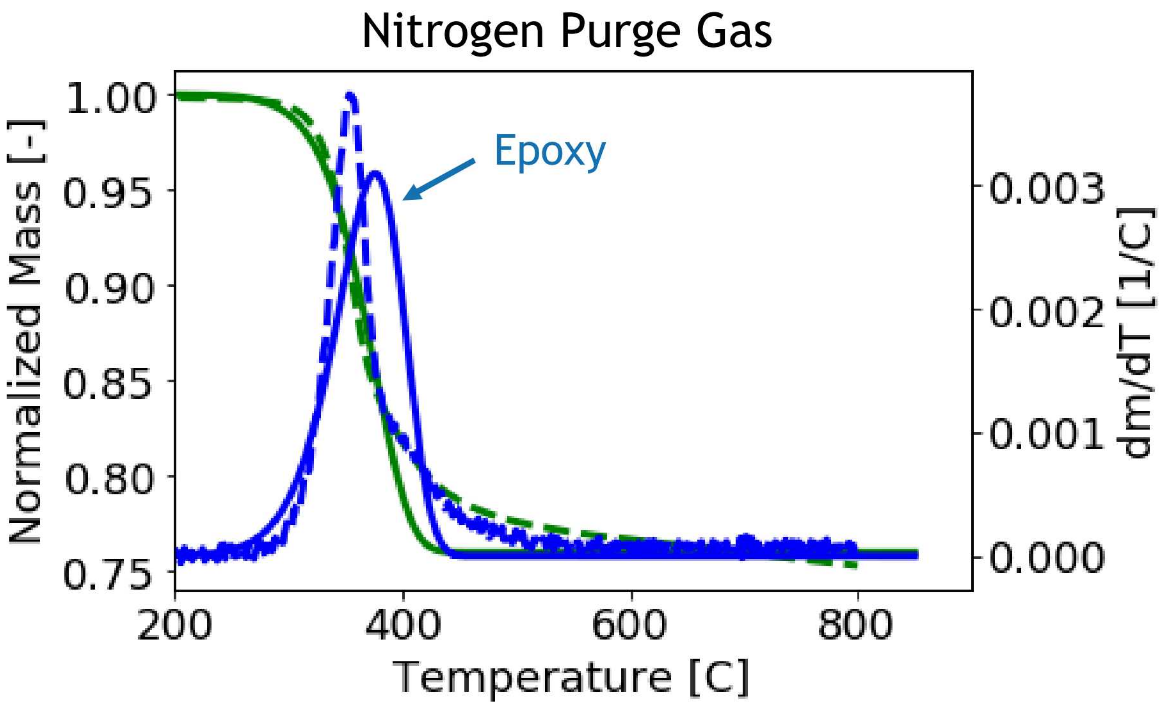
Continuity, species, and enthalpy equations
- Solved for in condensed and gas phases
- Gas velocity solved using Darcy's approximation for flow through a porous material
- Ideal gas law used to relate density to pressure
- Radiative and Convective boundary conditions

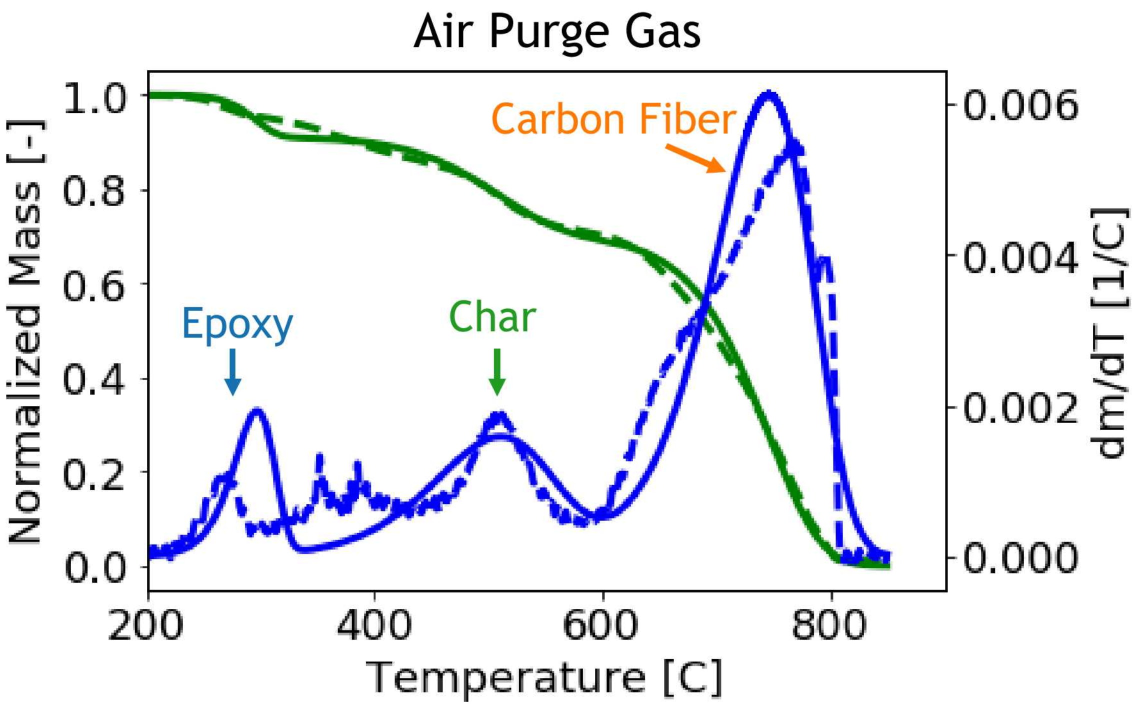
Material Properties
- Composite Effective Conductivity, Porosity, Permeability
  - Function of reaction
- Other material properties
  - Constant or function of temperature

Pyrolysis and Smoldering Mechanism



Pyrolysis and Smoldering Mechanism





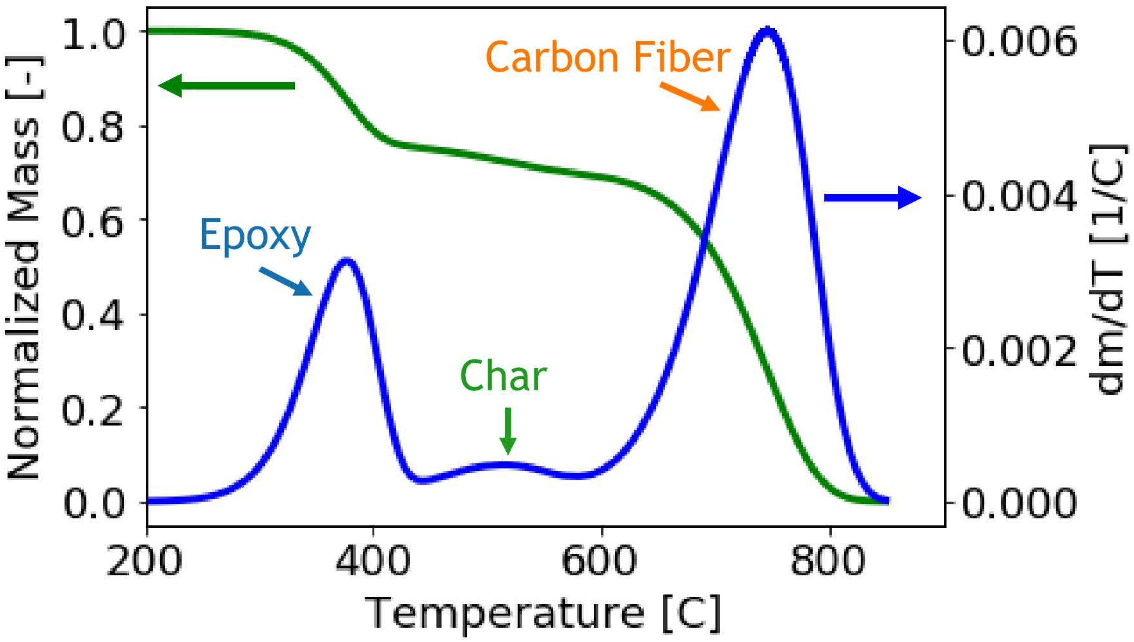
$Epoxy \rightarrow Char + fuel$

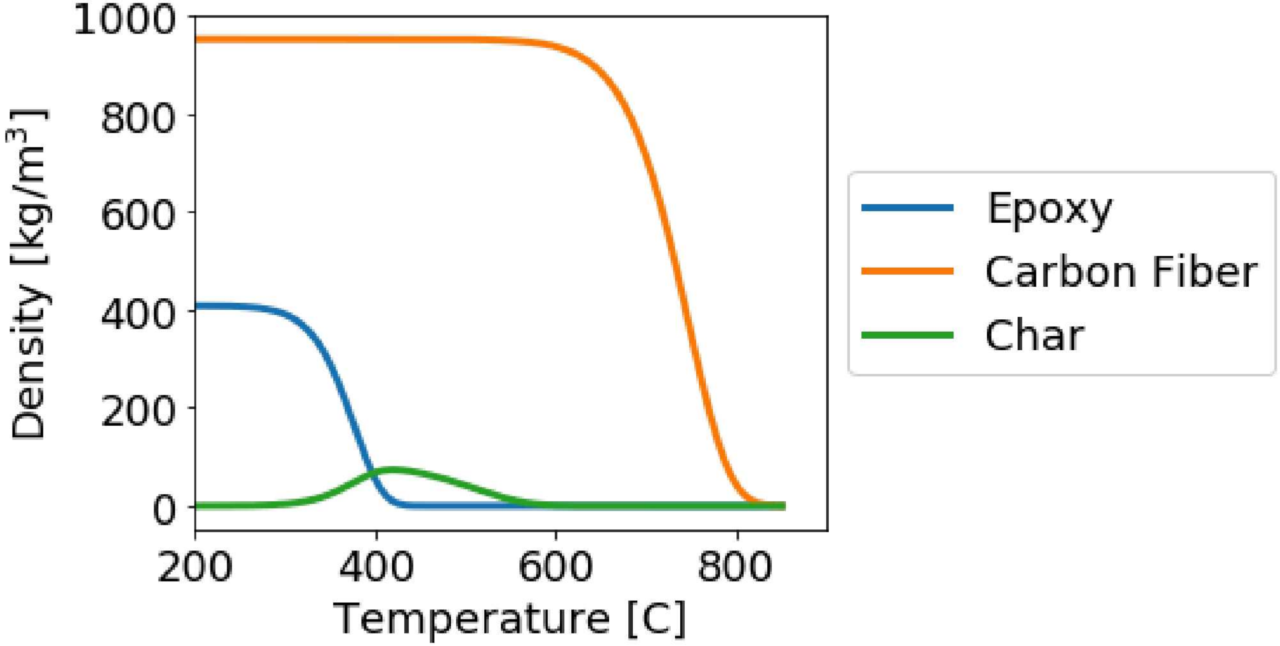
$Epoxy + O_2 \rightarrow Char + fuel$

$Char + O_2 \rightarrow Residue + gas$

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

Pyrolysis and Smoldering Mechanism





$$Epoxy \rightarrow Char + fuel$$

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

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

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

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:

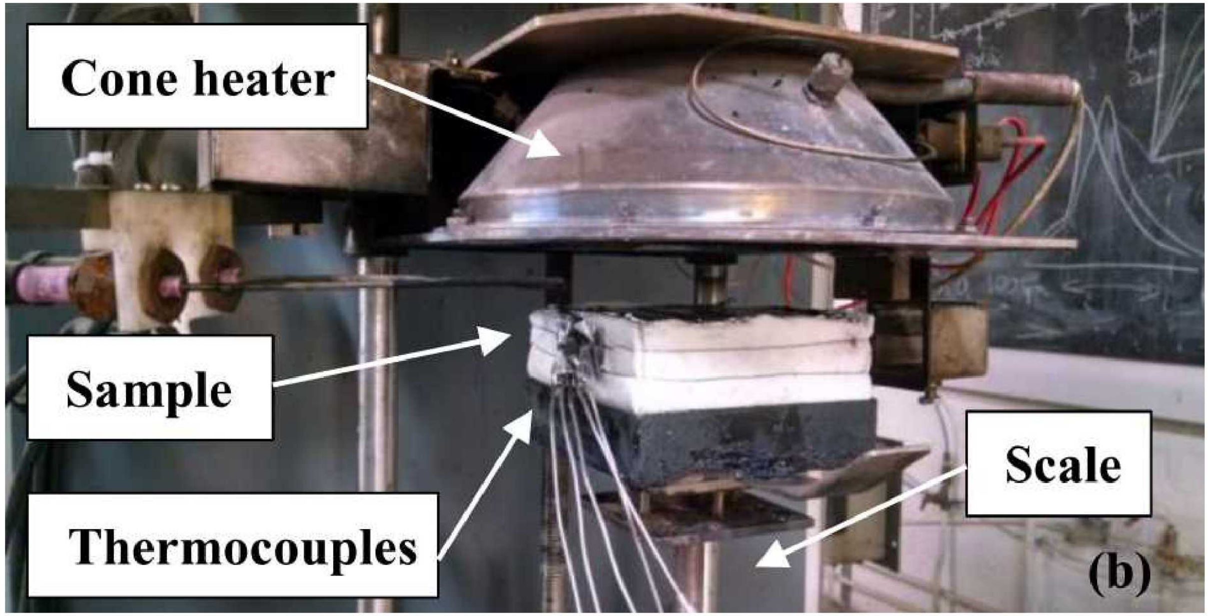
- Conductivity (k)
- Volumetric Heat Capacity (ρc_p)
- Emissivity (ϵ)

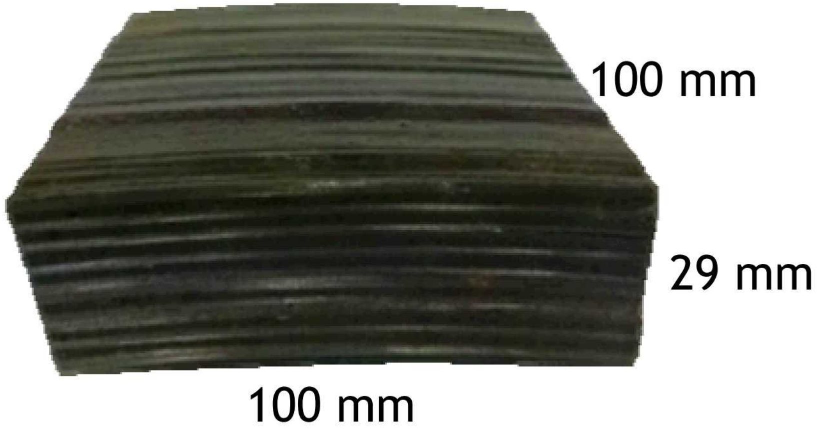
Boundary Conditions:

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

Model Validation, Uncertainty, and Sensitivity

Experiment





Sample thicknesses: 29 mm

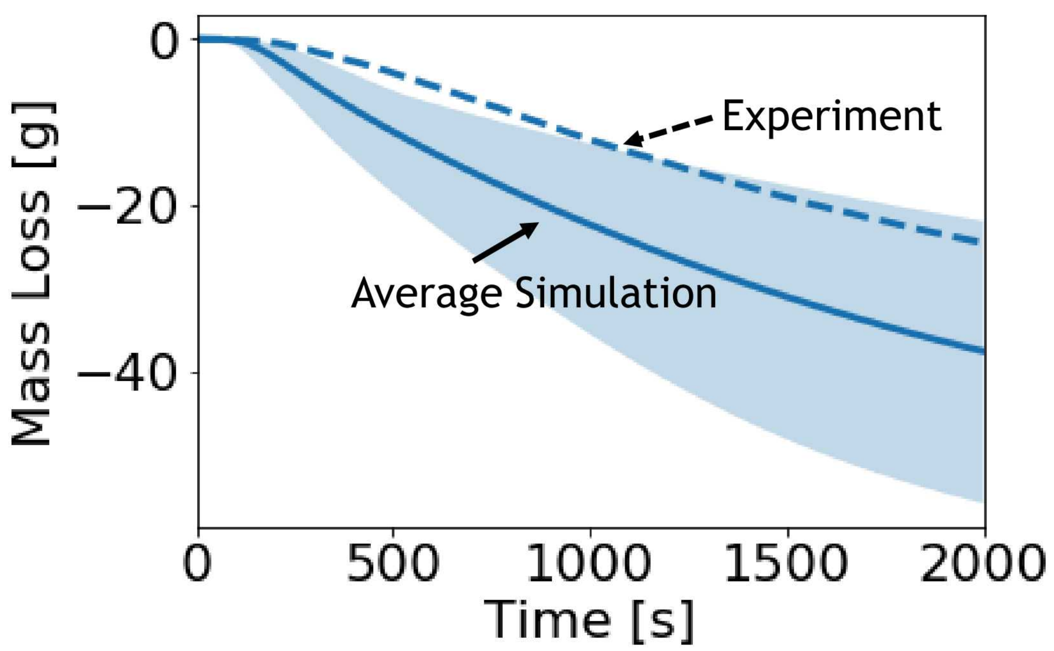
Sample holder material: Aluminum

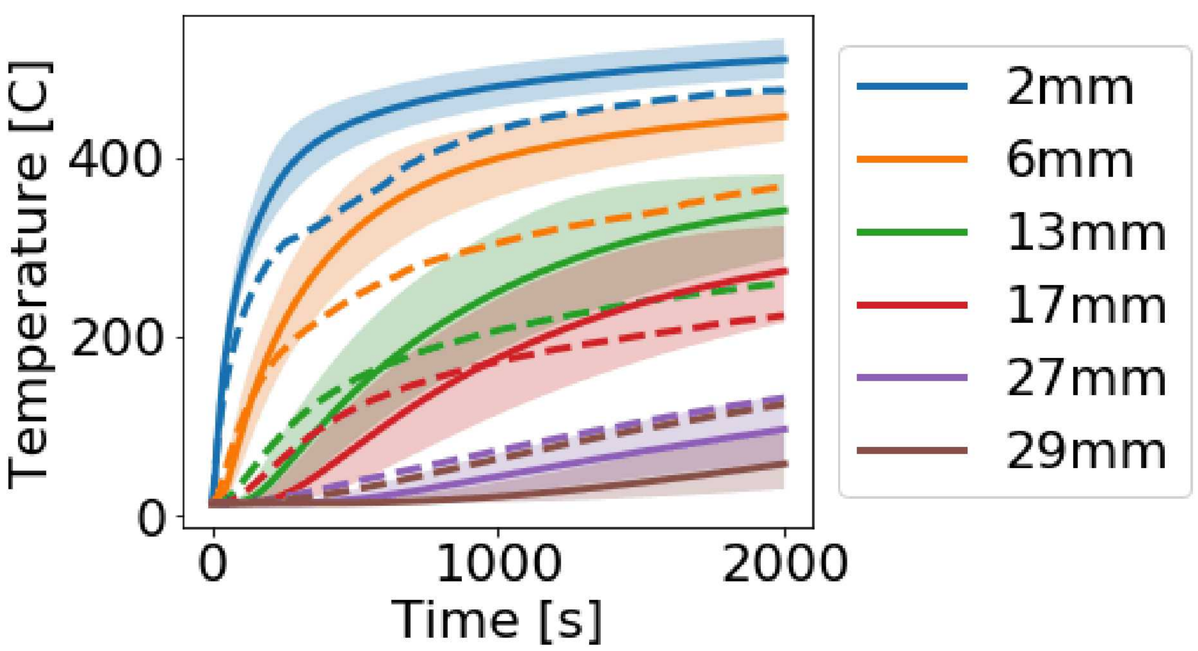
Heat flux: 30 kW/m^2

Temperature and mass loss recorded

Flaming Ignition: No

29 mm Thick Sample – 30 kW/m²





270 simulation in the ensemble

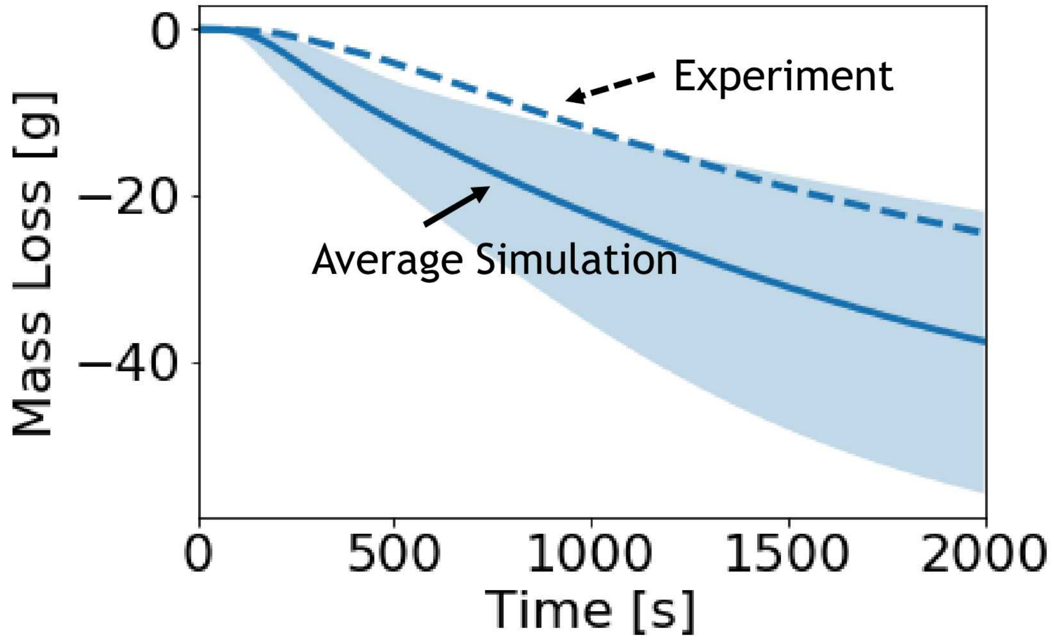
Average Simulation presented with min/max bounds

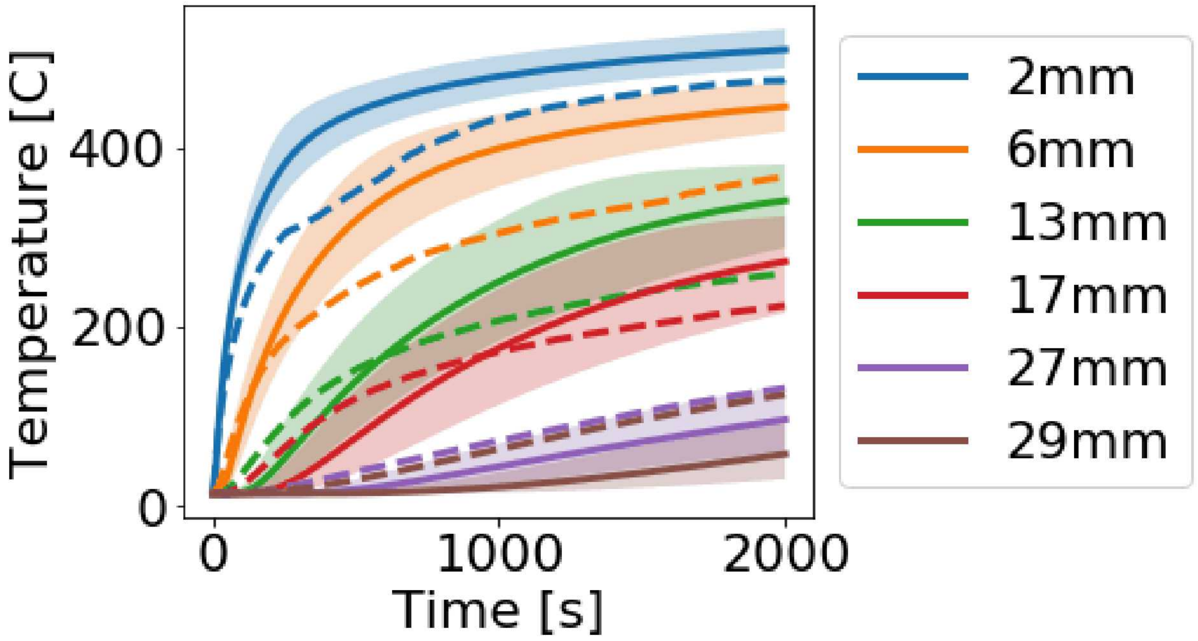
TC locations measured from top of the sample

Mass loss: good qualitative agreement

Temperature: Over predicting 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

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

- 27 input parameters varied to improve understanding of uncertainty
- Mass loss showed good qualitative agreement
- Ratio of carbon fiber to epoxy, followed by volumetric heat capacity and conductivity were most important the mass loss prediction
- Temperature over predicted in the middle of the sample
- Volumetric heat capacity and conductivity were most important to the temperature prediction

Future Work

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

- Anisotropic properties

Model gas phase combustion to increase range of experiments that can be compared to

Couple solid phase model to gas phase model

Questions?

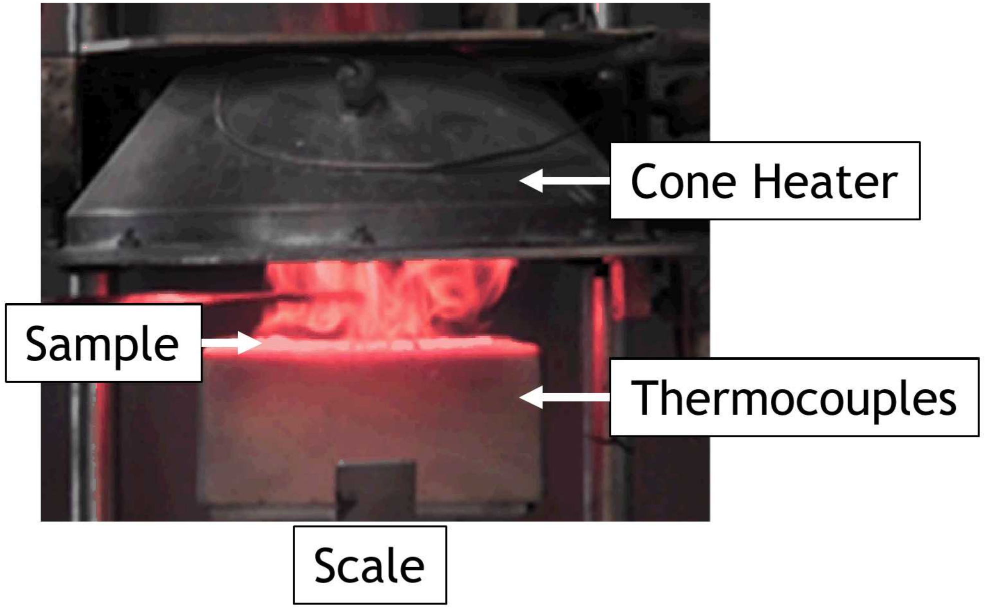
Model Parameters

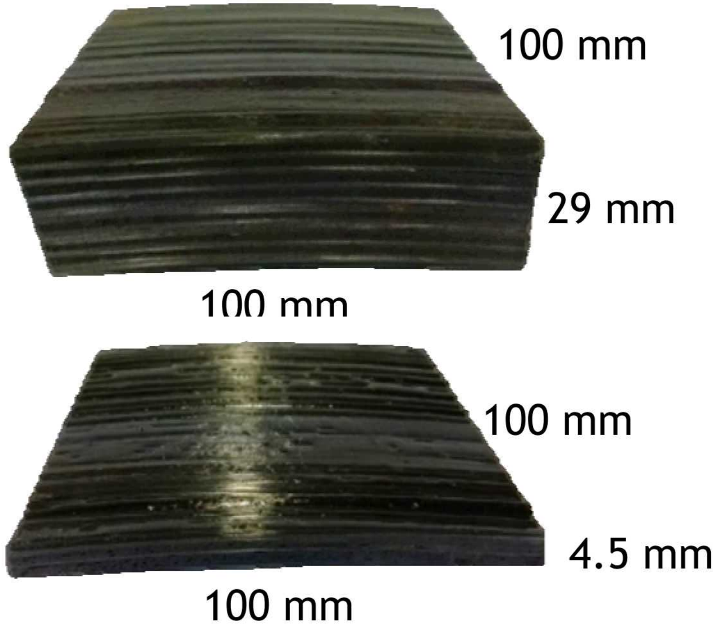
Parameter	Value / Correlation	Uncertainty	Units
Conductivity (k)			W/(mK)
Epoxy	0.145	±35%	
Carbon Fiber	$0.335\ln(T) - 1.8257$	±35%	
Char	0.029	±70%	
Residue	0.00725	±70%	
Density (ρ)			kg/m^3
Epoxy	408	±20%	
Carbon Fiber	952	±20%	
Char	650	±20%	
Residue	2000	±20%	
Specific Heat (c_p)			J/(kgK)
Epoxy	866	±20%	
Carbon Fiber	$4.0997\,\mathrm{T} - 369.12$	±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





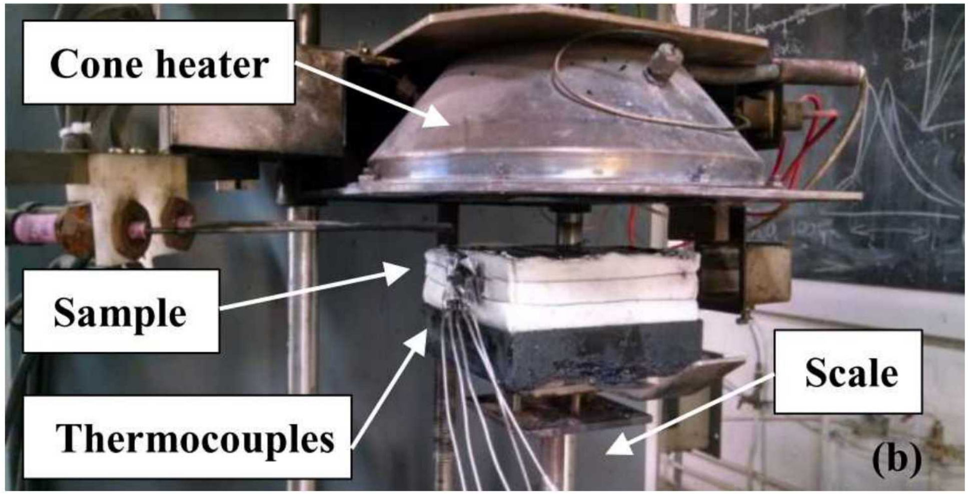
Two sample thicknesses: 4.5 mm and 29 mm

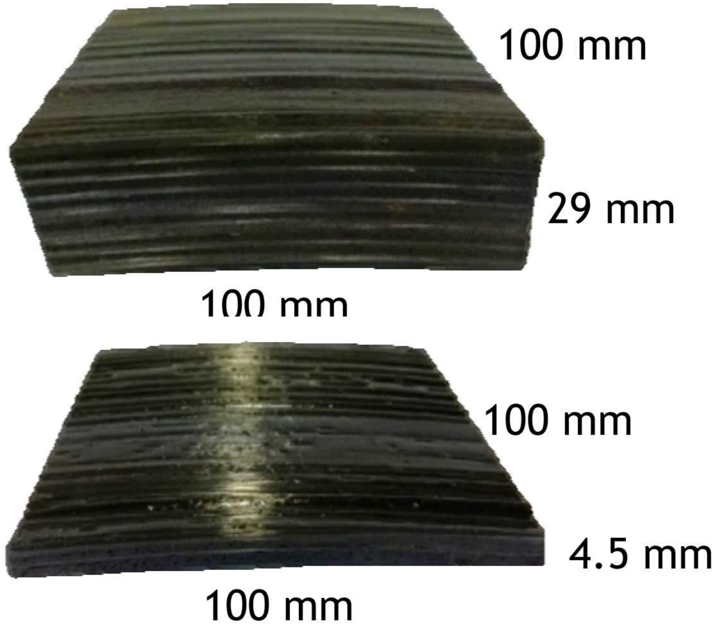
Two sample holder materials: Aluminum and Ceramic

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

Temperature and mass loss recorded

Experiments





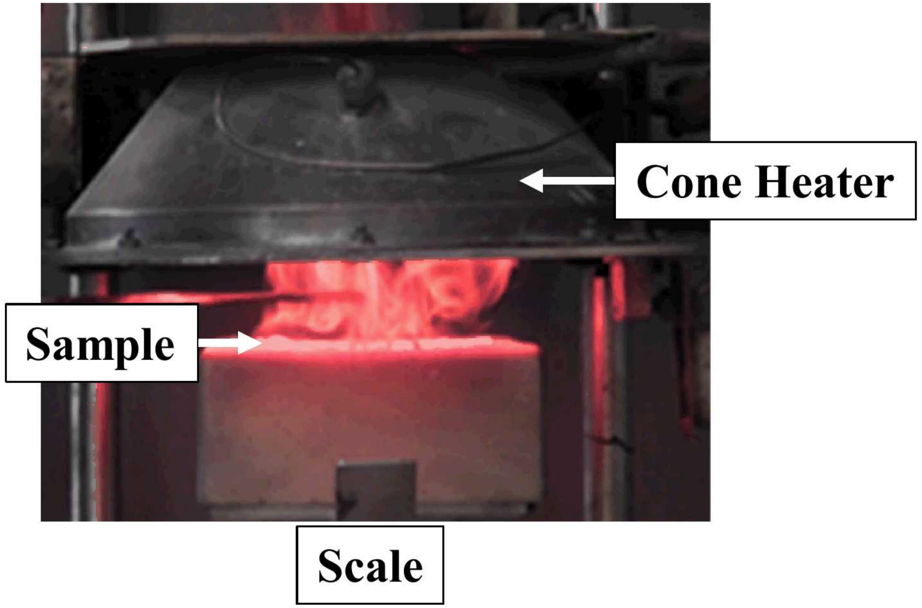
Two sample thicknesses: 4.5 mm and 29 mm

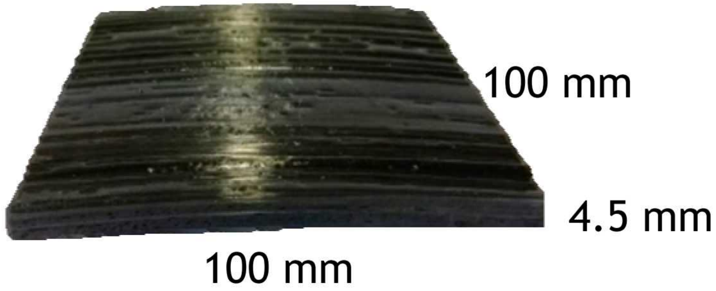
Two sample holder materials: Aluminum and Ceramic

Heat flux: 30 kW/m^2

Temperature and mass loss recorded

"Thin" Sample





Sample thicknesses: 4.5 mm

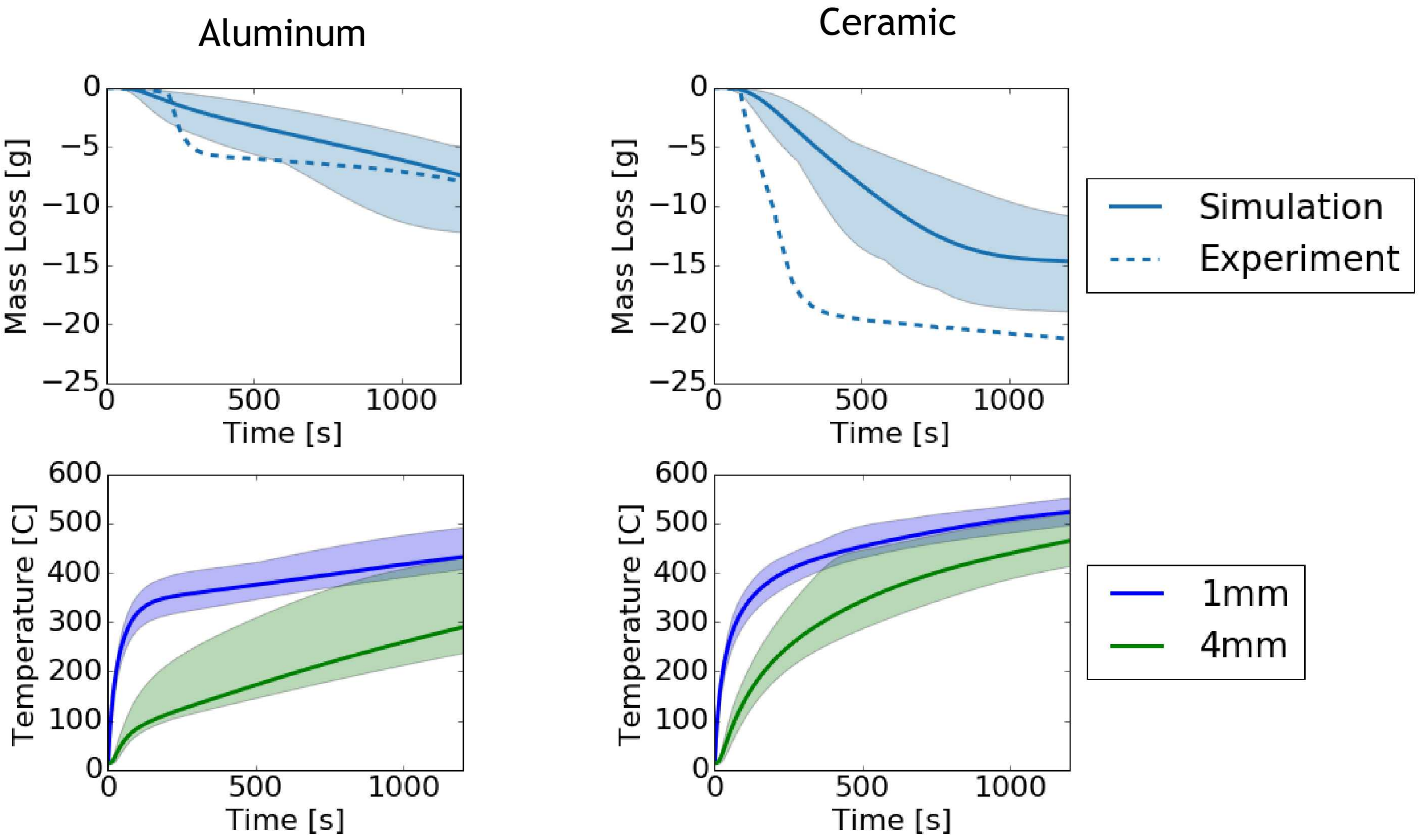
Two sample holder materials: Aluminum and Ceramic

Heat flux: 30 kW/m^2

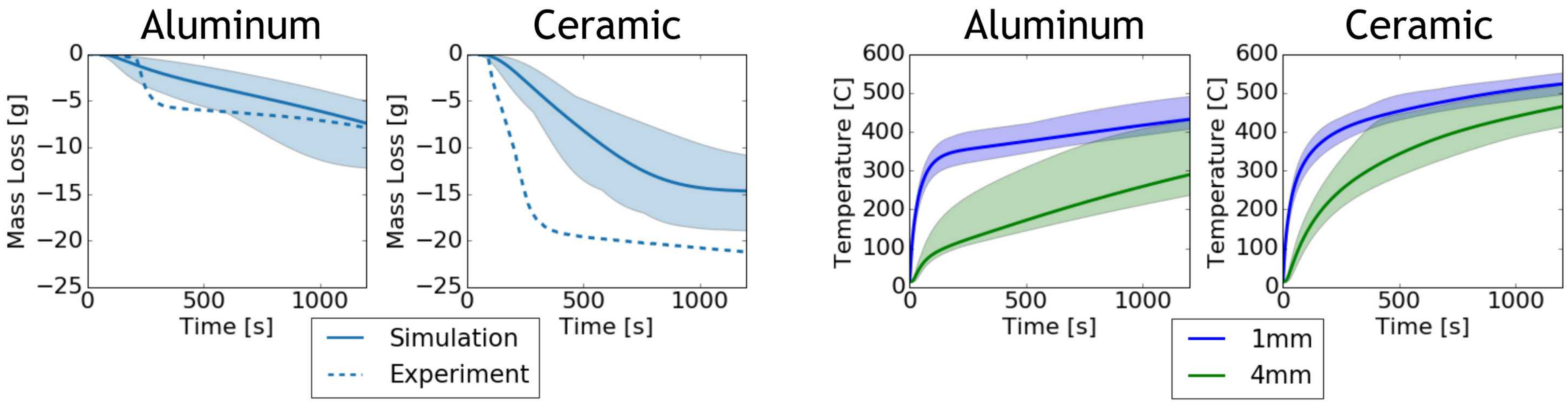
Mass loss recorded

Flaming Ignition: Yes

4.5 mm "Thin" Sample – 30 kW/m²



4.5 mm “Thin” Sample – 30 kW/m²



	1mm	2mm	3mm	4mm	Mass Loss
Aluminum	Carbon fiber k	R_c	R_c	Carbon fiber k	$\%CF$
	Composite ϵ	Carbon fiber k	Carbon fiber k	R_c	Carbon fiber k
	R_c	Aluminum ρc_p	Aluminum ρc_p	Aluminum ρc_p	R_c
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_c
	Carbon fiber k	Composite ϵ	Composite ϵ	Ceramic ρc_p	ν