SAND2012-3983C

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Several fire-related problems of interest to Sandia

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FM Global Open Source CFD Fire Modeling Workshop
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Outline

- Flame aerosol interactions and soot.
- Composite fires and solid combustion.
- Sodium smoldering.
- Cantera: an open source code.

Modeling Differential Diffusion in Nonpremixed Combustion: Soot transport in mixture fraction space

- Overall Goal: To develop predictive capability describing heat transfer due to fire.
  - Soot radiant heat transfer is dominant. Depends on the correlation of soot mass fraction and temperature.

$$E_s \propto Y_s T^5$$

- Understanding flame-soot interactions through one-dimensional turbulence (ODT) modeling of buoyant diffusion flame,
  - Identified new CMC formulation describing soot-mixture fraction differential diffusion.
  - Model suggested turbulent diffusive process for soot and other aerosols.

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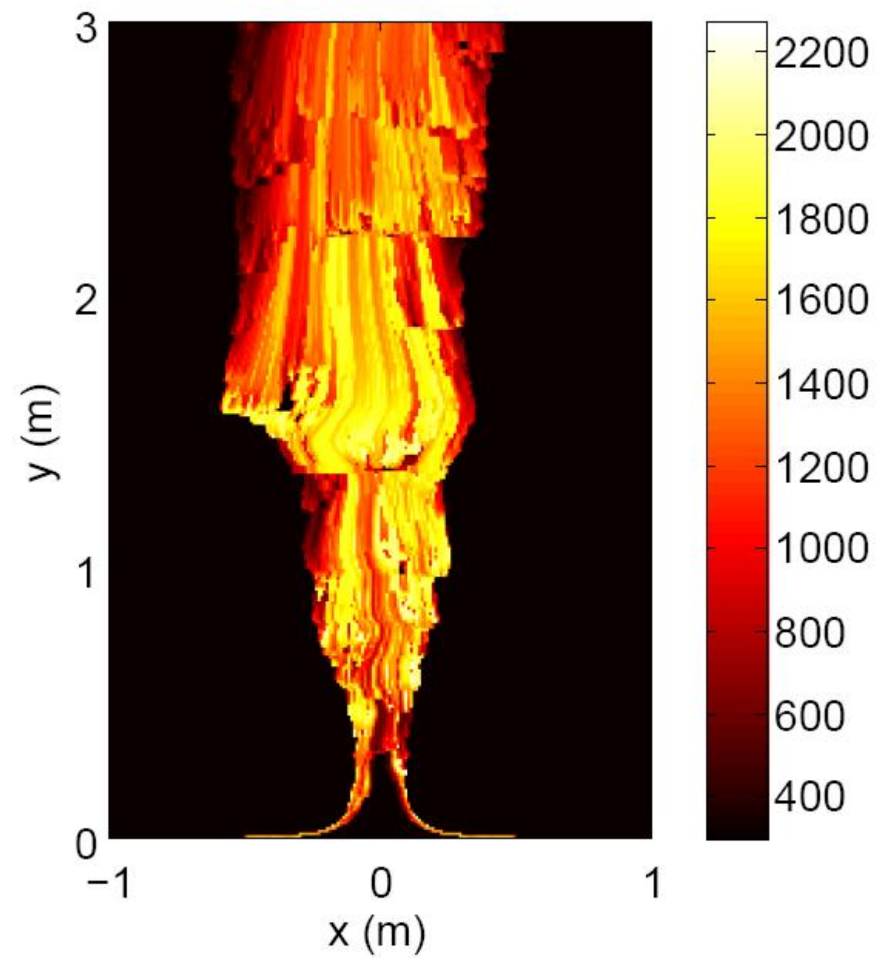
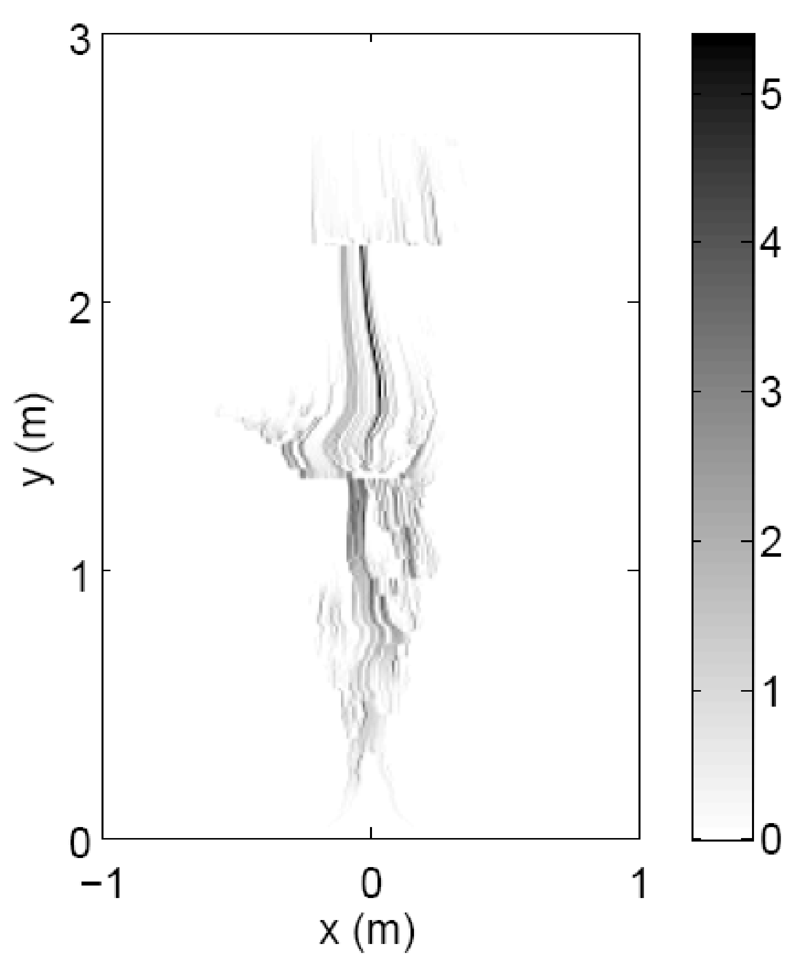
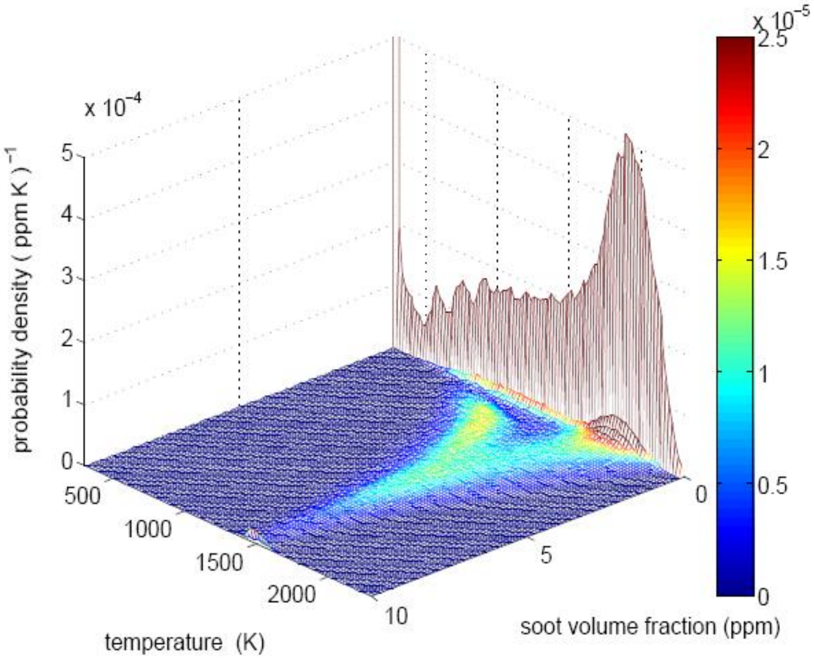
ODT simulations provide high-fidelity data to evaluate closures





ODT simulations provide high-fidelity data to evaluate closures

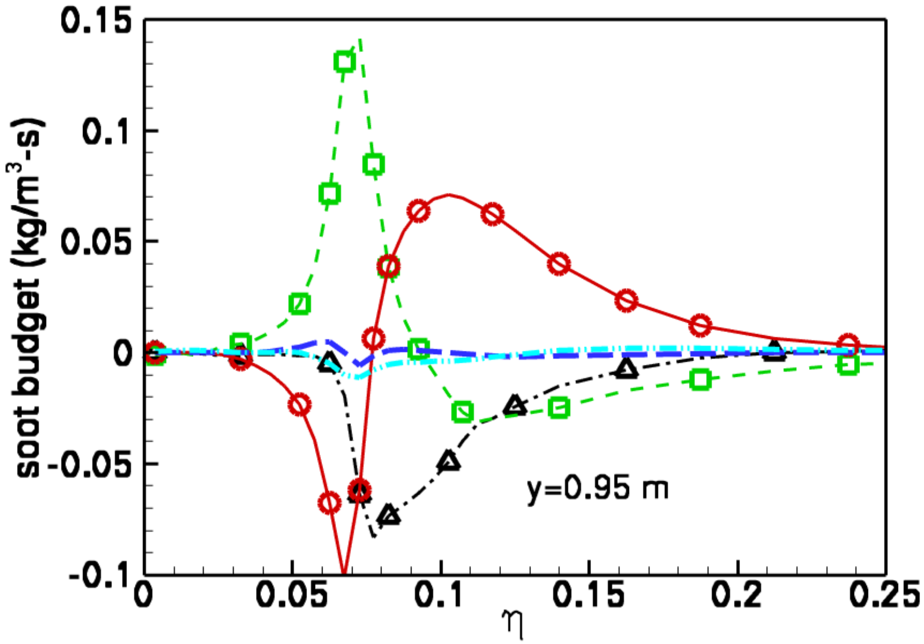
- Buoyant 1 m wide ethene plume (line fire) spatially evolving ODT simulation.
- Simple soot model (Fairweather *et al.* 1992) with steady laminar flamelet source terms tabulated by enthalpy and mixture fraction.
- Generate statistical quantities like soot-temperature joint PDF.



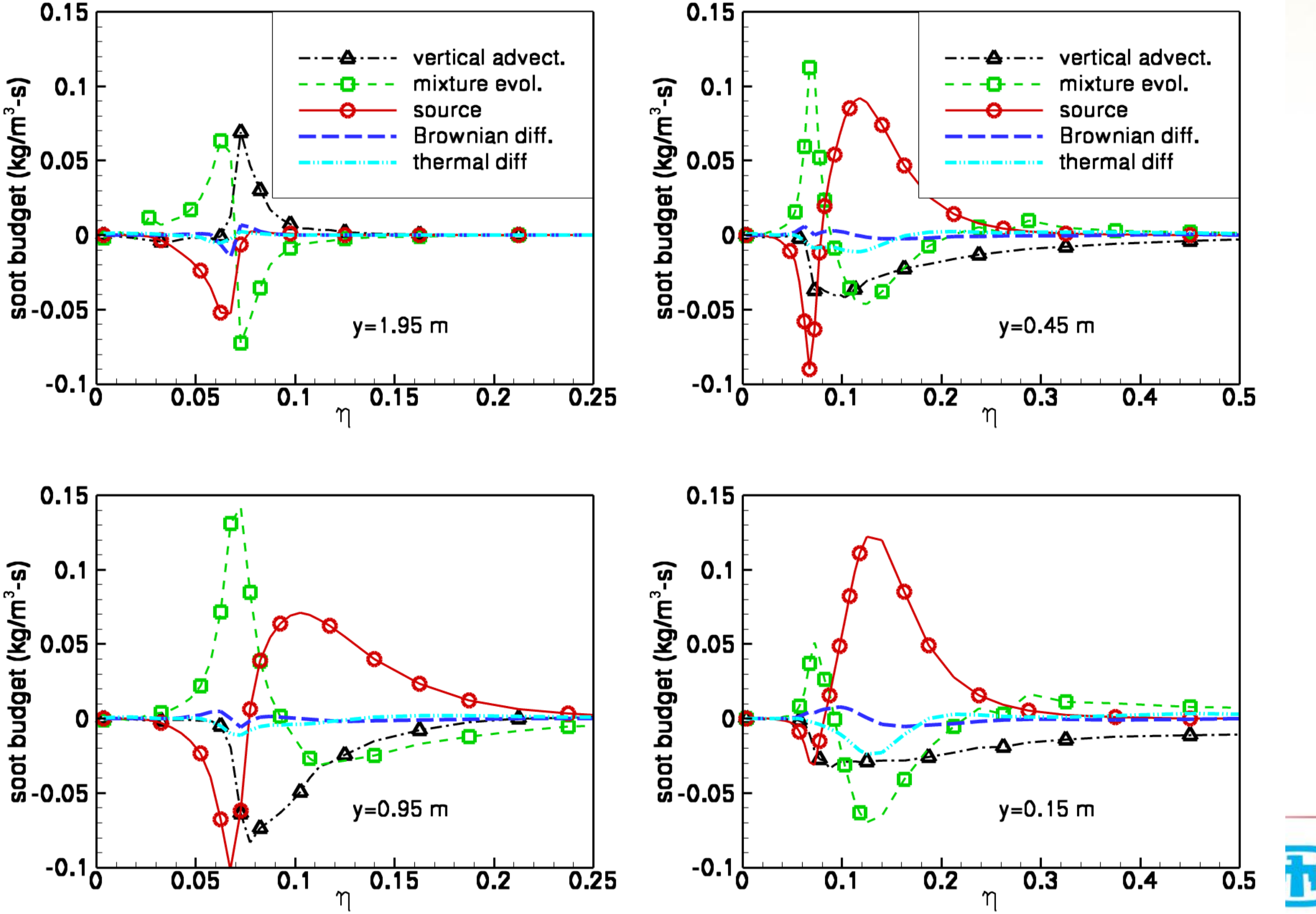
ODT results – conditional budgets for soot

$$
\begin{aligned}
\partial_y\left(\langle \rho v Y_s | \eta\rangle P(\eta)\right) = & -\partial_x\left(\langle \rho u Y_s | \eta\rangle P(\eta)\right) && \text{advection} \\
& + \langle S_{Y_s} | \eta\rangle P(\eta) && \text{chemical source} \\
& + \langle \partial_x(\mu\, \partial_x Y_s)/Sc_s | \eta\rangle P(\eta) && \text{Brownian diffusion} \\
& + \langle \partial_x(0.55\,\mu Y_s\, \partial_x \ln T) | \eta\rangle P(\eta) && \text{thermal diffusion} \\
& - \partial_\eta\left[\left\langle Y_s\left[\partial_x\left(\frac{\mu \partial_x f_g}{Sc}\right) - S_{Y_s} - \partial_x\left(\rho u'_{corr,g}\, f_g\right)\right] \middle| \eta\right\rangle P(\eta)\right] && \text{mixture evolution}
\end{aligned}
$$

Ricks, A. J., J. C. Hewson, et al. (2010). Combust. Sci. Technol. 182(1): 60-101.



ODT results – conditional budgets for soot



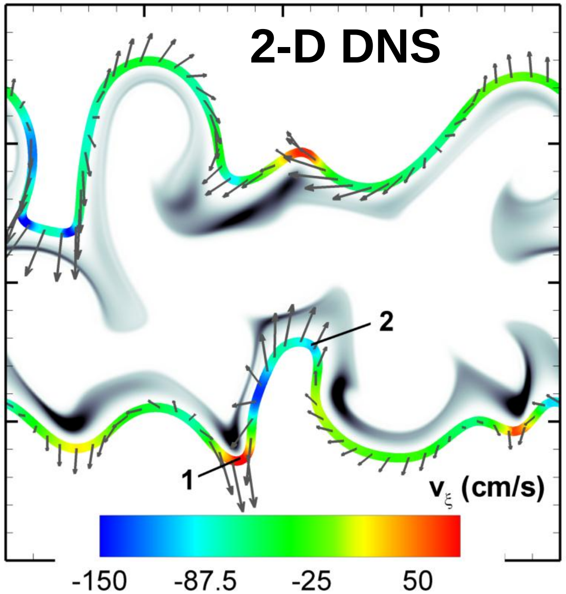
Aerosol mixing differs from that of gases

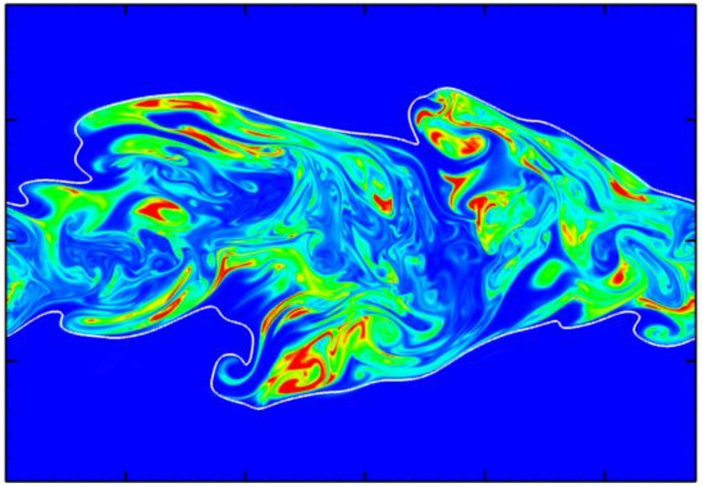
- Soot is example of species for which differential diffusion is significant.
  - Zero soot diffusivity.
  - Mixture fraction diffuses.

- Diff-diff dominated by high wave-numbers:
  - Random directions

- More complex structure in 3-D

Vectors show flux of soot through flame





3-D DNS, Lignell

A new CMC formulation to address differential diffusion in turbulence

- Using PDF approach to conditional-moment closure (CMC) derivation but use aerosol Lewis number (infinite) in derivation…
- Differential diffusion manifest in term

$$\frac{\partial}{\partial \eta}\left[\left\langle \nabla\cdot\left(\rho (D_\xi - D_k)\nabla \xi \right) Y_k \middle| \vec{\eta} \right\rangle P(\vec{\eta}) \right]$$

[Mix frac/time] **Density**

Scalar

  - Looks like total scalar-flux term, but in the mixture fraction coordinate.
  - Closure: separate using $\langle VY|\eta\rangle \approx \langle V|\eta\rangle\langle Y|\eta\rangle + \langle v''y''|\eta\rangle$

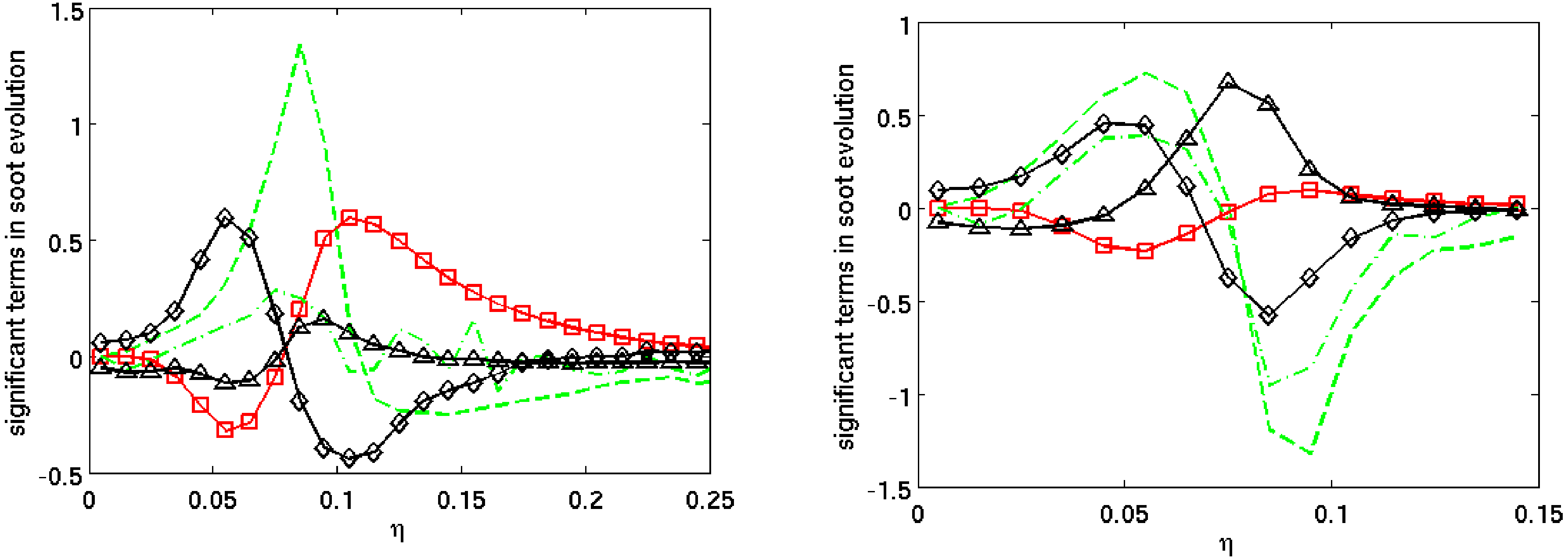
- Diff-diff flux by means related to mean PDF evolution

$$\frac{\partial}{\partial \eta}\left[\langle V|\eta\rangle\langle Y|\eta\rangle P(\vec{\eta}) \right] = \frac{\partial}{\partial \eta}\left[\left\langle \nabla\cdot\left(\rho (D_\xi - D_k)\nabla \xi \right) \middle| \vec{\eta} \right\rangle P(\vec{\eta}) Q_k \right]$$

Looks like PDF evolution

ODT results

•Terms plotted below for heights in ODT simulations where mixture fraction pdf is centered on production (left) and on oxidation (right).



Advection (dash), pdf flux (dash-dot) -- long-term evolution of soot.
Soot source (squares).
Diff-diff by evolution of pdf (triangles) -- long-time advection in mixture fraction.
Diff-diff fluctuations R_{DD} (diamonds) -- short-time diffusion in mixture fraction.

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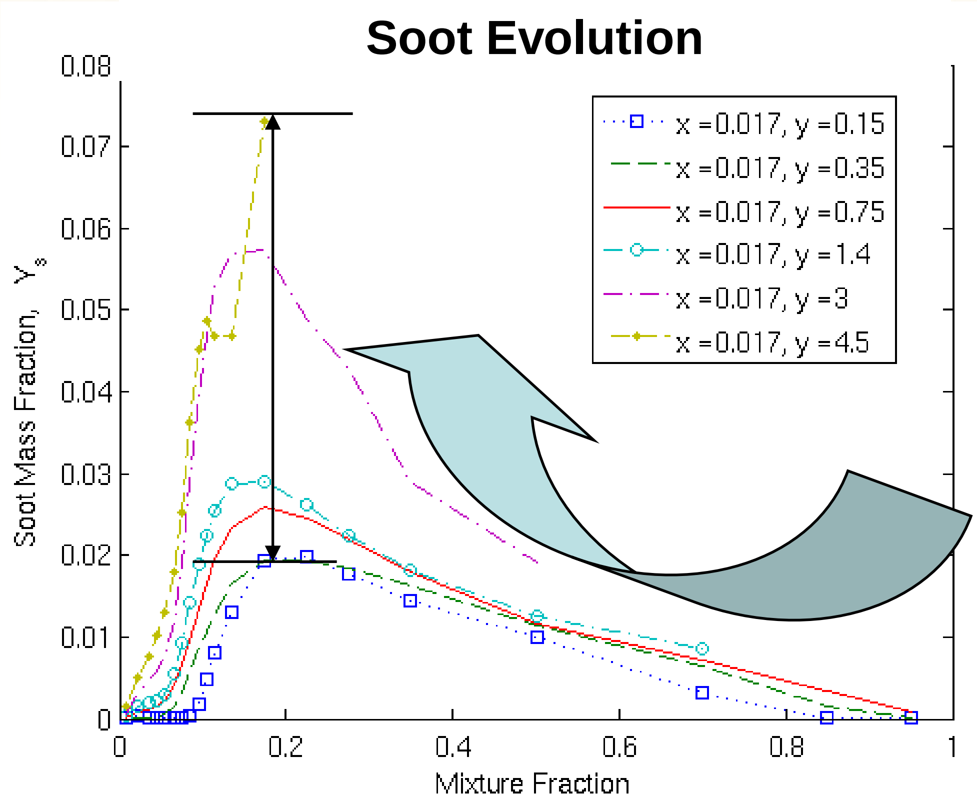
Soot Transport by Mean PDF



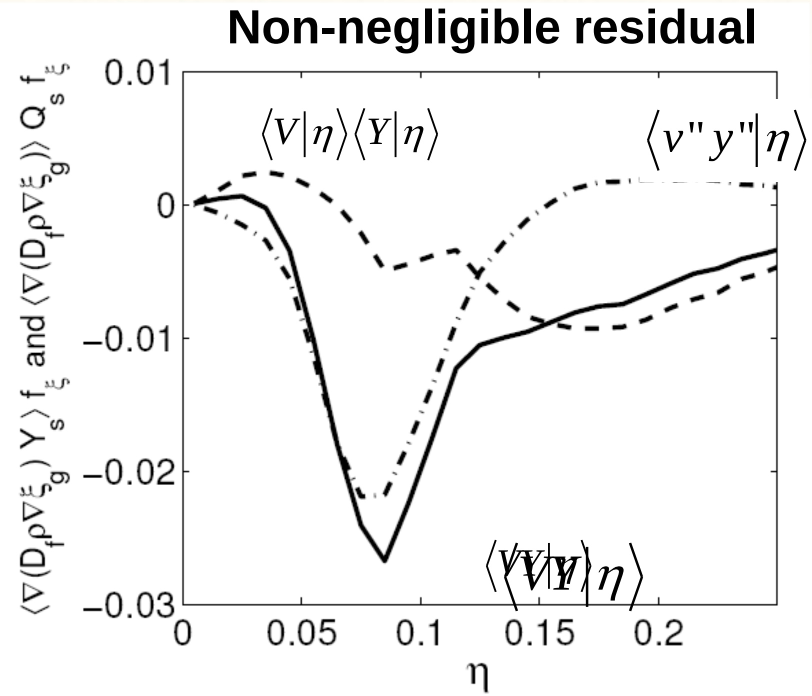
- Global fire scale PDF(ξ) evolution sweeps soot toward and then from the fuel-rich side as the PDF evolves from rich to lean.

Closure for new CMC formulation to address differential diffusion in turbulence

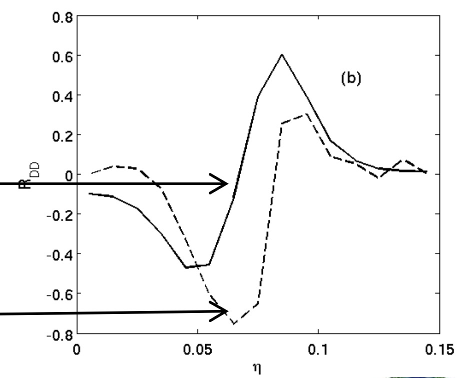
- Prior slides demonstrated primary closure of diff-diff term, but residual (fluctuations) are also important.

$$\langle v''y''|\eta\rangle \approx \langle V|\eta\rangle\langle Y|\eta\rangle - \langle VY|\eta\rangle$$

- Diff-diff dominated by high wave-number structures:
  - Random directions
  - Like turbulent scalar flux in mixture-fraction coordinate.
  - Model as diffusion process



$$R_{DD} = \frac{\partial}{\partial\eta}\langle v''y''|\eta\rangle \approx \frac{\rho_\eta\chi_\eta f_\xi}{2Le_{DD,t}}\frac{\partial^2 Q_s}{\partial\eta^2}$$



J. C. Hewson, et al., "*On the Transport of Soot Relative to a Flame: Modeling Differential Diffusion for Soot Evolution in Fire*," in *Combustion Generated Fine Carbonaceous Particles*, H. Bockhorn, *et al.*, Editors. Karlsruhe University Press: Karlsruhe, Germany. p. 571-587, 2009

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Summary: A new CMC evolution equation for soot and other species with strong diff-diff

$$\frac{\partial Q_s}{\partial t} + \langle \vec{\mathbf{u}} | \eta \rangle \bullet \nabla Q_s = \langle \omega_s | \eta \rangle$$ Species Source Term

$$+ \frac{\langle \chi | \eta \rangle}{2\mathrm{Le_s}} \frac{\partial^2 Q_s}{\partial \eta^2}$$ Species Diffusion

$$+ \frac{1}{2\rho_\eta f_\xi(\eta)} \frac{\partial}{\partial \eta}\left[\rho_\eta \left(\frac{1}{\mathrm{Le_s}} - 1\right)\langle \chi | \eta \rangle f_\xi(\eta)\right]\frac{\partial Q_s}{\partial \eta}$$ Transport by PDF evolution

Current Focus

$$+ \left(1 - \frac{1}{\mathrm{Le_s}}\right)\frac{\langle \chi | \eta \rangle}{2\mathrm{Le_{DD}}} \frac{\partial^2 Q_s}{\partial \eta^2}$$ Turbulent differential diffusion

+other terms

- Derived from combined PDF and soot conservation equations without the primary closure hypotheses.
- Turbulent diffusion term is new model from Hewson et al.
- Some definitions for above:

$$Q_s \equiv \langle Y_s | \eta \rangle \quad \langle \chi | \eta \rangle \equiv \left\langle 2D(\nabla \xi)^2 | \eta \right\rangle \qquad f_\xi(\eta) \text{ is PDF}(\xi)$$

J. C. Hewson, et al., "*On the Transport of Soot Relative to a Flame: Modeling Differential Diffusion for Soot Evolution in Fire*," in *Combustion Generated Fine Carbonaceous Particles*, H. Bockhorn, *et al.*, Editors. Karlsruhe University Press: Karlsruhe, Germany. p. 571-587, 2009

Composite material fire: Background

- Increased numbers of aircraft with composite materials
- Boeing 777 (20% composite)
  - Used on wings, trailing edge panel, flaps, spoilers, floor beams, landing gear doors, etc.
- Boeing 787 (50% composite)
  - Used on fuselage, wings, tail, doors and interior
- F22 (24% composite)
  - Used on fuselage, doors, wings, skins
- F35 (40% composite)
- Composite materials behave differently from conventional fuel sources and have the potential to smolder and burn for extended time periods

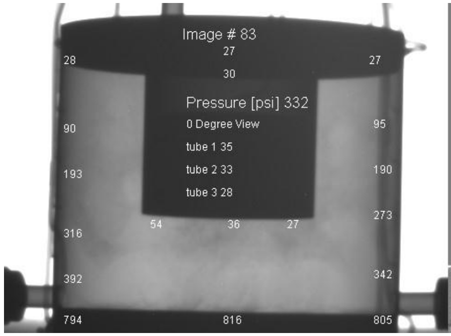
Fighter Aircraft	U.S. Europe Russia	AV-8B, F16, F14, F18, YF23, F22, JSF, UCAV Harrier GR7, Gripen JAS39, Mirage 2000, Rafael, Eurofighter, Lavi, EADS Mako MIG29, Su Series
Bomber	U.S.	B2
Transport	U.S. Europe	KC135, C17, 777, 767, MD11 A320, A340, A380, Tu204. ATR42, Falcon 900, A300-600
General Aviation		Piaggio, Starship, Premier 1
Rotary Aircraft		V22, Eurocopter, Comanche, RAH66, BA609, EH101, Super Lynx 300, S92

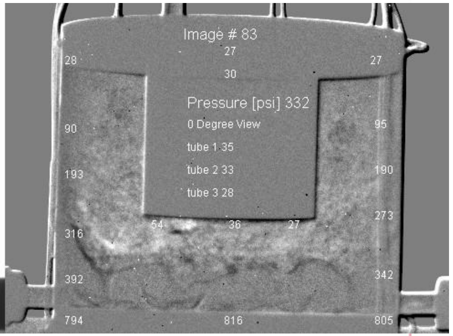
Quilter, A. "Composites in Aerospace Applications," An IHS White Paper, http://uk.ihs.com/NR/rdonlyres/AEF9A38E-56C3-4264-980C-D8D6980A4C84/0/444.pdf

*Percentages are by weight

Composite and Organic Material Fires Overview

- Problems of Interest
  - Composite material fires
    - Experimental response
    - Phenomenology
    - Preliminary modeling approach
  - Organic material decomposition
    - Experimental response
    - Phenomenology
    - Current/past modeling approach
- Path forward
  - Modeling Approaches
    - Porous media
    - Fluid region
  - Long term plans
    - Computationally
    - Experimentally





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Carbon-fiber epoxy composites: fire experiments

	Characteristic Length Scales	*Characteristic Mass*	*Experiments*	*Purpose of Testing*
Very small	0.1 mm to 1 mm	Milligrams (initial mass)	TGA, DSC	Fundamental kinetic, chemistry, decomposition behavior, and property measurements
Small	mm to 10 cm	Hundreds of grams	Cone calorimetry, radiant heat	Burn rate and scaled dynamics determination, simple validation testing
Intermediate	10-100 cm	0.1-100 kg	Radiant heat and environmental chamber tests	Bridge the gap between small and very small scale and large scale testing to discover dynamics not exposed at the smaller scales that will be present at larger scales
Large	Meters and above	Hundreds of kg and above	Full-scale fire testing	Full-scale with all physics represented in appropriate scale range

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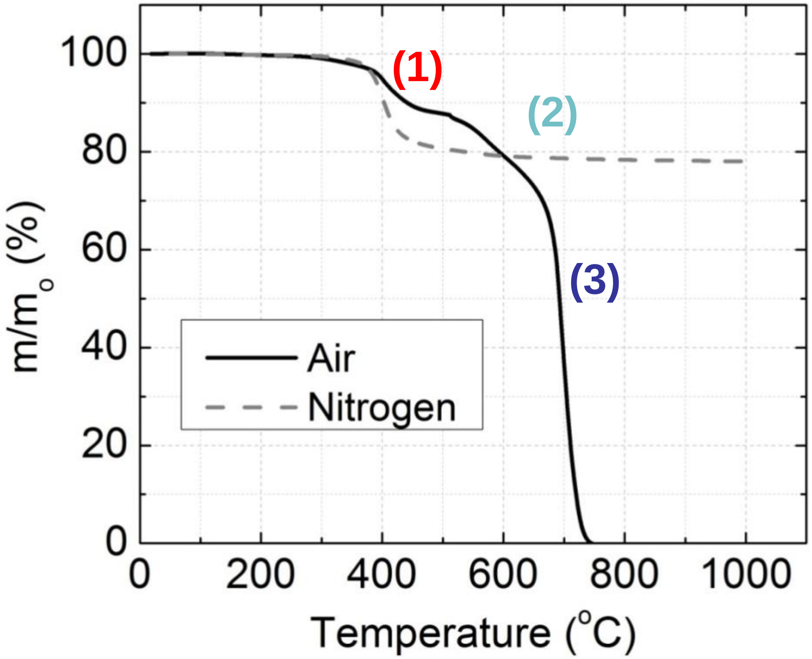
TGA Results, 3 Regimes



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

TGA Details:

- 1-2 mg samples
- 20ºC/min
- Cytec 977-3 resin
- IM7 Fibers
- Single sheet cured in 1 atm oven

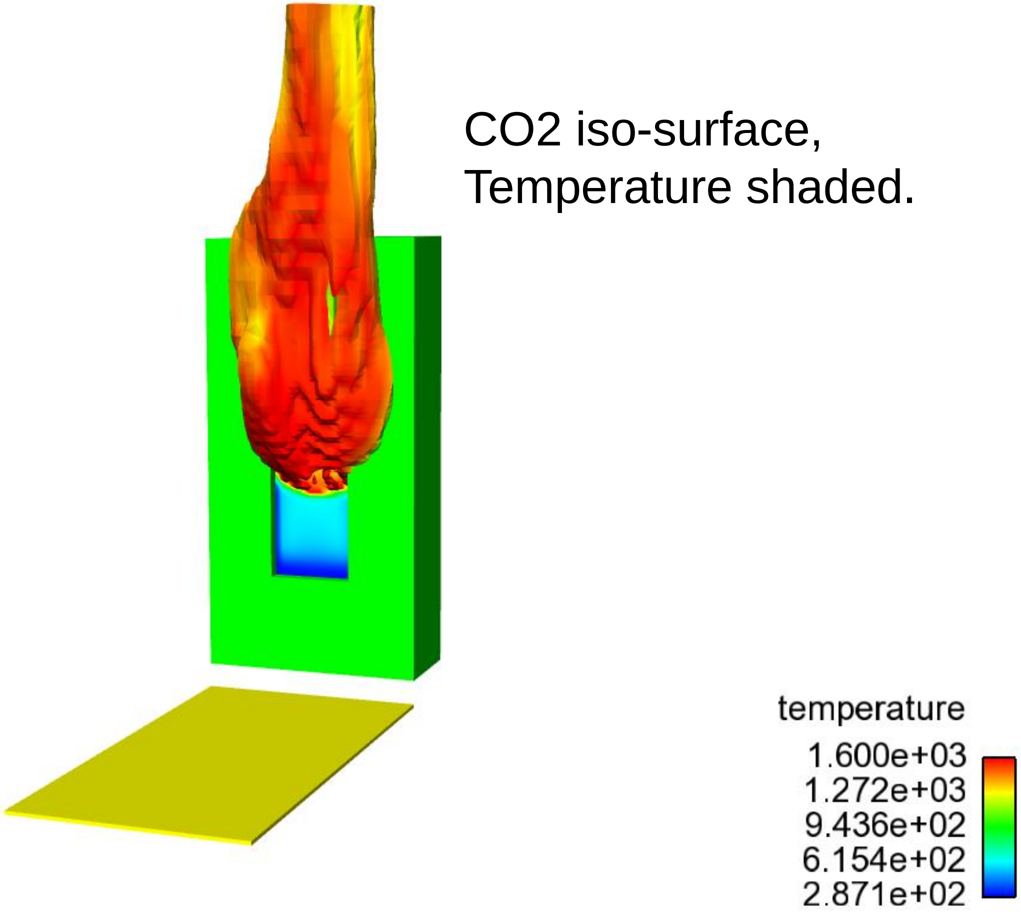
- In N_2, pyrolysis reaction generate organic vapors/fuel and char
- In air, O_2 interacts with the epoxy and changes rate at which organic vapors are generated
- Char formation inhibits combustion of carbon fibers
- Char oxidation occurs BEFORE carbon fiber oxidation

Composite modeling capability status

- Modeling: Multi-path approach
  - Fuego (Simplified One-Dimensional Energy Equation Model)
  - Aria (reacting porous medium coupled to Fuego or reacting medium)
- Physics include:
  - Condensed-phase conduction and
  - Epoxy decomposition.
    - Reaction mechanism developed over range of oxygen concentrations at temperature schedules (5 C/min to 500 C/min).
    - Based on TGA/DSC/FTIR/Cone
  - Gas-phase oxidation of epoxy products.
  - Interphase coupling through conduction, convection, radiation.
  - Coming from sodium-smoldering work:
    - Oxidizer transport through porous layers.
    - Structural deformation through Aria – Adagio coupling.

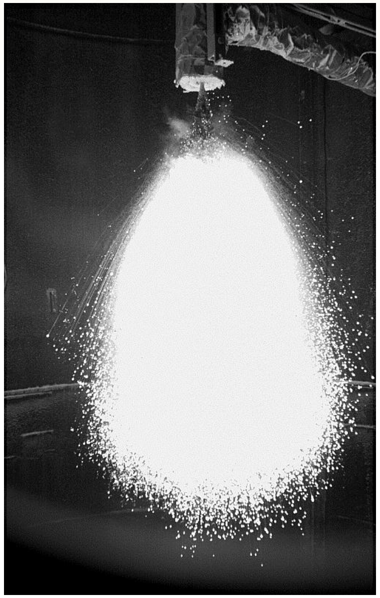
Computational modeling: Composite ignition by radiant panel

CO2 iso-surface,
Temperature shaded.



Sodium fires and reactor safety

- Nuclear energy: renewed interest
  - New reactor designs include fast reactors.
- Fast reactors:
  - Liquid sodium for neutronics and cooling
- Safety implications for these facilities
  - Sodium is highly reactive, and ignites at relevant temperatures.
  - Critical components vulnerable to thermal damage
  - Nuclear materials can be dispersed in sodium fires.
- Hazard mitigation required during regular operation, transportation, maintenance



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Sodium Pool Fire Test

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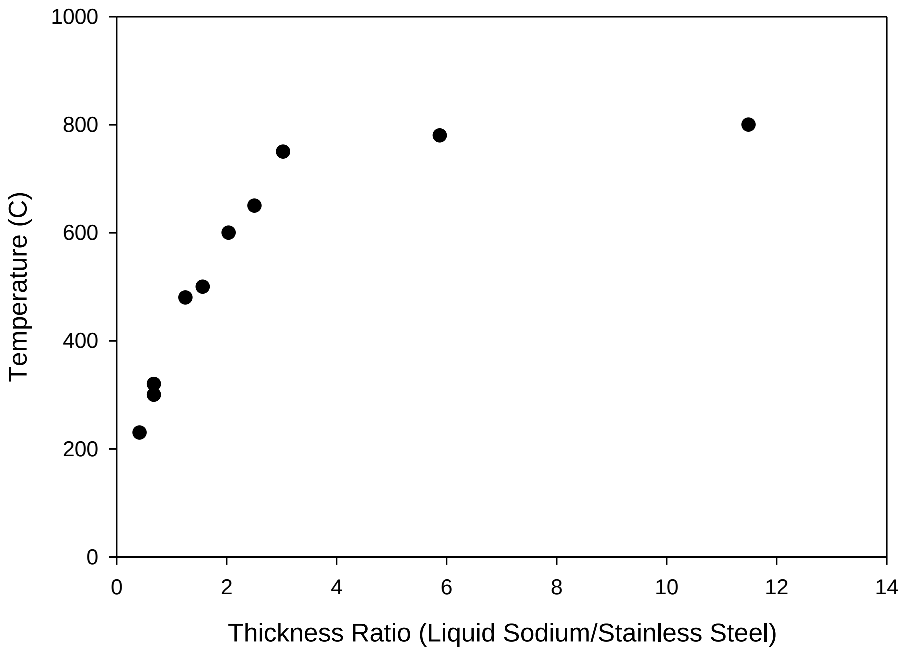
Sodium pool fire temperatures

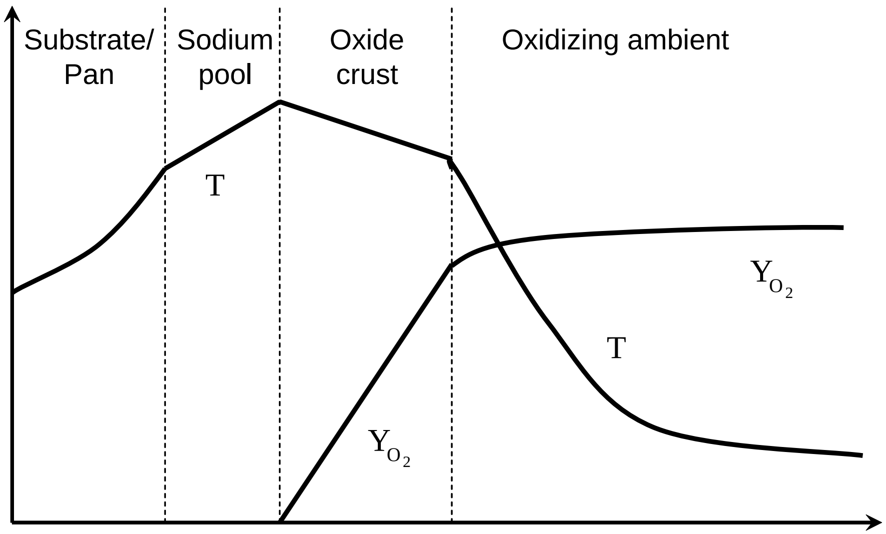
- Sodium pool fires well-studied in quasi-steady ‘deep pool’ configuration.
- But sodium-cooled reactor systems designed to drain leaked sodium into inert vessels: Only thin layers will remain.

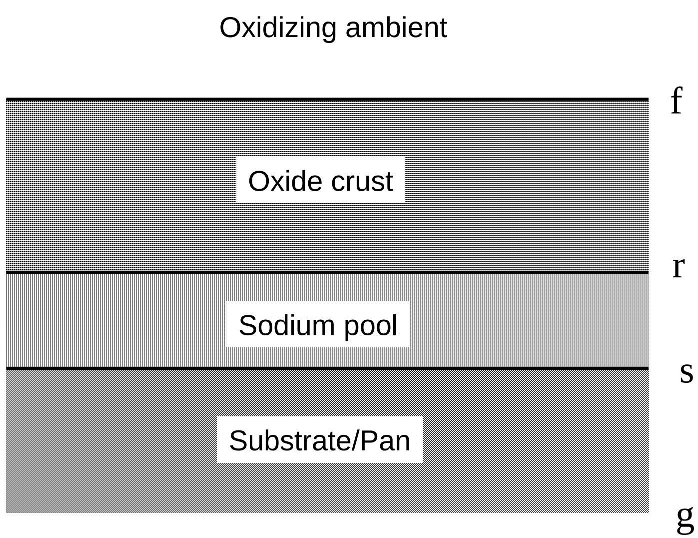
All Sodium Pool Tests: Measured Peak of Average Bottom Pan Temperature vs Thickness Ratio (Liquid Sodium/Stainless Steel)



- Experiments show shallow pools exhibit different thermal evolution.
- Dominated by oxide crust.

Model Configuration





- Thermal evolution driven by heat release versus heat loss
  - Heat release determined by oxygen transport to sodium.
    - Driving potential is oxygen mass fraction.
    - Resistance is across boundary layer and across oxide layer.
  - Heat transfer into “pool + pan + ground” versus transfer away from surface.
    - Driving potential is temperature difference.
- Presence of oxide crust introduces resistance that more strongly resists oxygen transport than heat transport.

Conceptual/Simplified Model for Smoldering Sodium Pool Fires

- Consider potential-resistance-flux analogy:
  - Potential is oxygen concentration or temperature difference.
  - Resistance is inverse of diffusivities.
  - Flux is burning rate, heat release rate, and heat transfer rates.

- Additional resistance associated with oxide crust alters dynamics
  - Thermal diffusivity of crust is greater than mass diffusivity.
  - Oxide crust tends to reduce heat release rates leading to cooler systems.

Fluxes **Driving potentials**

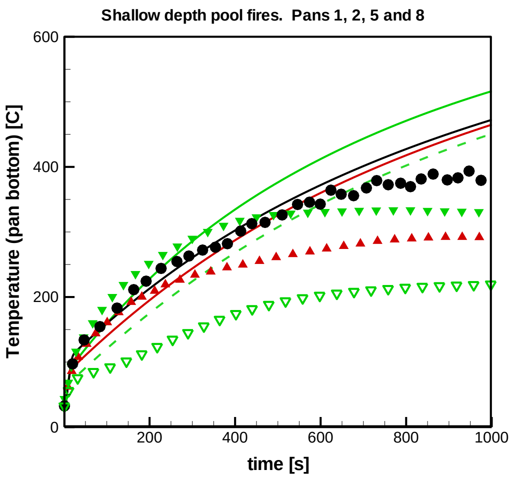
$$\dot{m} = A' \frac{Y_{O_2}}{\frac{L}{Sh\,D} + \frac{\delta}{D_{eff}}}$$

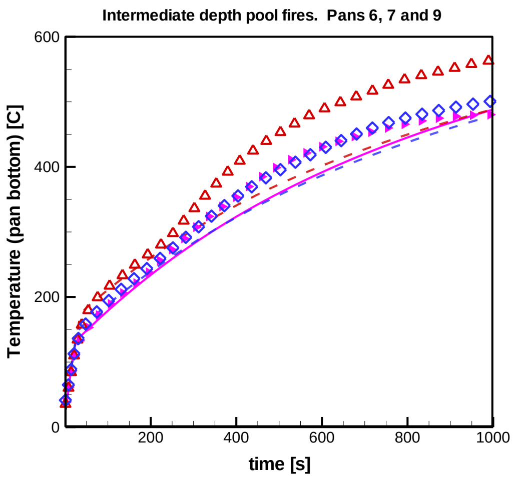
$$\dot{Q}_{pool+pan+ins} = A \frac{q\,Y_{O_2}}{\frac{L}{Sh\,D} + \frac{\delta}{D_{eff}}} + B \frac{(T_r - T_\infty)}{\frac{L}{Sh\,\lambda} + \frac{\delta}{\lambda_{eff}}}$$

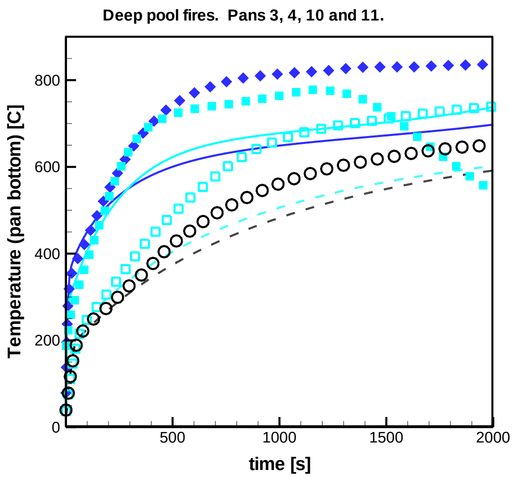
Boundary layer resistances **Oxide crust resistances**

Temperature Evolution Predictions

- **New model can predict shallow pool burning**
  - **Oxide crust inhibits oxidation heat release.**
  - **Transition to deep pool burning still needs work, but we can go back to deep pool model that ignores oxide crust.**
  - **Very recent comparison with experiments suggests more oxide sinking in early phase will aid that transition and also improve shallow pool predictions.**

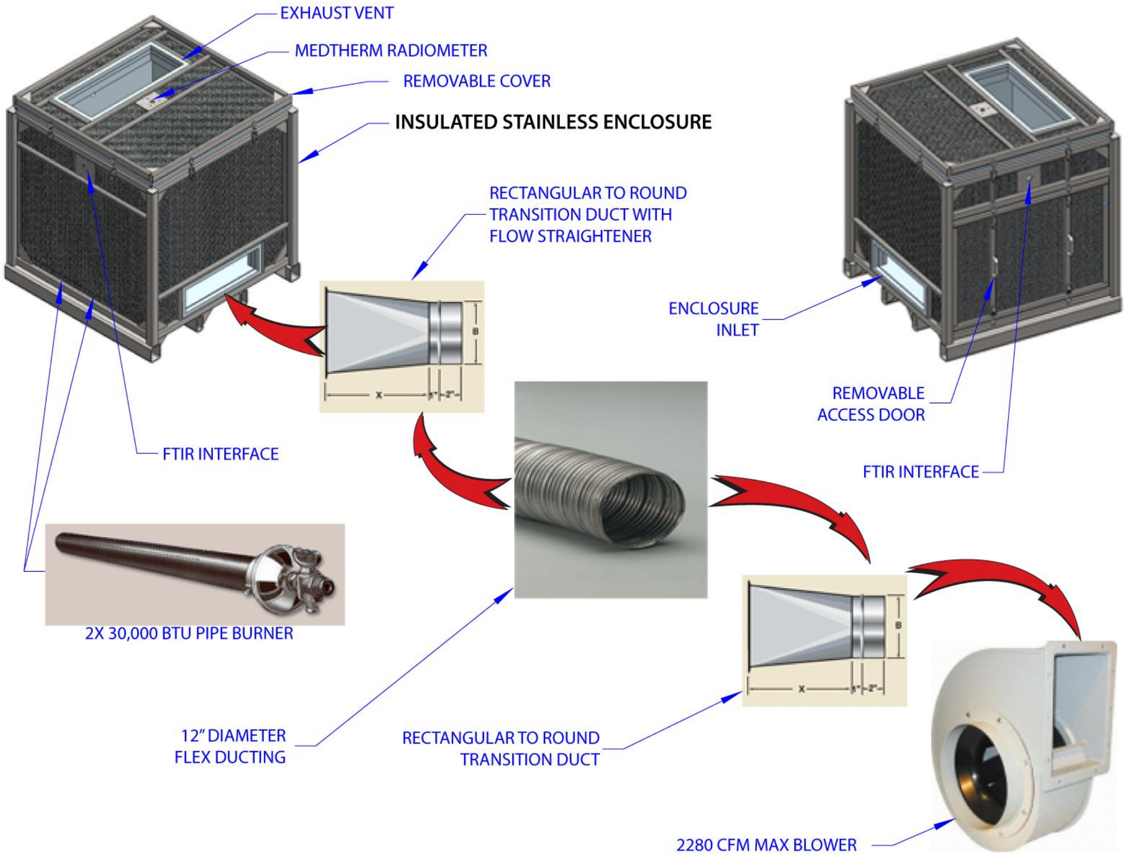






Composite fire test enclosure

- 91.0 cm aspirated internal cube designed to create an idealized semi-adiabatic environment

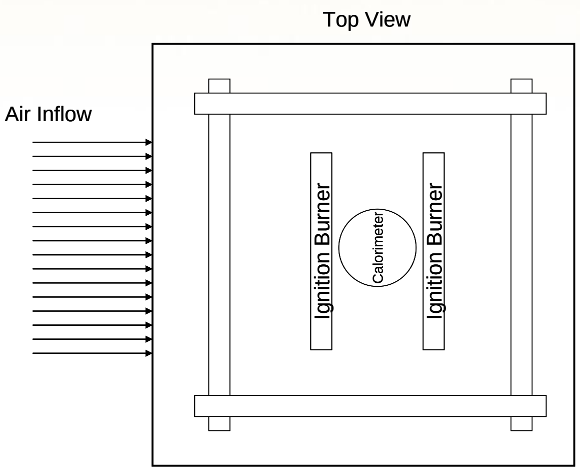


Instrumentation

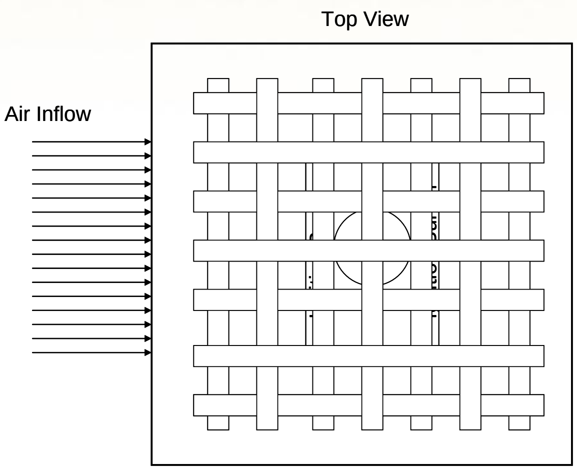
- **FTIR**
- **RGA/Mass Spec.**
- **Radiometers**
- **Calorimeter**
- **Thermocouples**
- **Pitot Velocity Probe**
- **Video**

Composite fire test

Lower Layer



Upper Layer



→ **Air inflow was significantly varied for this test**

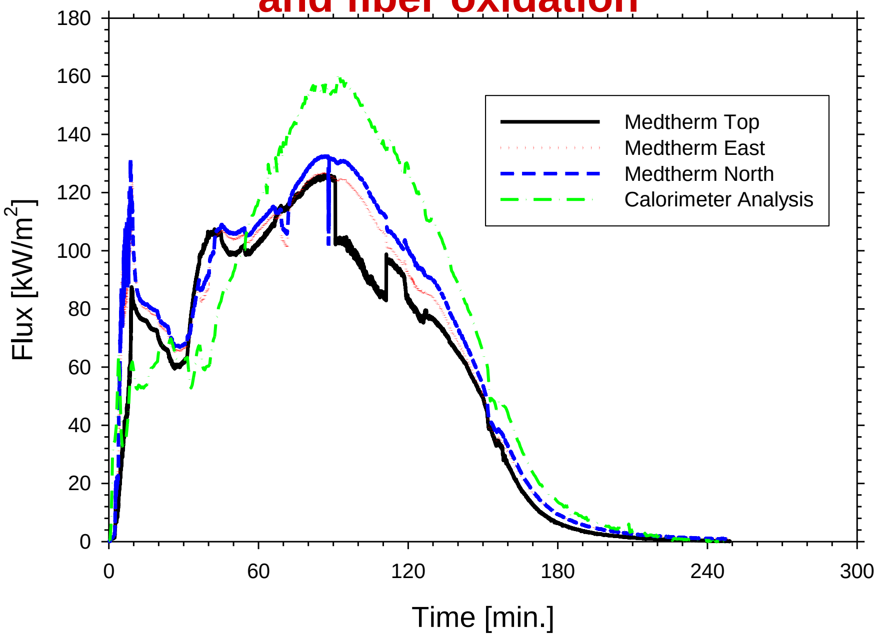
Composite I-beams fire video frames

Frames show the progression of the reactions through the glowing combustion phase

Composite I-beams fire:
Heat Flux and Calorimeter Results

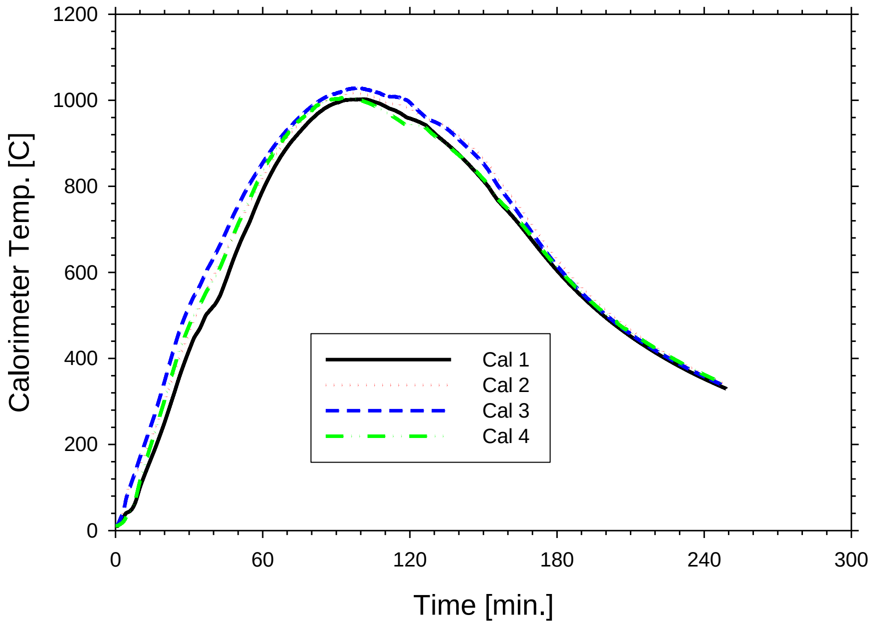
Measured heat fluxes

Heat flux maxima associated with epoxy devolatilization and fiber oxidation



Large calorimeter temperatures

bottom center of enclosure

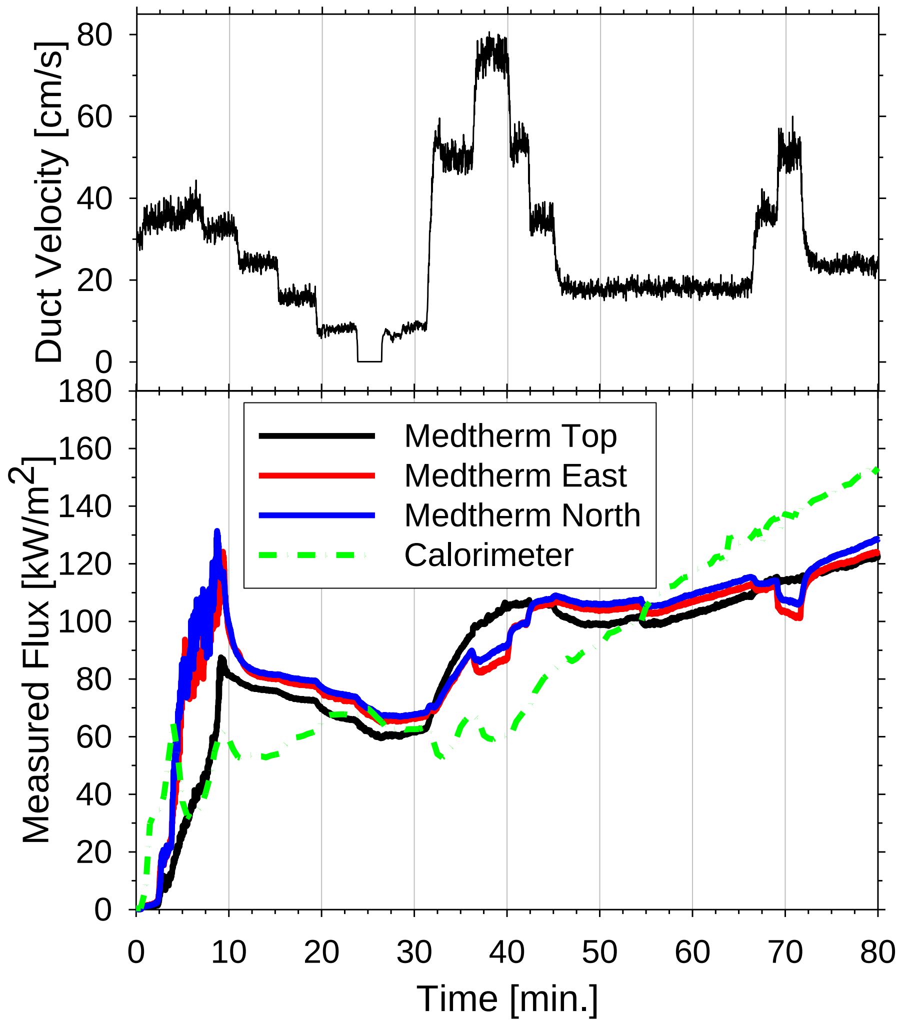


Calorimeter shows lower flux during flaming, higher during glowing combustion times

Fluxes as high as 160 kW/m^2 are found during glowing combustion in the bed

Composite I-beams fire: Sensitivity to air flow

Air supply varied with time during char oxidation



Minor effect of velocity on measured flux. Reversing trends suggestive of a transitional region between diffusion and kinetic reaction control.

Composite fire summary

- Multi-scale experiments: small scale to develop subgrid models and then to validate at mid-scales and larger.
- Epoxy devolatilization: flaming and sooting combustion for 10-30 minutes followed by 4-8 hours of glowing surface oxidation reactions.
- Evidence of both diffusion and kinetic reaction control with low air in-flow.
- Thermally driven surface combustion models, but more to be done.

Cantera

Chemical Kinetics • Thermodynamics • Transport Processes

- Cantera – open source software.
  - Thermodynamics, transport, kinetics.
  - Zero-dim and one-dim geometries as examples. Users have linked to CFD.
  - C++, Matlab and python interfaces.
- Version 1.8 is stable: http://code.google.com/p/cantera/
  - Version 1.8 has most everything needed for gas-phase combustion and possibly surface combustion, too.
- Version 2.0 is in beta: http://cantera.github.com/docs/sphinx/html/index.html.
  - Version 2.0 adds a great deal of non-ideal solution chemistry and probably much more…

Backup material

Composite fire problem of interest

- What is the heat flux and duration in such fires?
- Materials contributing to fire load
  - Composite
  - Honeycomb
  - Fuel on board aircraft
  - Other materials
- Phenomena
  - Gas phase combustion
  - Condensed phase combustion: pyrolysis, oxidation
  - Swelling
  - Complex flow paths
  - Complex heat transfer paths
- Future questions: how do you extinguish a composite material fire?

Composite Fires: Experimental and Modeling Efforts

- Objective: To develop an understanding of composite material fires and a modeling capability to assess a wide range of scenarios
- Approach:
  - Small scale experimental data (TGA/DSC/FTIR/Cone) to develop decomposition models
  - Perform medium-scale experiments to evaluate models
  - Perform large-scale experiments and modeling to determine scalability of model
  - Modeling: Multi-path approach
    - Fuego (Simplified One-Dimensional Energy Equation Model)
    - Aria (reacting porous medium coupled to Fuego or reacting medium)

Porous Media Capability Status

- Porous media capability has been implemented
  - Solve conservation equations for:
    - Mass (gas phase, condensed phase)
    - Species (gas phase, condensed phase)
    - Energy (gas phase, condensed phase)
  - Physics include:
    - Condensed phase and gas phase conduction
    - Gas phase convection
    - Species diffusion
    - Darcy flow
    - Generalized reaction capability
- Interface with Fluid region is currently ongoing

Testing Summary

Table 6. A summary of various results from six tests.

	Test	Initial Mass	Residual Mass	Peak Flux	Flaming Duration	Total Duration	SA/V	Mean Consumption Rate
	#	*kg*	*%*	*kW/m²*	*min*	*min*	*cm⁻¹*	*g/s*
Wood	1	40.8	-	220	-	90	2.4	7.56
	2	31.8	-	220	-	60	1.3	8.82
Composites	4	36.5	9.56	180	25	330	-	1.84
	5	38.5	2.59	175	30	420	2.0	1.53
	6	39.3	6.74	220	20	300	9.2	2.18
	7	26.5	10.34	160	10	240	6.9	1.84

Compared to wood, peak fluxes tend lower, consumption rates are much lower, thermal release duration is much longer.

Surface Area to Volume appears to relate to consumption rate.

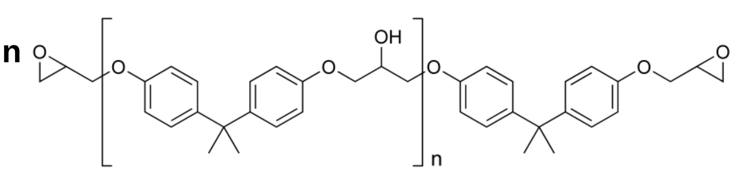
Very low residual mass.

About Carbon Fiber Epoxy Aircraft Composites

- Around ~35% epoxy, ~65% carbon fiber
- Fabric (woven) or uni-tape sheets, usually multiple layers thick
- Possibly sandwich material with high void fraction material between two composite sheets
- Pressed and cured in an autoclave
- Fibers around 5 μm diameter, 95% carbon

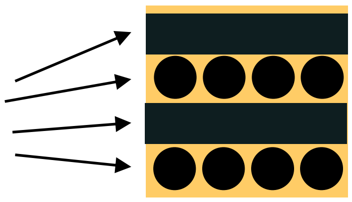
Epoxy and TETA hardener (From wikipedia):

$[C_{12}H_{20}O_3]_n$



A four layer cross-section illustration:

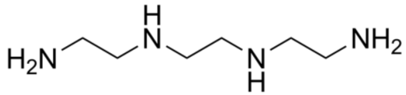
Fibers in varying orientation



Key:

Carbon Fibers

Epoxy Resin



$C_6H_{18}N_4$