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Fire Science & Technology

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# Numerical study of pyrolysis and combustion of a carbon fiber-epoxy composite

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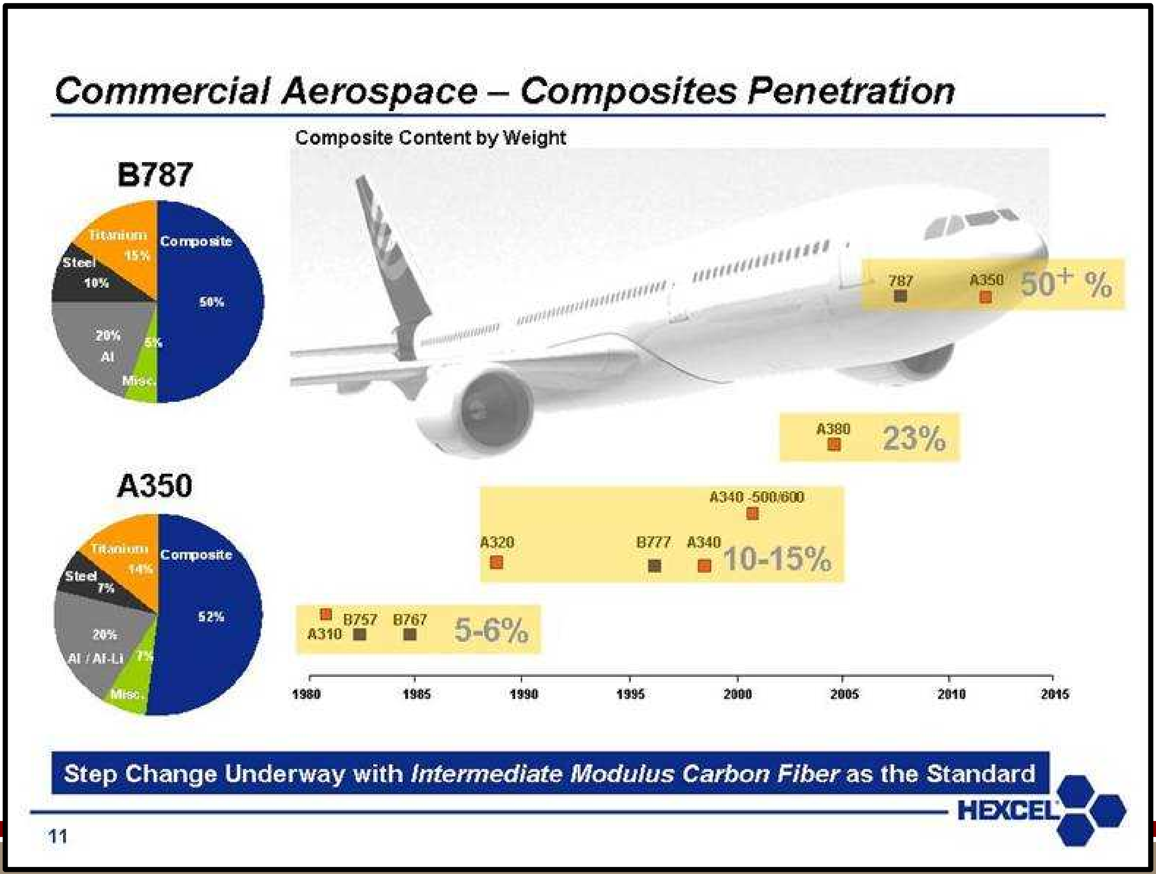
# Composites in the Aviation Industry

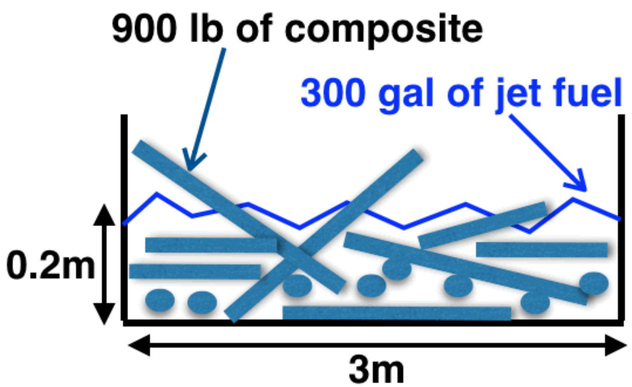
- Modern aircraft uses increasing quantities of composites
  - Reduce weight while preserving strength
  - Lower fuel consumption: efficiency ↑, emission ↓
  - Carbon fiber-epoxy materials are heavily used in new design




from hexcel.com

# Composites and the Safety

- Sandia has been focusing on understanding potential fire environment
  - Fire experiments were performed at various scales and scenarios
- In 2014, a rubble fire test was performed that replicates an aircraft accident
  - Carbon fiber epoxy composite rubbles were soaked in jet fuel

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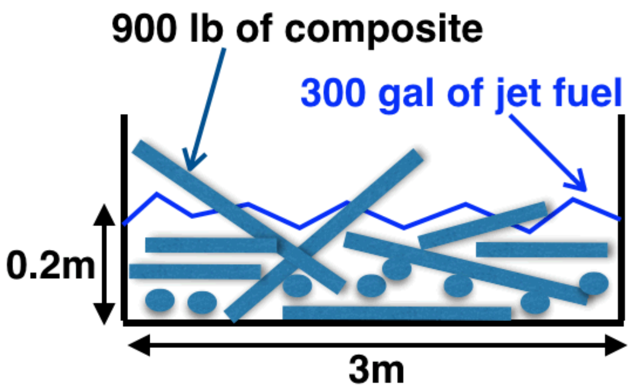



- Test lasted 14+ hours before suspended
- Burning is slow but constant due to the rubble presence
- Burning characteristics of soaked composite needs to be modeled
  - Which requires a 3-phase combustion solver

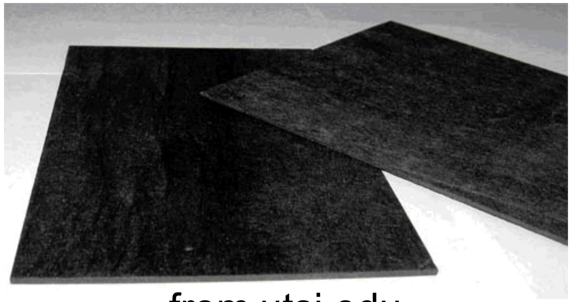
# Available Tools & Objectives

- SIERRA: Sandia's engineering mechanics simulation code suite
  - Fuego: low-Ma reacting turbulent flow solver
  - Aria: low-Re multi-phase reaction & heat transfer solver
  - Syrinx: radiation solver
  - Several solid-gas, liquid-gas 2-phase combustion models are available
  - Full 3-phase combustion capability is currently under development

- Objective: develop a rigorous solid combustion model for carbon fiber epoxy
  - Revisit solid-gas 2-phase combustion model
  - Simulate two experiments

# Carbon Fiber Epoxy

- 65% carbon fiber, 35% epoxy resin
- Fabric (woven) or uni-tape sheets, usually multiple layers thick
  - Results in the exceptional strength and directional properties
- Thermal characteristics depend on the details of composition and manufacturing (curing) process
  - Woven CYTEC 977-3, cured in 1 atm oven with IM7 fibers, is tested



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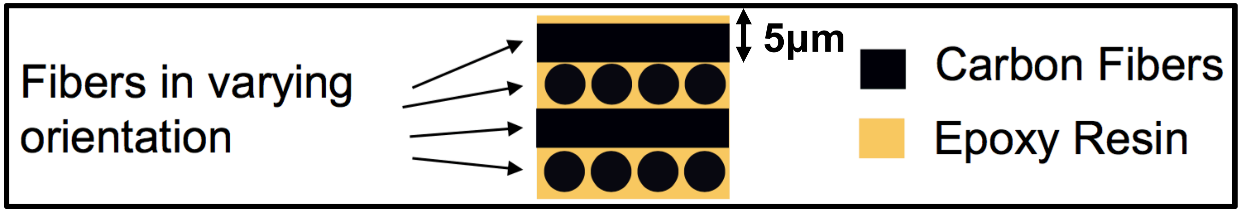
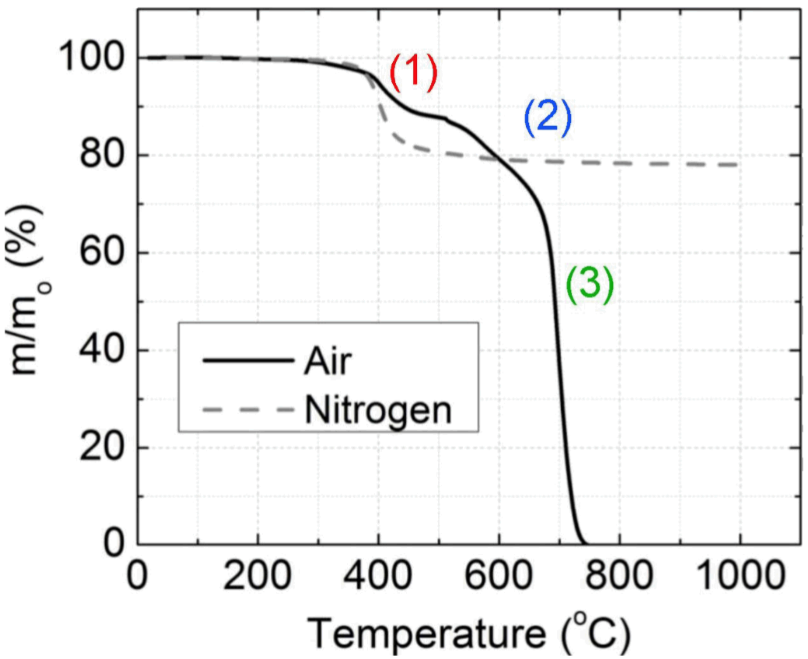


# TGA Results

- 20°C/min
- Epoxy pyrolysis generates gaseous fuel and char
- In air, epoxy oxidizes before char and carbon fiber

Brown et al. (2012)

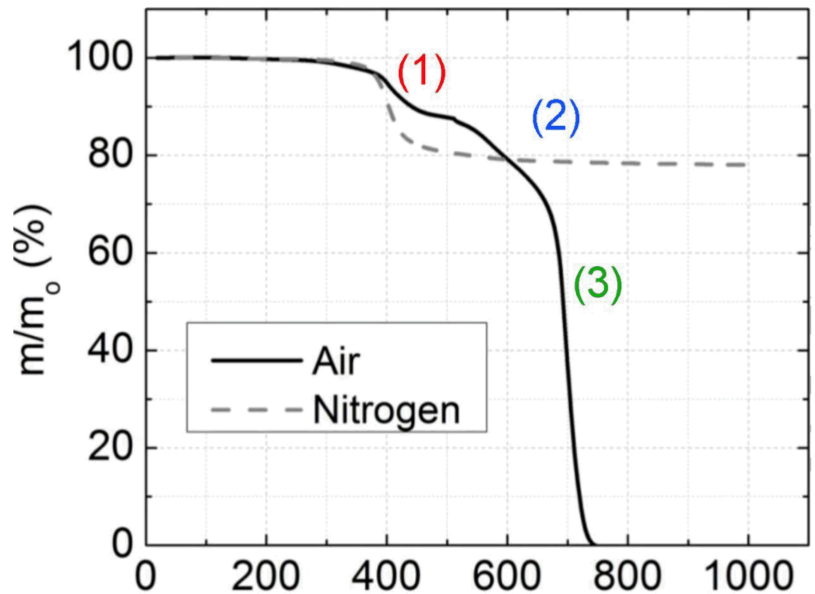



(1) Epoxy Decomposition (both Thermal and Oxidative Pyrolysis) and Char Formation
(2) Slow Char Oxidation
(3) Carbon Fiber Oxidation

# TGA Results

- 20$^{o}$C/min
- Epoxy pyrolysis generates gaseous fuel and char
- In air, epoxy oxidizes before char and carbon fiber
- Different sample results in different TGA

Brown et al. (2012)




Quintiere et al. (2007)
Different company

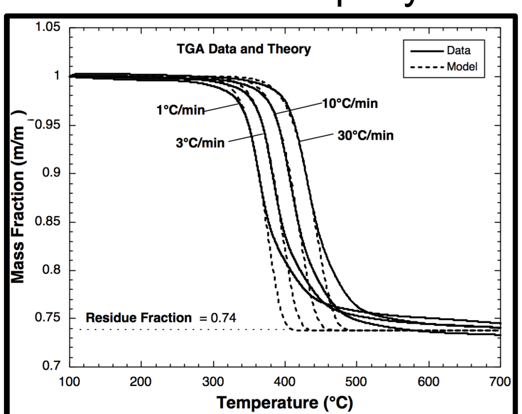



Figure 7. The TGA Results and Comparison to First-Order Model

Murthy et al. (2015)
Different composition

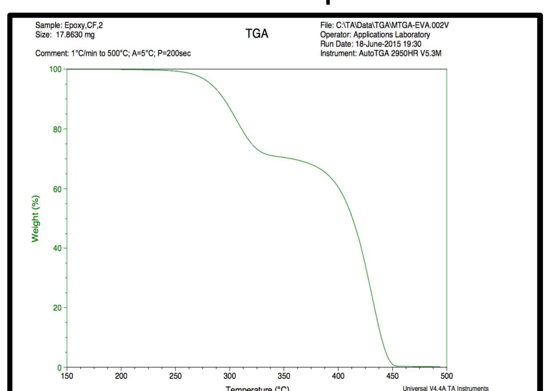
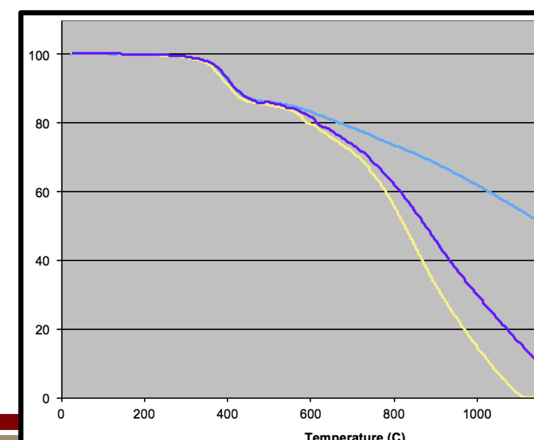



**Figure 17:** Thermo Gravimetric Analysis for Specimen 2 of System 1.

Dodd et al. (2013)
Sampled different parts



# Reaction Mechanism

- Fitted mechanism with the TGA (Dodd et al. 2013)
- For a solid-gas reaction, defining pre-exponent factor needs a caution

Gas species: $$\frac{\partial \rho_g Y_{CH_4}}{\partial t} + \nabla \cdot (\rho_g \mathbf{u} Y_{CH_4} + \rho_g D \nabla Y_{CH_4}) = \dot{\omega_{EDC}} + 0.5\dot{\omega_1} + \dot{\omega_2}$$

Solid composition: $$\frac{d\rho_s Y_{epoxy}}{dt} = -\dot{\omega_1} - \dot{\omega_2}$$

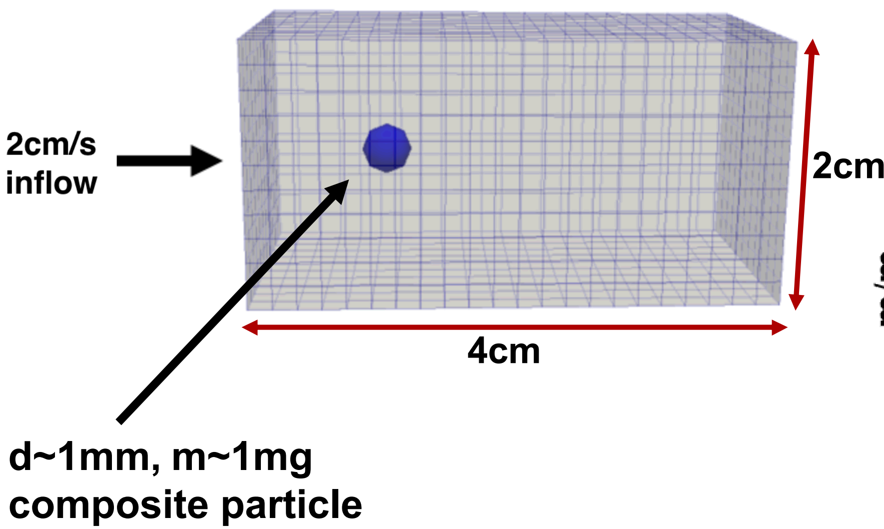
Reaction rates: $$\dot{\omega_1} = \rho_s Y_{r,s} A e^{-E_a/RT}$$

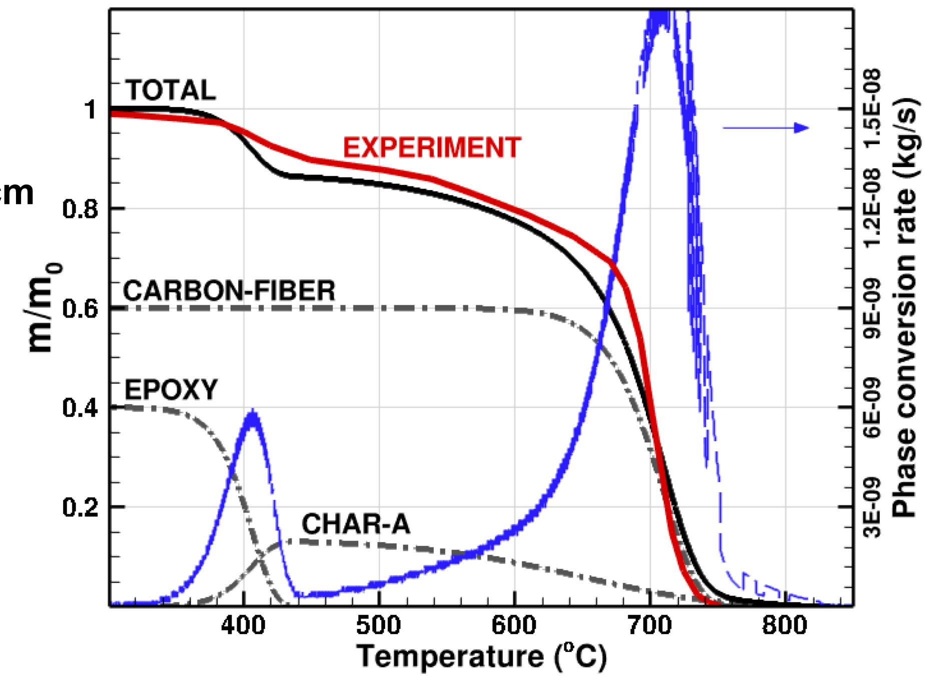
$$\dot{\omega_{2-5}} = \rho_s Y_{r,s} \rho_g Y_{r,g} A e^{-E_a/RT}$$

| | | |
|---|---|---|
| 1 pyrolysis | Epoxy → 0.5 CharA + 0.5 $CH_4$ | A=3.33E15, $E_a$/R=27200 |
| 2 oxid. | Epoxy + $O_2$ → CharB + $CH_4$ | A=5.3E15/$\rho_g$, $E_a$/R=27200 |
| 3 oxid. | CharA + $O_2$ → Residue + CO | A=7.58E2/$\rho_g$, $E_a$/R=10000, ΔH=12730kJ/kg |
| 4 oxid. | CharB + $O_2$ → Residue + CO | A=7.58E2/$\rho_g$, $E_a$/R=10000, ΔH=12730kJ/kg |
| 5 oxid. | Carbon-Fiber + $O_2$ → Residue + $CO_2$ | A=3.79E15/$\rho_g$, $E_a$/R=38000, ΔH=24770kJ/kg |

# TGA Simulation

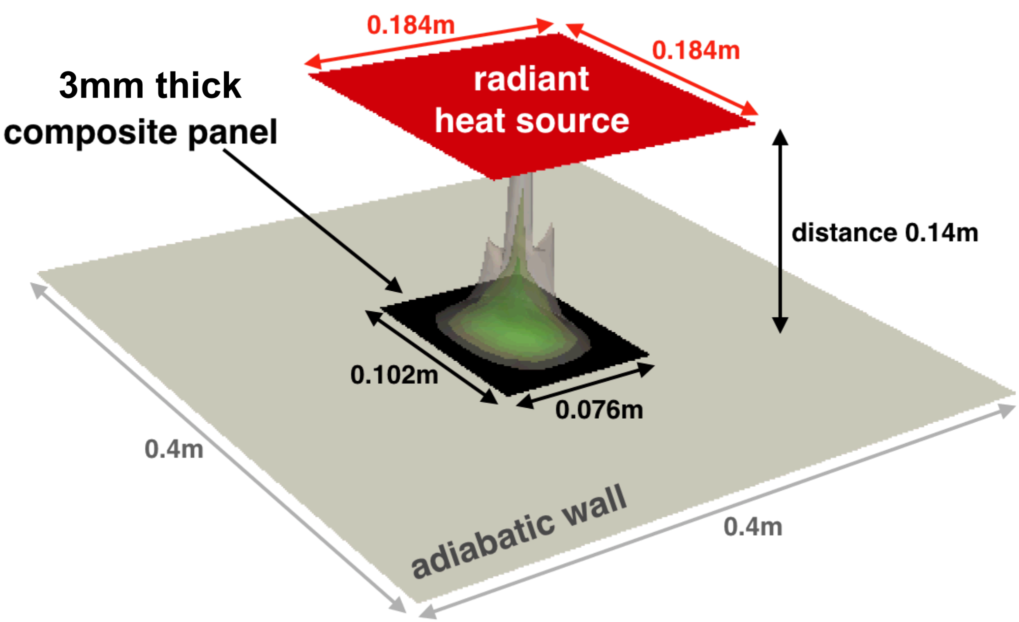
- An immovable Lagrangian particle represents TGA sample
- An ODE solver handles the 5-step mechanism
- Fuego result closely matches the TGA degradation rate

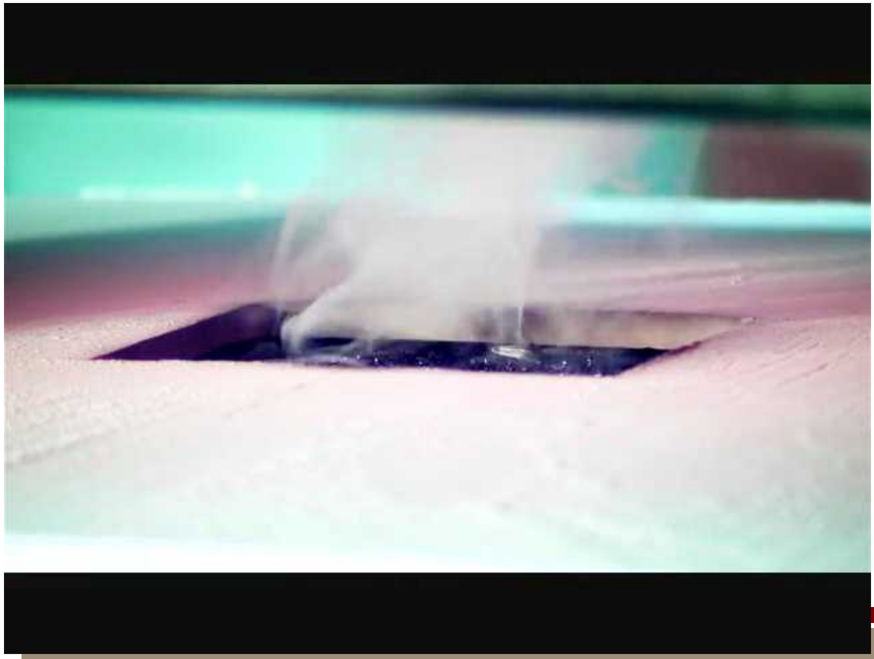


# Composite Panel Experiment

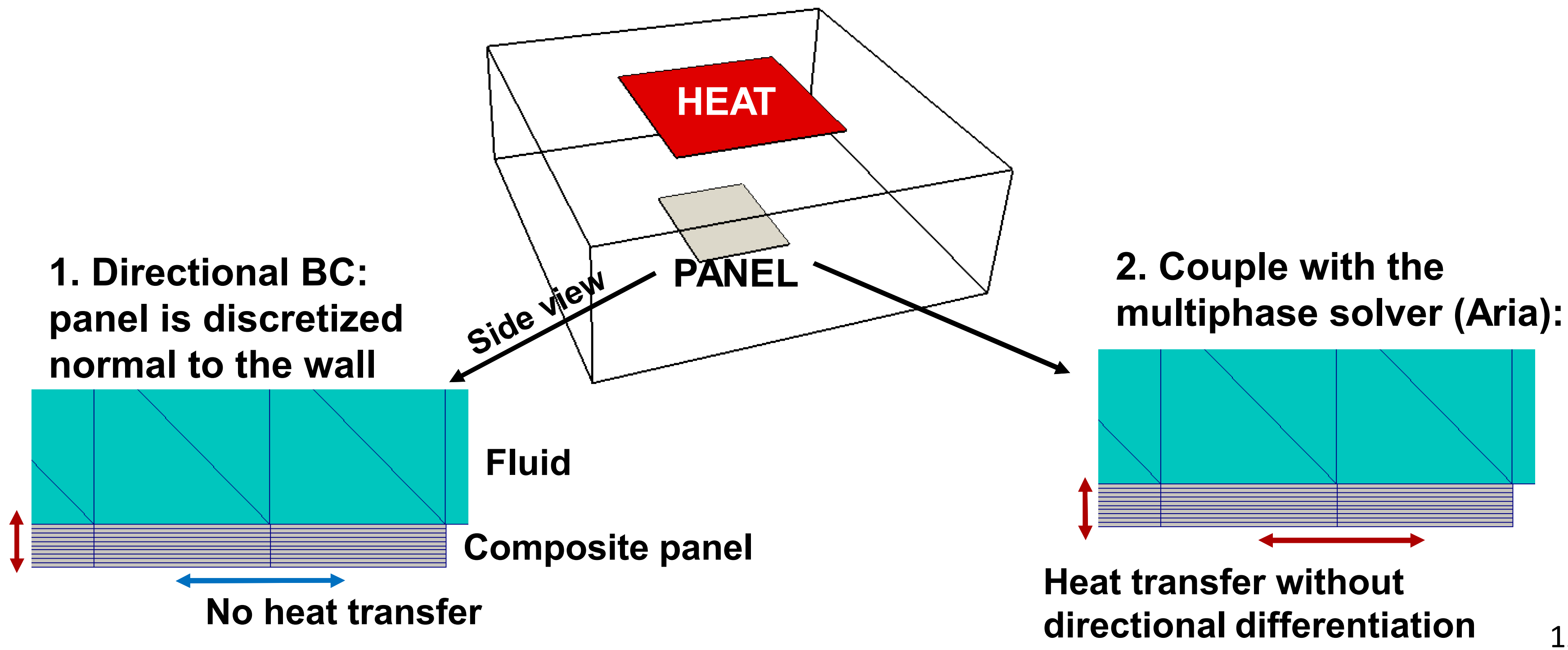
- Exposed composite panel degrades under a radiant heat (Hubbard et al., 2011)
  - Upper panel is heated up to 800°C
  - Duration of visible gasification (smoke) and backside panel temperature profiles are available



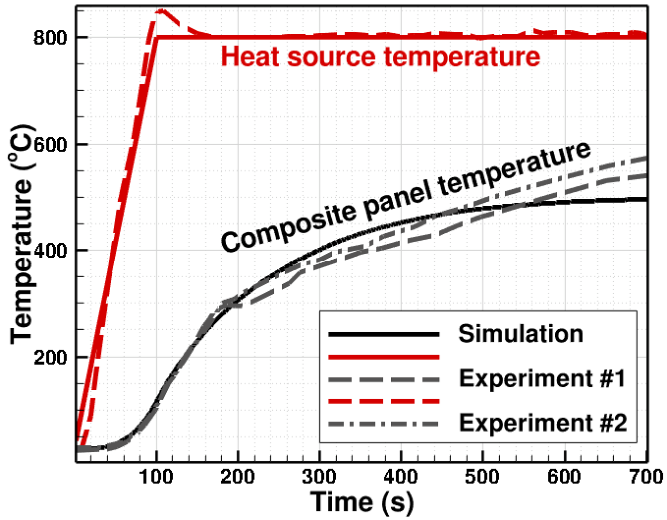



# Numerical Approaches

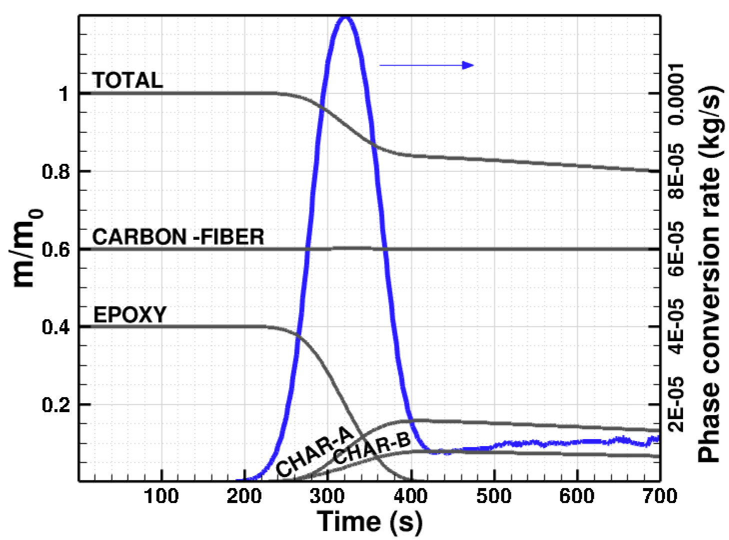
- LES with a transport equation of subgrid scale kinetic energy
  - $\mu_t = \rho C_\mu \Delta k^{sgs\frac{1}{2}}$ cf> $\mu_t = \rho \left(C_s \Delta\right)^2 |\tilde{S}|$
- Two approaches are tested
  - With or without lateral heat transfer, due to code availability
  - Mesh size ~ 5mm, total 0.1M grid; no gas-phase reaction



# 1. Directional Boundary Condition

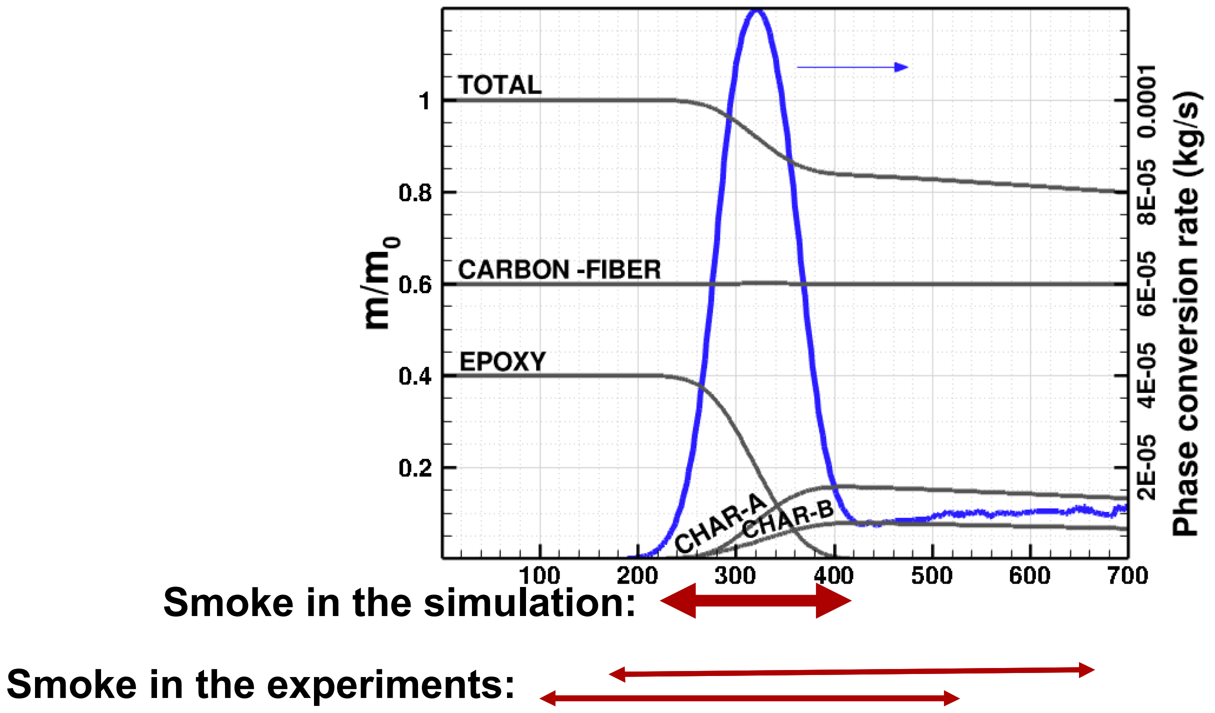






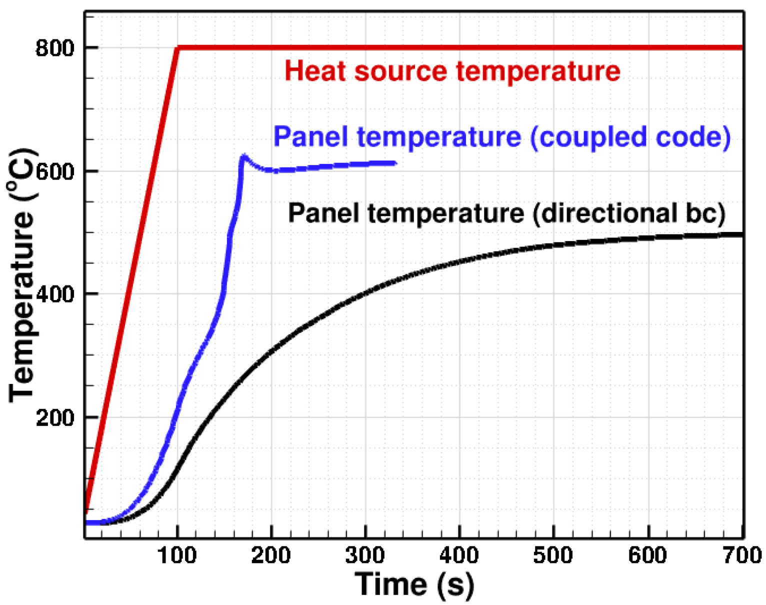

# 1. Directional Boundary Condition

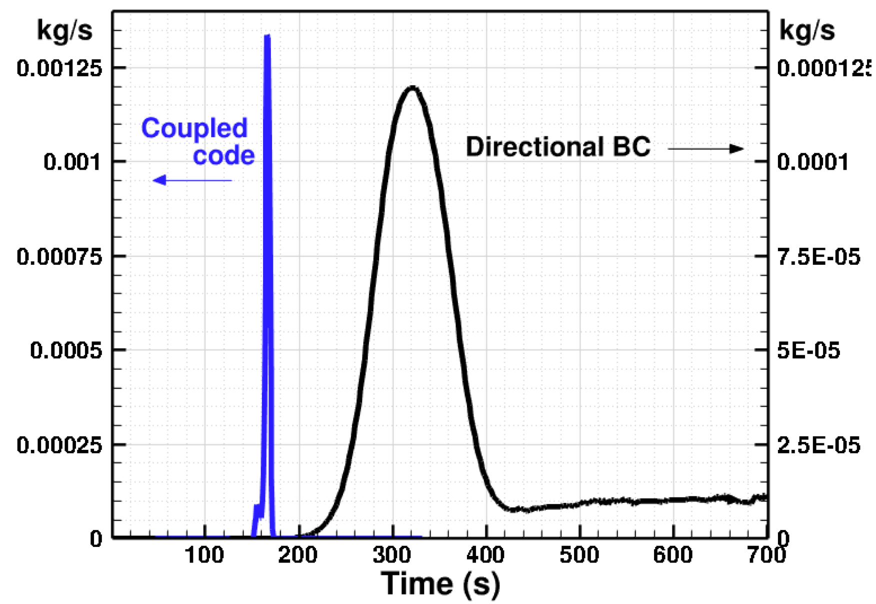
- Phase conversion is active between 240s and 400s
  - Minimal conversion continues after 400s
  - Experiment reported visible smoke durations as 165-660s and 100-520s



# 2. Couple with the Multiphase Solver

- Phase conversion begins earlier but does not sustain



# Conclusion

- Composite pyrolysis and oxidation procedures were correctly modeled using CFD solvers
  - Parameter definitions were revisited
  - TGA and the panel exposed to a radiant heat tests were simulated
- Solid response (TGA degradation) and heat transfers (panel backside T) were correctly predicted
  - Detailed composition of the gas phase release needs further work