SAND2011-3223P

Multiphase Coupling of Solid Material Decomposition with Fluid Flow and Combustion

Amanda Dodd, A. L. Brown, K. L. Erickson, and J. A. Hubbard

Sandia National Laboratories
Albuquerque, NM

3rd FM Global Open Source

CFD Fire Modeling Workshop

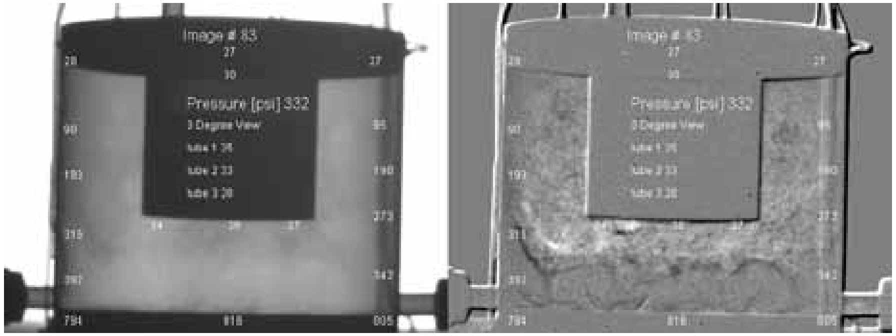
Norwood, MA

May 9-10, 2011

Sandia is a multi program laboratory operated by Sandia Corporation, a Lockheed Martin Company,
for the United States Department of Energy's National Nuclear Security Administration
under contract DE-AC04-94AL85000.

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



Sandia National Laboratories

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 I
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

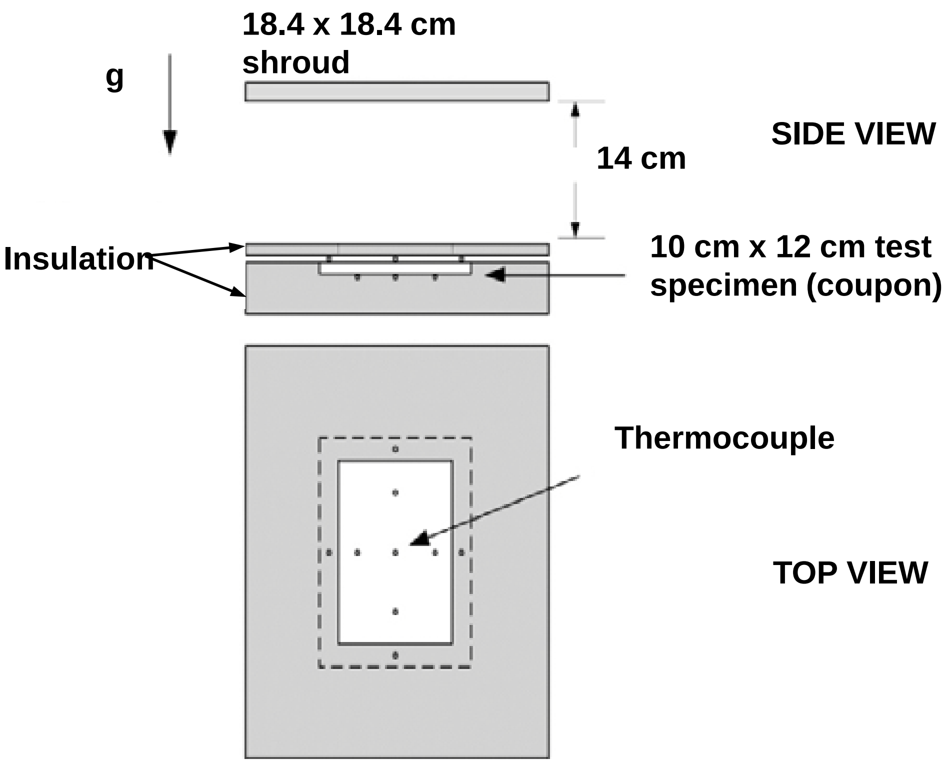
http://en.wikipedia.org/wiki/File:B787-1869.jpg

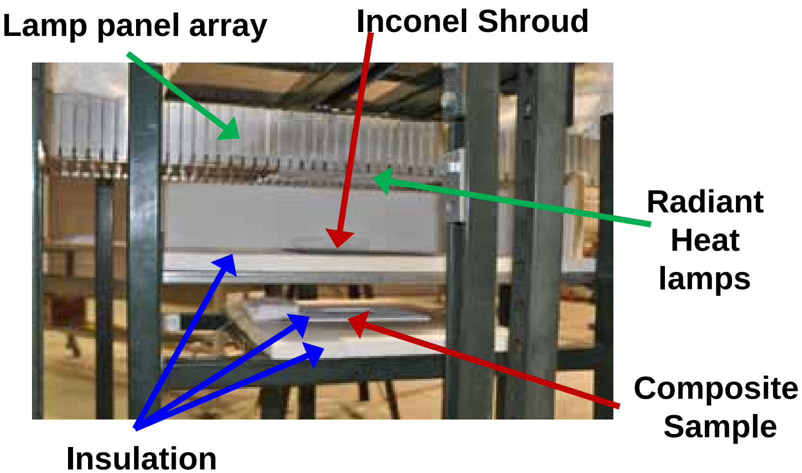
http://www.airforce-technology.com/projects/f22/f222.html

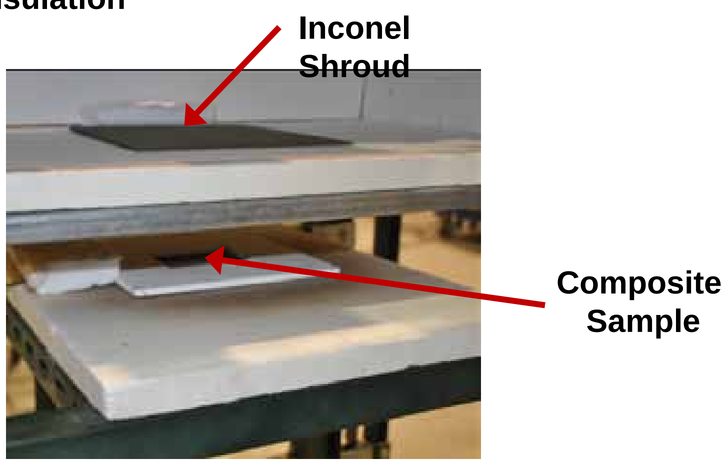
*Percentages are by weight

Composite Material
Mid-scale Experiments

Radiant Heat Experiments

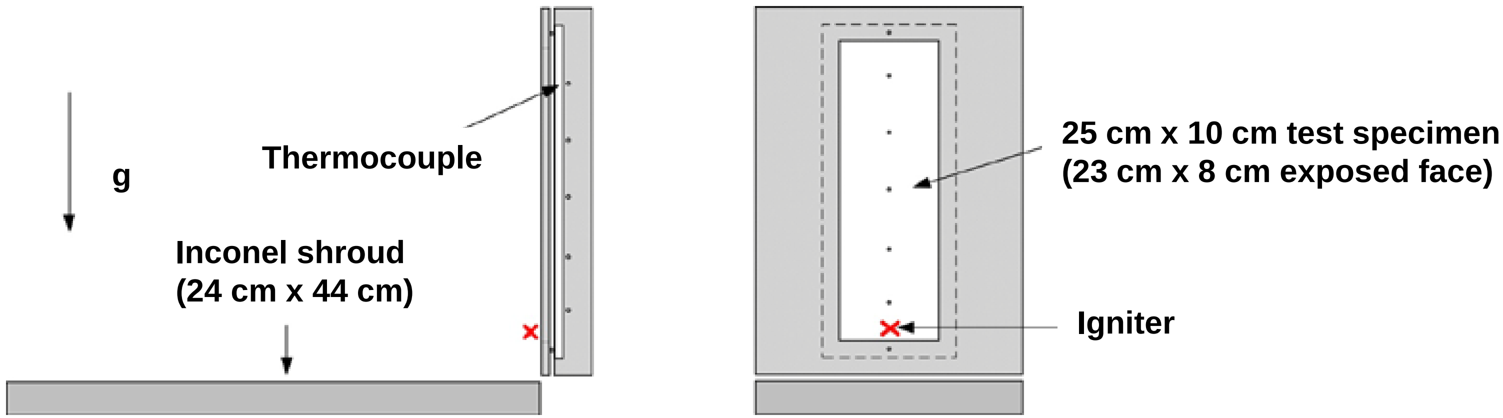


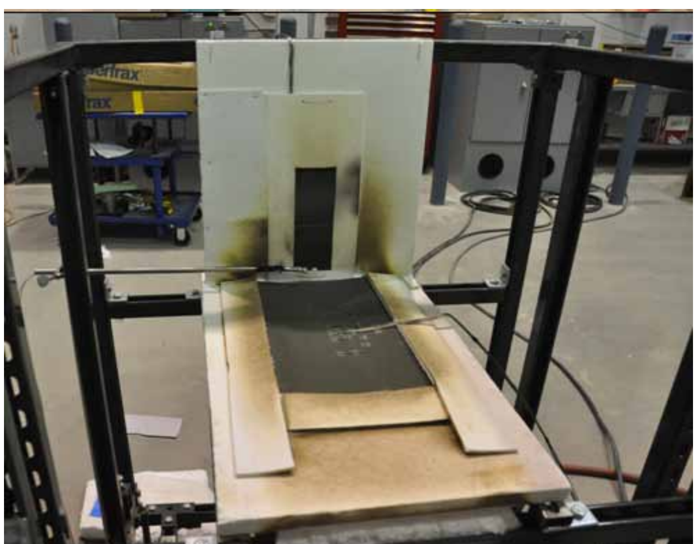


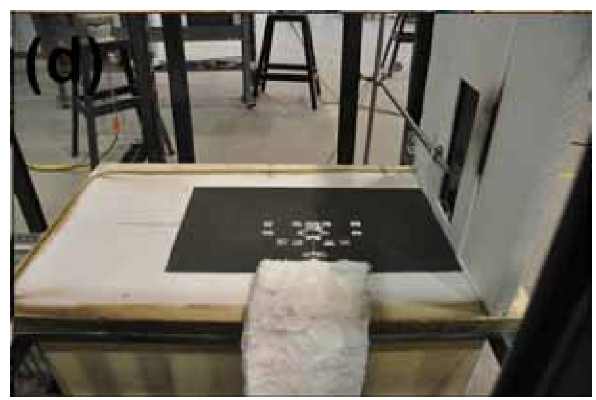


Composite Material
Mid-scale Experiments

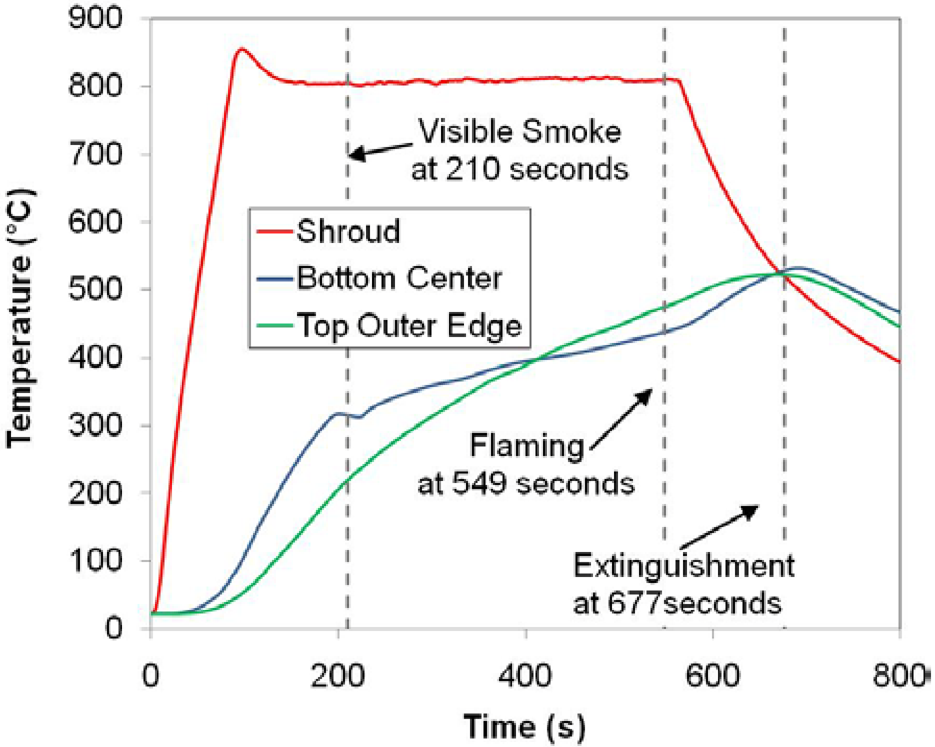
Flame Spread Experiments





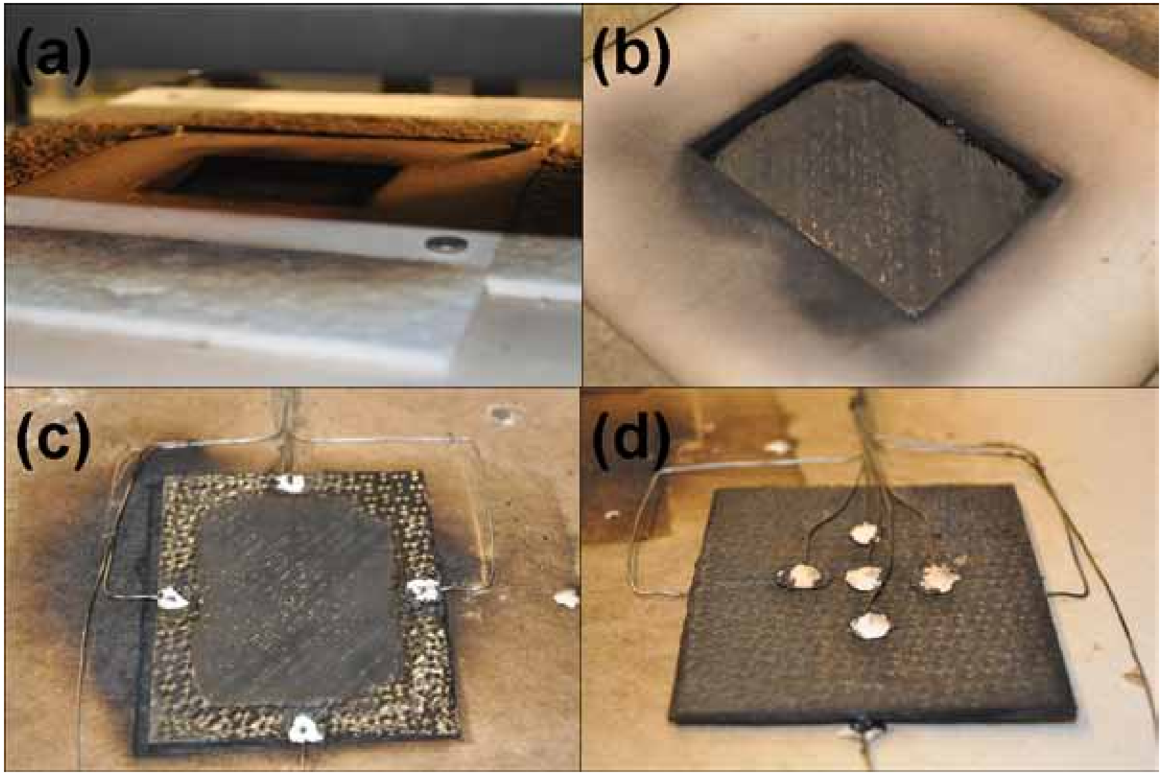


Experimental Results
BMI/Carbon Fiber Woven (Test 3)



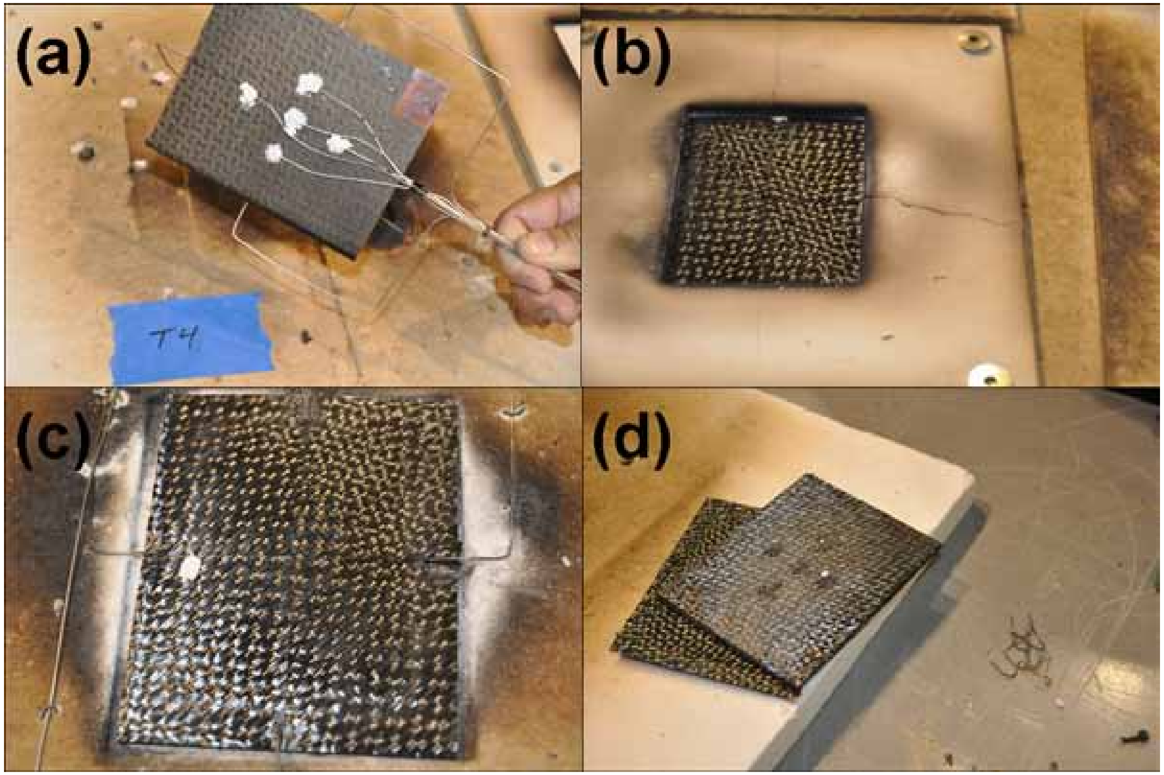
BMI/Carbon Fiber Composite
Initial swelling and smoking

BMI/Carbon Fiber Composite Post-Experiment Pictures



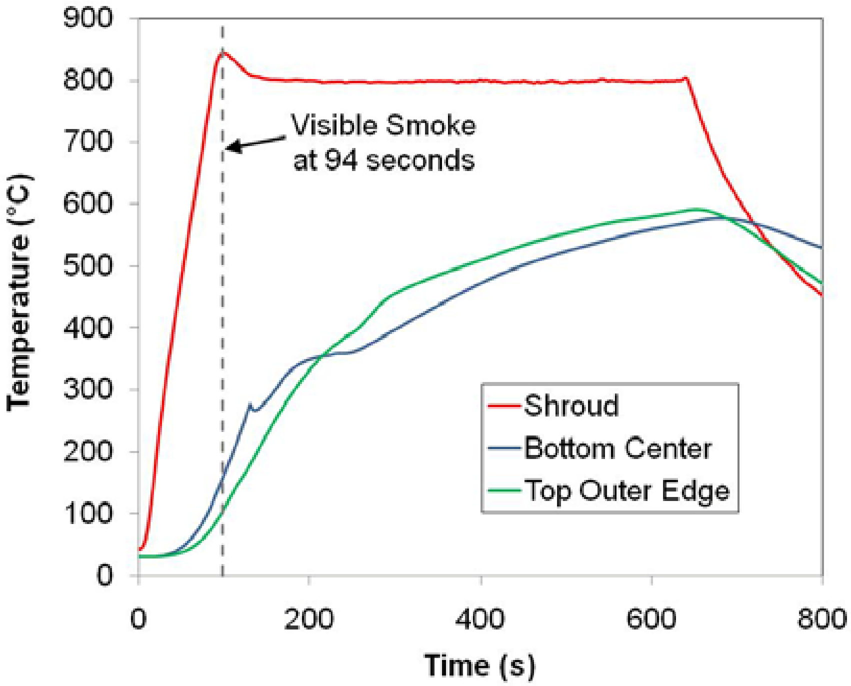
(a) Pre-test coupon in test apparatus
(b) Post-test top coupon face and zirconia board mask
(c) Post-test top coupon face (irradiated) surface
(d) Post-test bottom coupon face (insulated)

BMI/Carbon Fiber Composite Post-Experiment Pictures

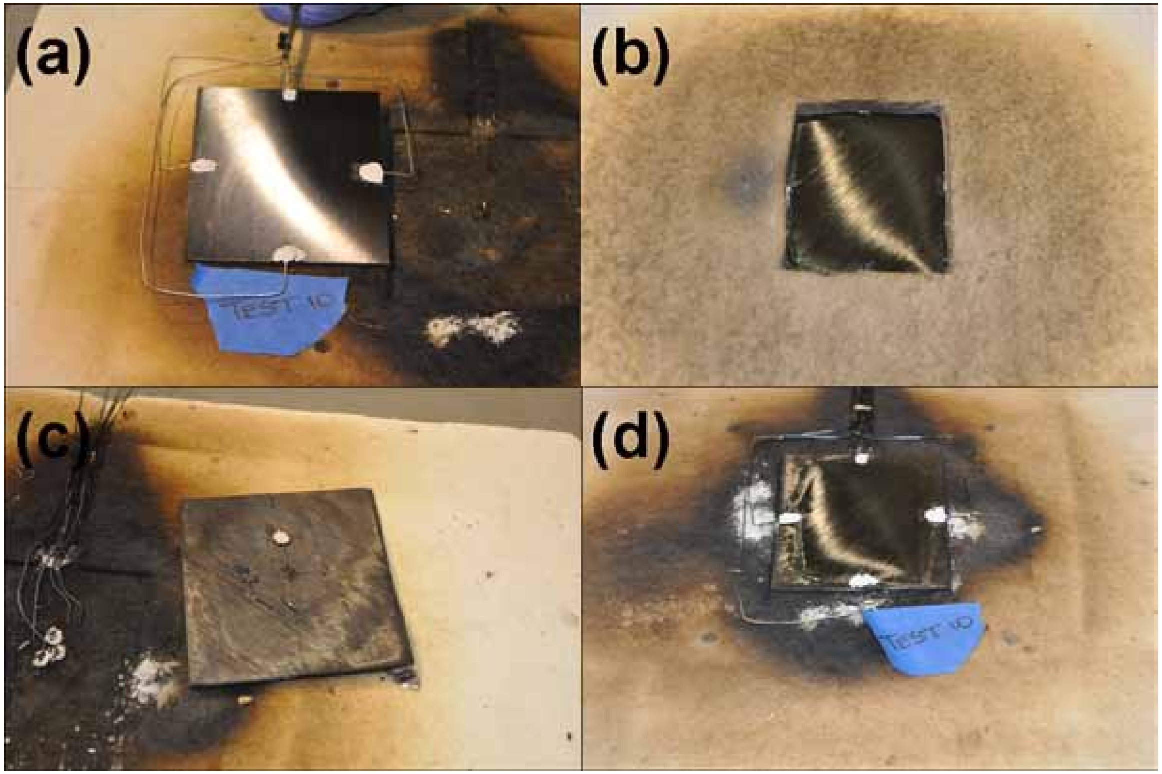


(a) Pre-test coupon, bottom face
(b) Post-test top coupon face and zirconia board mask
(c) Post-test top coupon face (irradiated) surface
(d) Post-test bottom coupon face (insulated), showing delamination of top surface (flaming did not occur)

Experimental Results
Epoxy/Carbon Fiber Tape (Test 10)

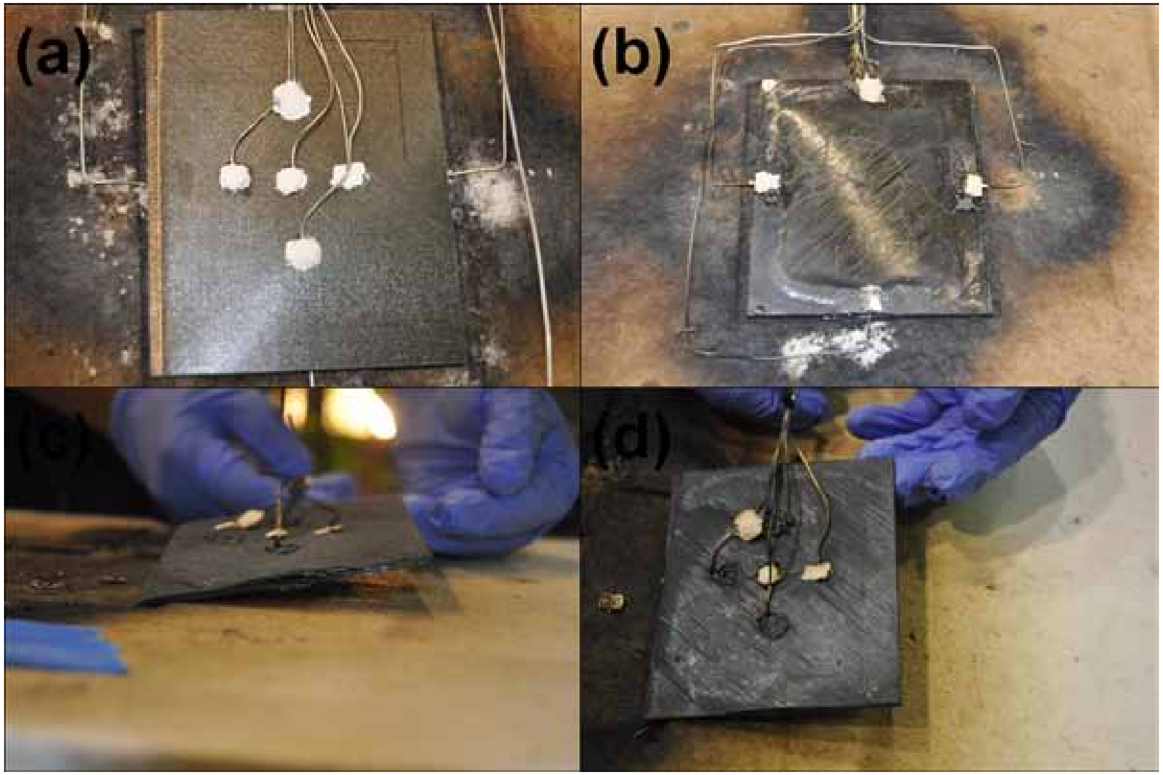


Epoxy/Carbon Fiber Composite Post-Experiment Pictures



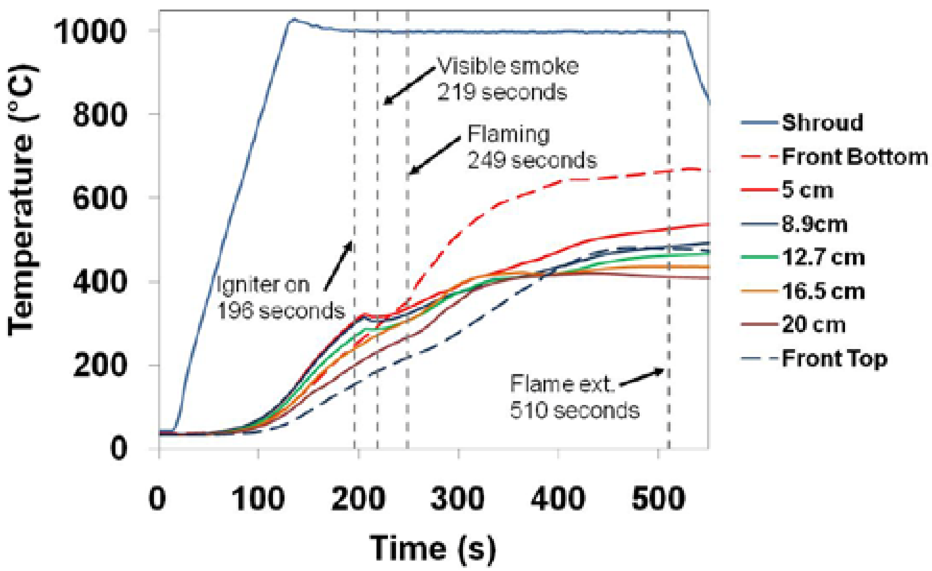
(a) Pre-test coupon, top face
(b) Post-test coupon, top face and fiber blanket mask
(c) Post-test bottom coupon face
(d) Post-test top coupon face

Epoxy/Carbon Fiber Composite Post-Experiment Pictures



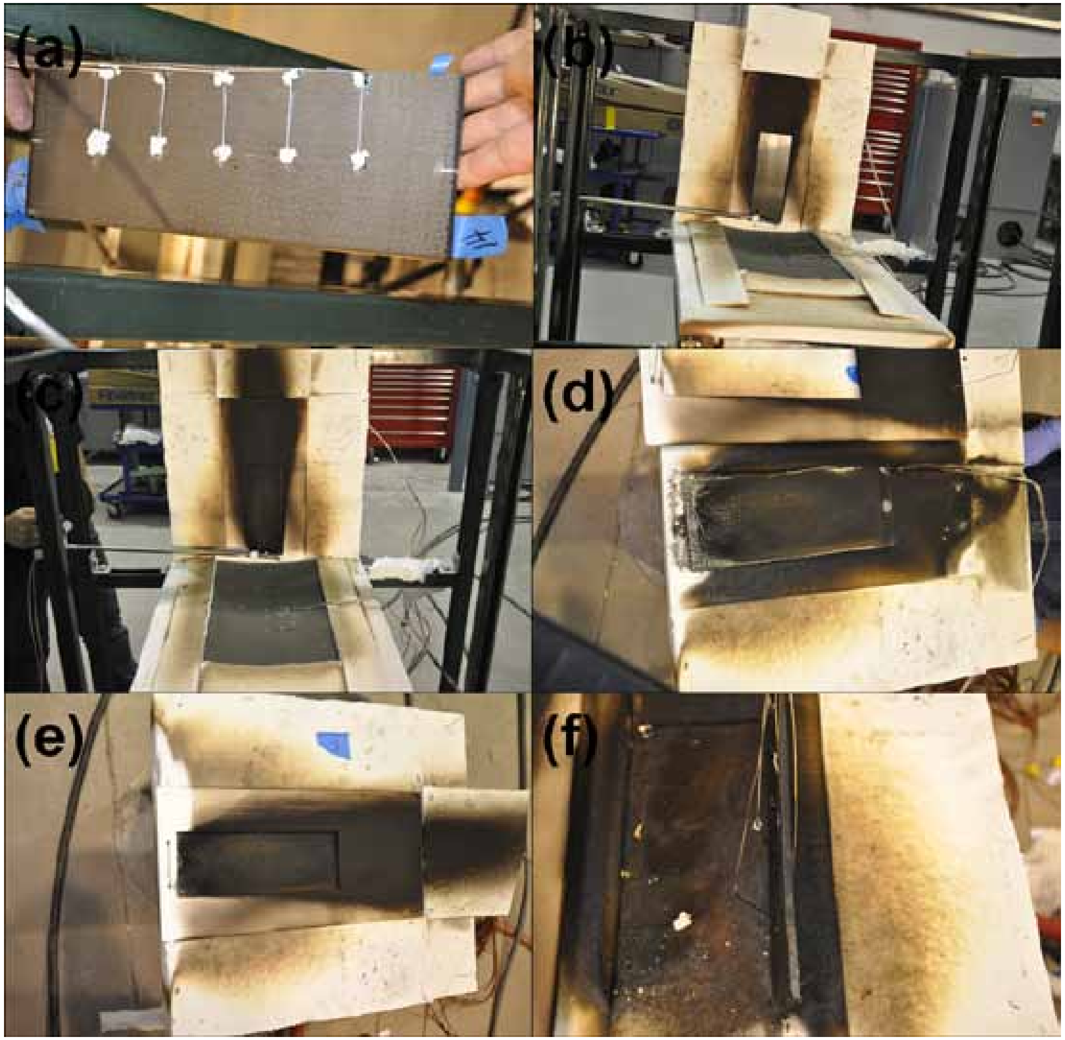
(a) Pre-test coupon, top face
(b) Post-test coupon, top face showing cracking
(c) Post-test coupon, side-view, showing significant delamination and expansion
(d) Post-test bottom coupon face, showing cracks parallel to fiber direction

Experimental Results
BMI/Carbon Fiber Woven (Test 14)



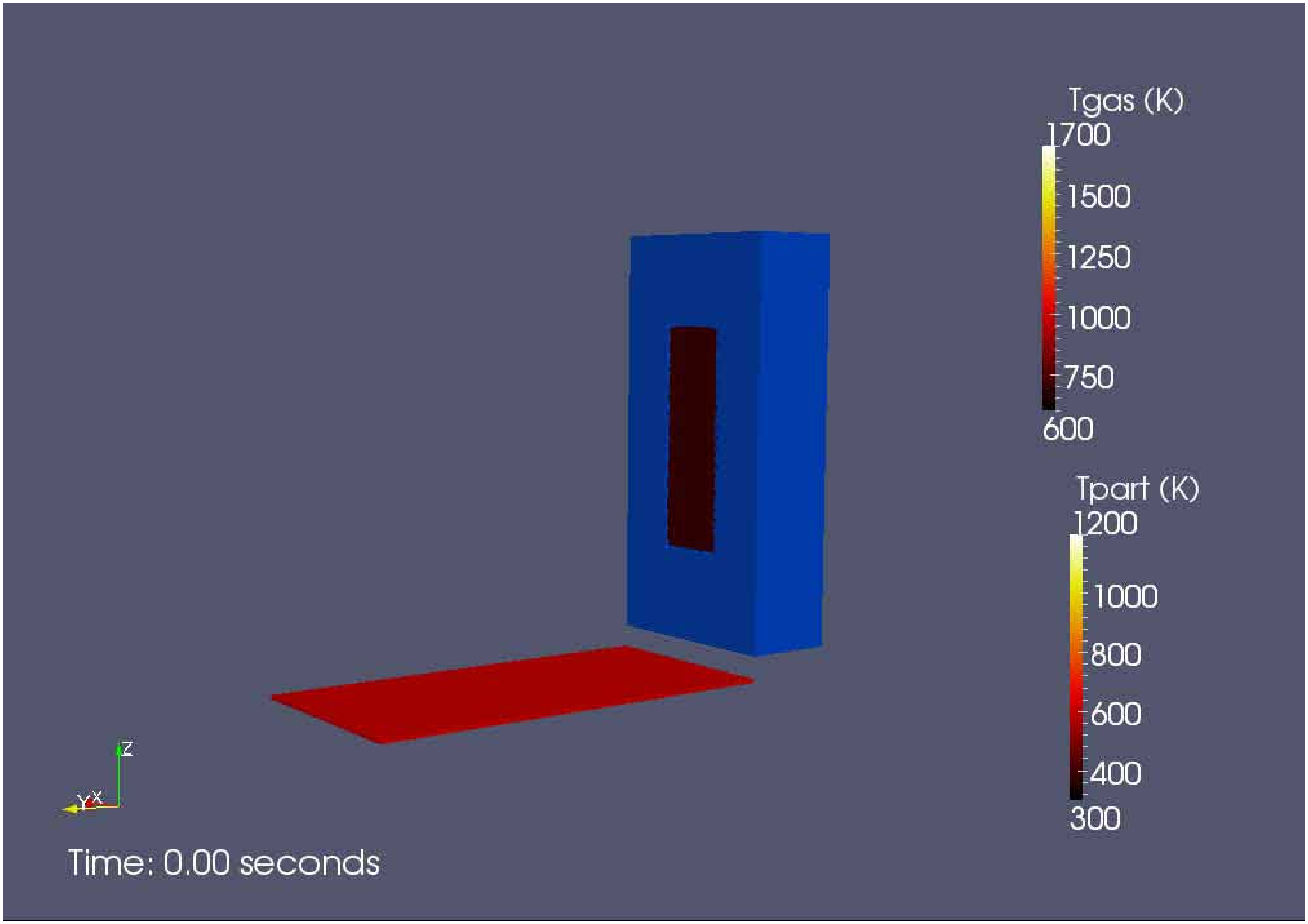
BMI/Carbon Fiber Composite
Smoking, Flaming, Reignition
(5x speed)

BMI/Carbon Fiber Composite Post-Experiment Pictures



(a) pre-test coupon back side (insulated)
(b) pre-test setup
(c) post-test setup
(d) post-test coupon front side (irradiated)
(e) post-test coupon front side
(f) post-test coupon back side (insulated

Computational Modeling: Flame Spread



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
- **Further questions: how do you extinguish a composite material fire?**

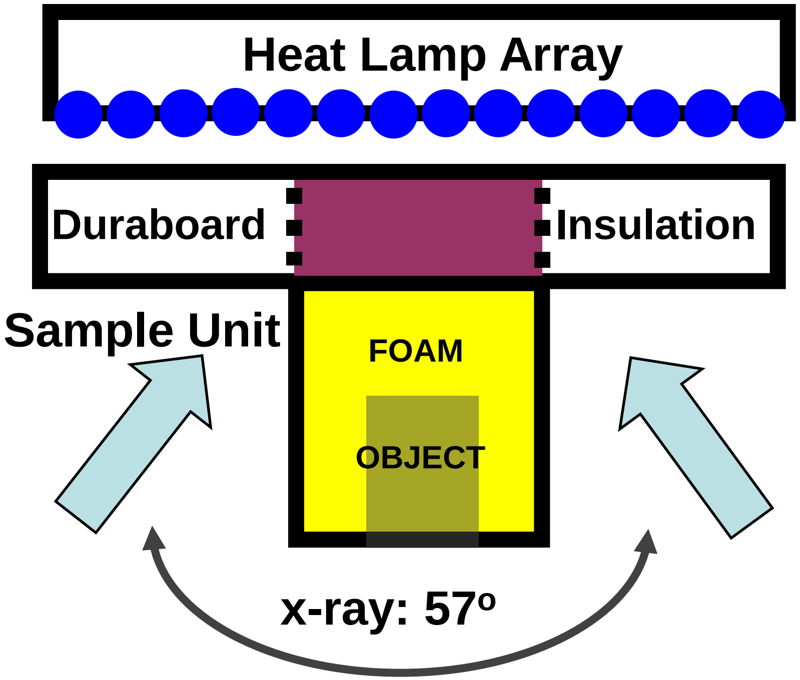
Organic Material Decompositon Background

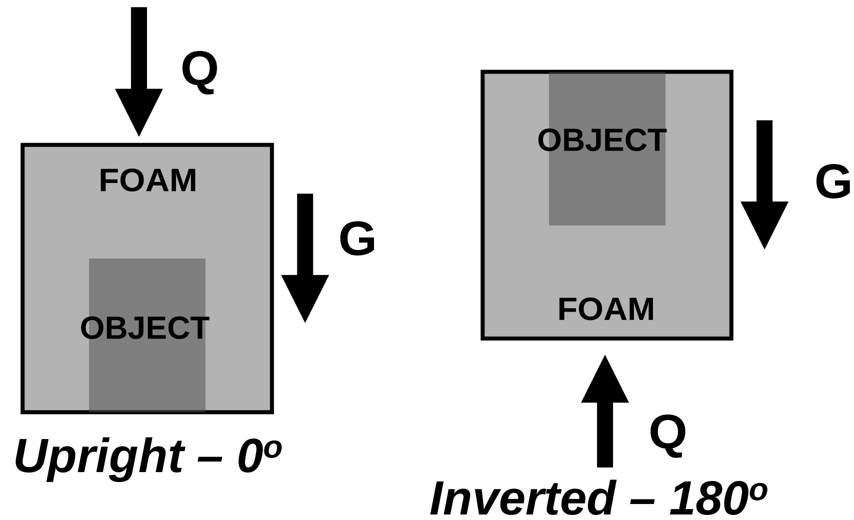
- **In fire environments, commonly used organic materials liquefy and flow during decomposition**
- **Evolved gases can cause pressurization and failure of sealed systems**
- **Previous analyses focused on heat transfer to components à now focus also involves predicting pressurization**
- **Complex physics**
  - Liquefaction/flow introduces convective heat transfer
  - Erosive channeling by hot gases exacerbates liquefaction/flow
  - Pressure depends on rate of gas generation, which depends on temperature history

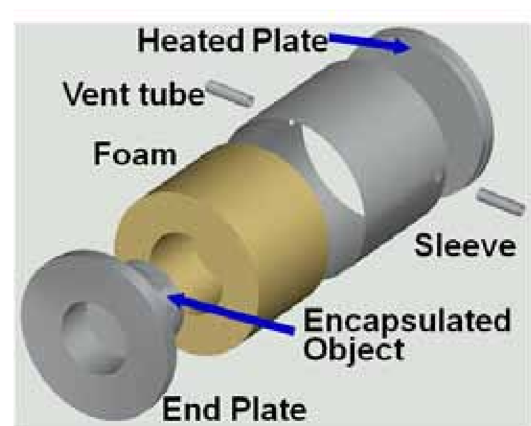
ASC

Sandia National Laboratories

Thermal transport and container pressurization experiments

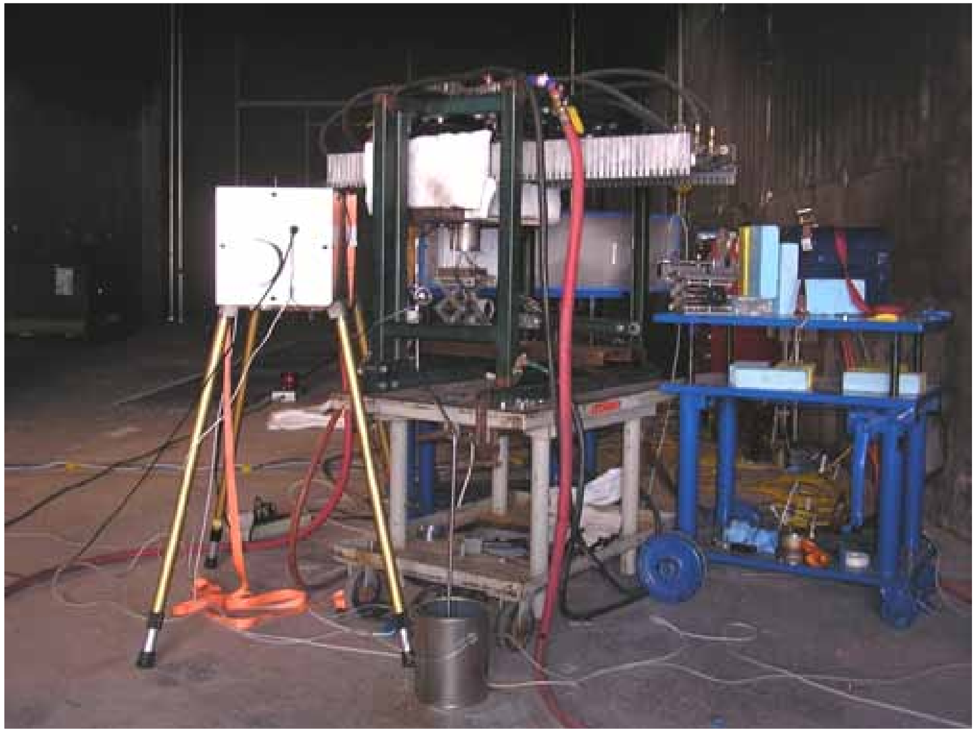






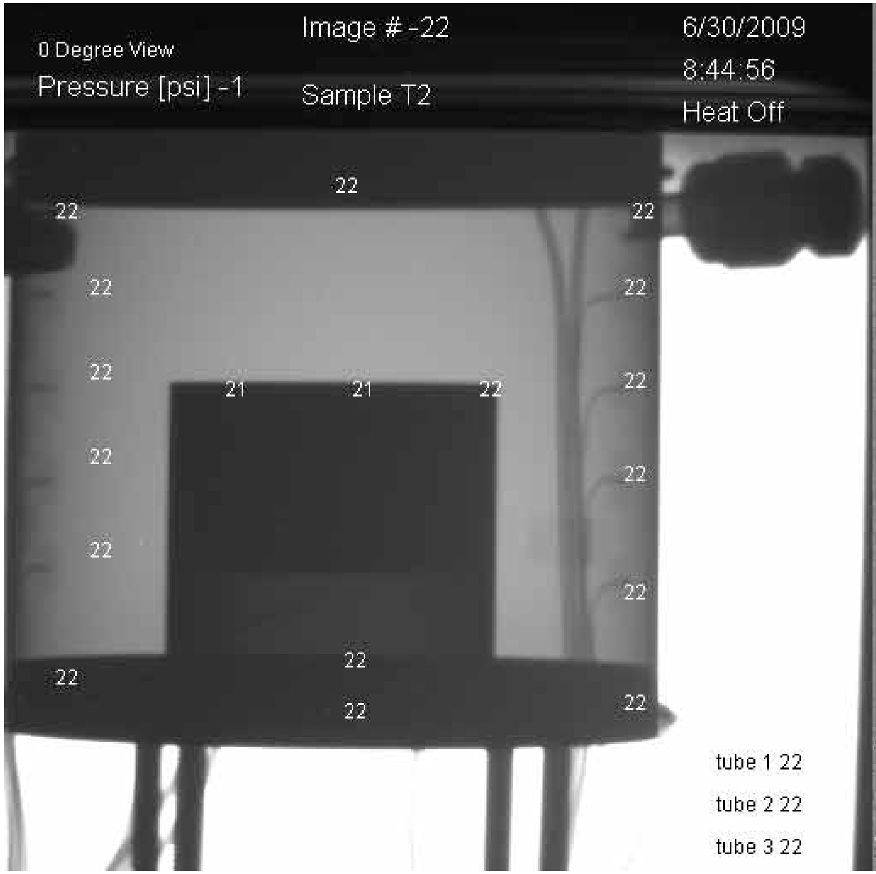
- **Plate temperatures: 600˚C & 900˚C**
- **Sealed samples for pressurization**

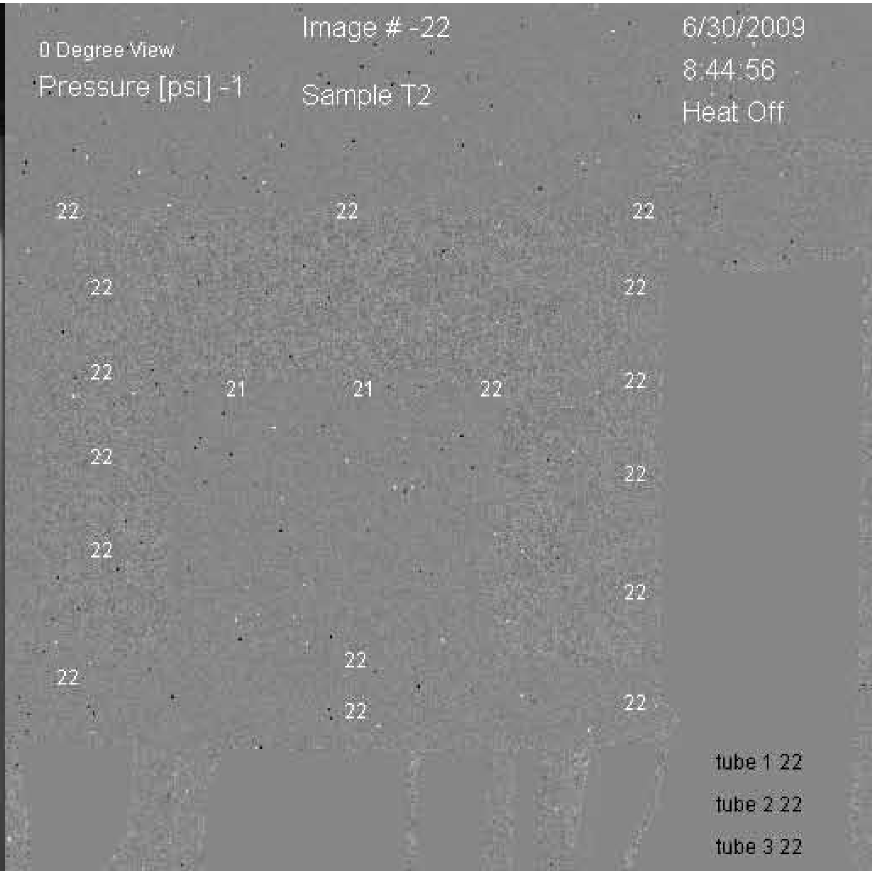
Experiments were performed at Thermal Test Complex



X-ray imaging gave insight into physical behavior of foam during experiments

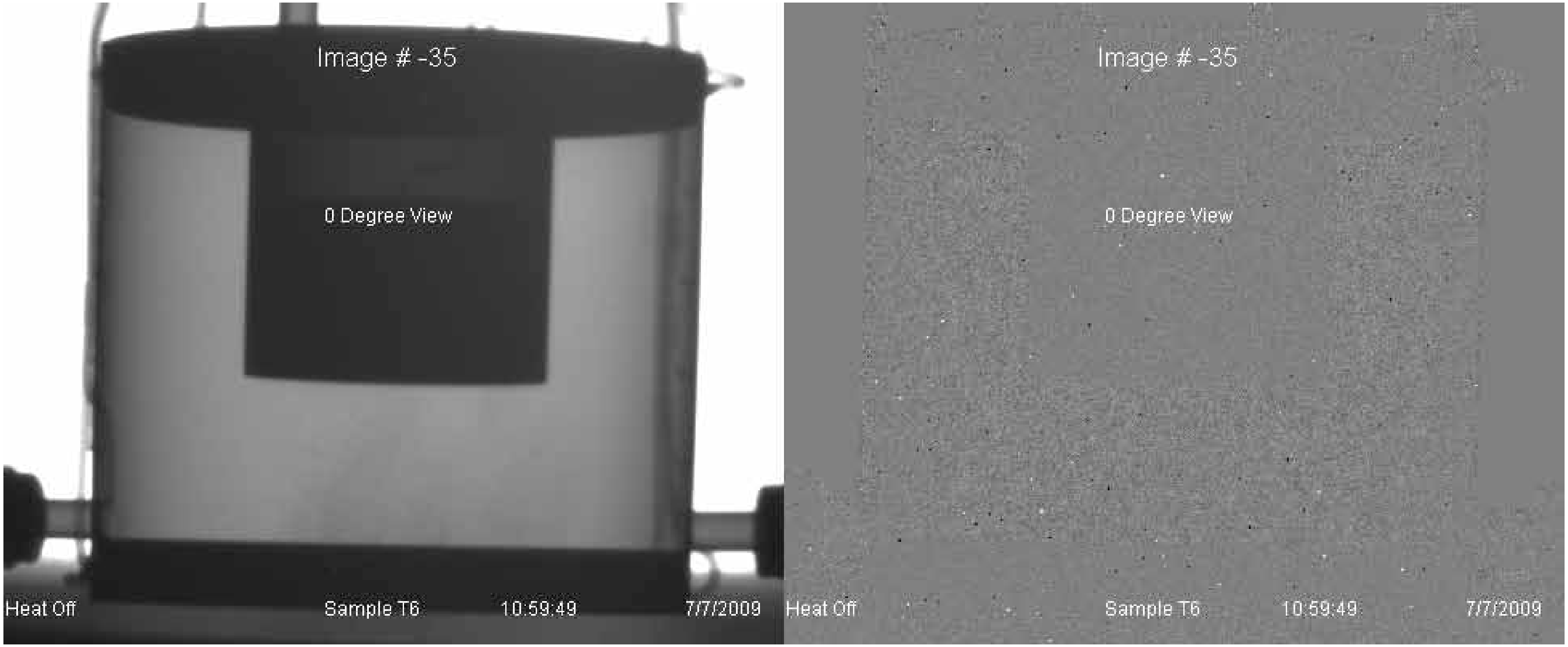
TDI (toluene diisocyanate)-based polyurethane (14 lb/ft^3): ramp 200 K/min to 1173 K





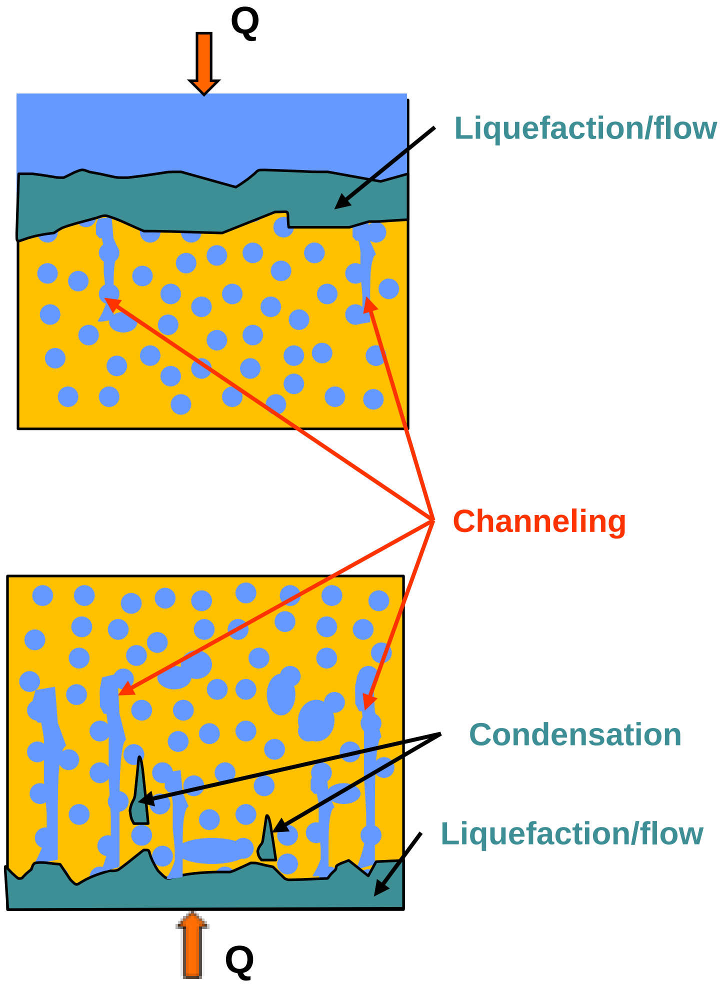
Difference between successive images showed channeling, liquefaction & flow

TDI-based polyurethane (14 lb/ft^3): ramp 200 K/min to 1173 K



Phenomenology

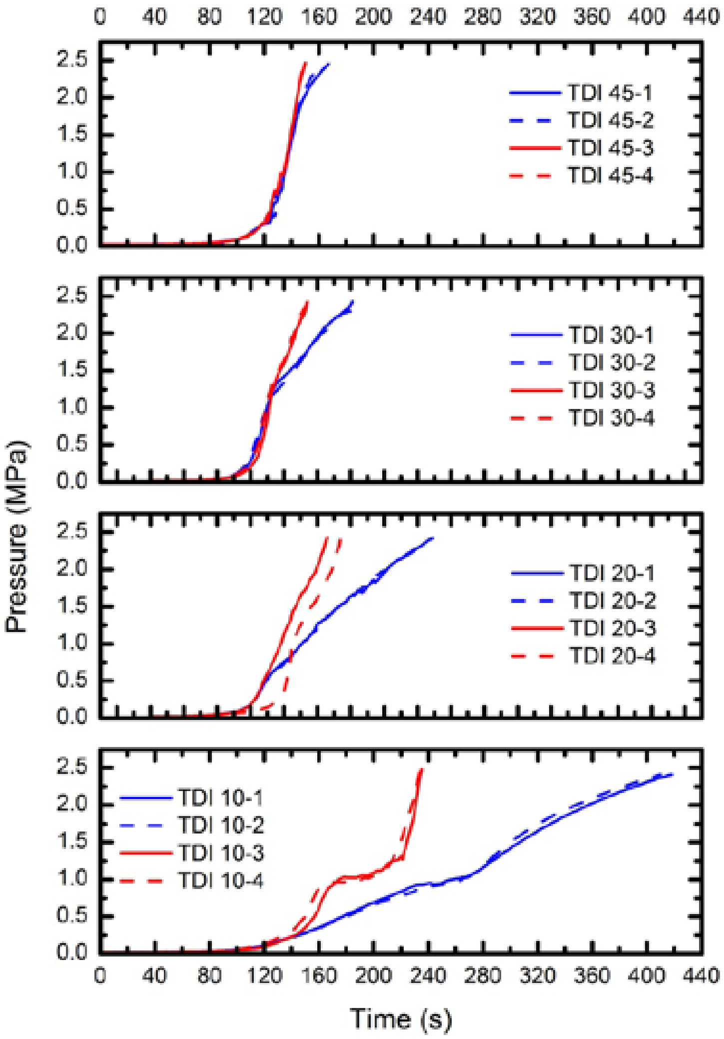
- **Heat transfer**
- **Mass transfer**
- **Chemistry**
- **Liquefaction/flow of decomposition products**
  - *Significantly impacts heat transfer to foam / rate of gas generation and container pressurization*
- **Erosive channeling by hot gas-phase decomposition products**
- **Vapor-Liquid Distribution of Organic Decomposition Products**



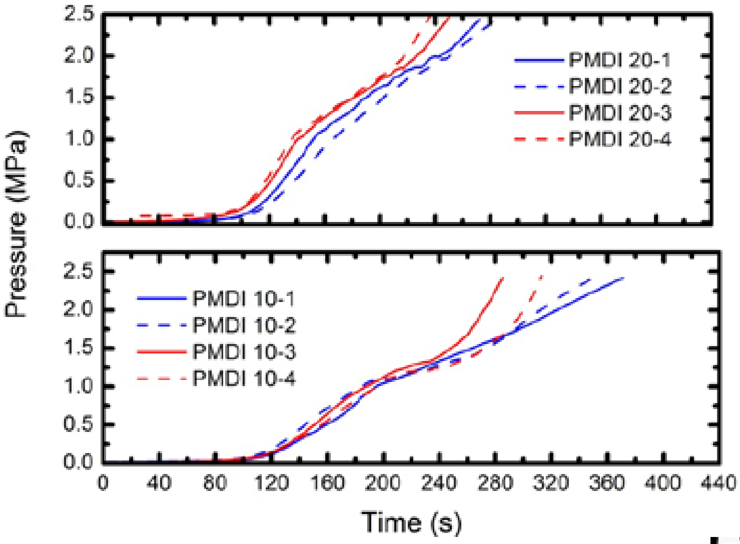
Sandia National Laboratories

Polyurethane Foams
Examining Density Effects

TDI (toluene diisocyanate)



PMDI (polymethylene diisocyanate)



Current Model Formulation

Energy Equation

Based on diffusive approximation for optically thick material

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot (k + k_e)\nabla T + \sum_i \rho r_i(-\Delta H_i)$$

$$k_e = \frac{16\sigma}{3(a + s_s)} T^3$$

Effective radiative conductivity k_e depends on absorption coeff. a and scattering coeff. s_s[1]

*•Note: Absorption coeff. a and scattering coeff. s_s were calculated using an analytical two-flux model for radiative transfer and the measured values of reflectance **R** and transmittance **T*** [2,3]

Decomposition Model

Decomposition reactions / rates (r_i)

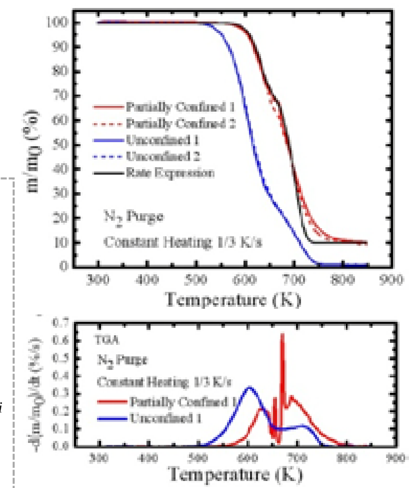
$$\text{Polymer} = w_1 A_1 + w_2 A_2 + \cdots$$

$$A_i \xrightarrow{r_i} \xi_{i1} B_{i1} + \xi_{i2} B_{i2} + \cdots$$

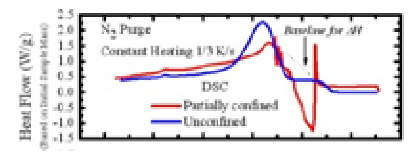
$$\frac{dw_{A_i}}{dt} = -k_i w_{A_i} = -r_i \qquad \frac{d\overline{r}_{B_{ij}}}{dt} = r_B^0 \frac{X_{ij} w_i^0}{\overline{M}_{B_{ij}}} k_i w_{A_i}$$

$$k_i = k_i^0 \exp(-Q_i / RT)$$

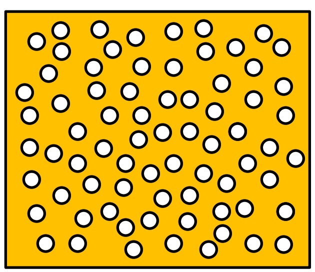
ThermoGravimetric Analysis (TGA)



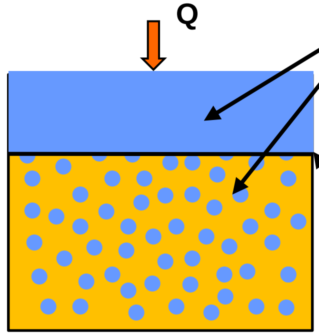
Differential Scanning Calorimetry (DSC)



Initial Foam



Partially Reacted



Gas/Vapors: CO_2, Cyclopentanone, Toluenediamine, Ethylacrolien, Other

Reaction Front

Pressure

- Gradients relax quickly
- Ideal gas law
- All decomp. prod.
- Gas occupies all free volume

Moles of gas

$$P = \frac{n_g R}{\int_{V_g} \frac{1}{T} dV_g} = \frac{n_g R}{\left(\int_{V_{fv}} \frac{1}{T} dV_{fv} + \int_{V_B^0} \frac{\Phi}{T} dV_B^0 \right)}$$

n_g= gas moles, , $f(K_{Bij}, T)$

Φ=porosity, $f(\varphi_0, SF, f_p)$

Free volume/ temperature

Gas Volume: reacted area and pore space

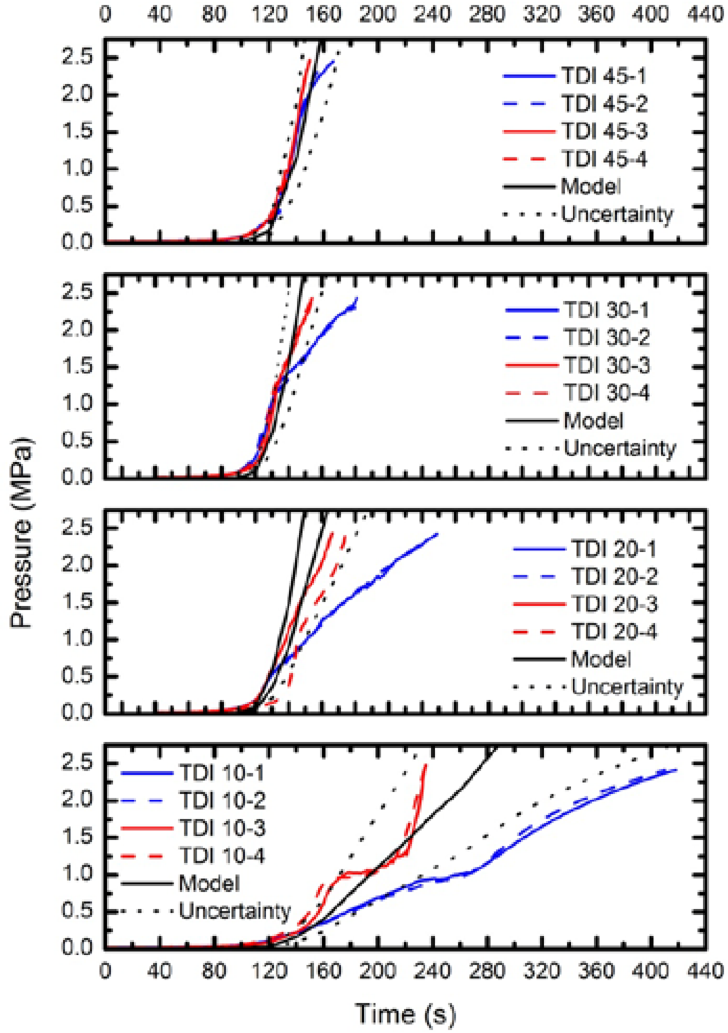
[1]Siegel, R. and Howell, J. R., Thermal Radiation Heat Transfer, 2nd ed., Hemisphere Publishing Corp., Cambridge, 1982, p497-p501.
[2]Reichman, J., *Applied Optics*, 12 (8), August 1973, p1811-p1815.
[3]Erickson et al., BCC 2009.

ASC

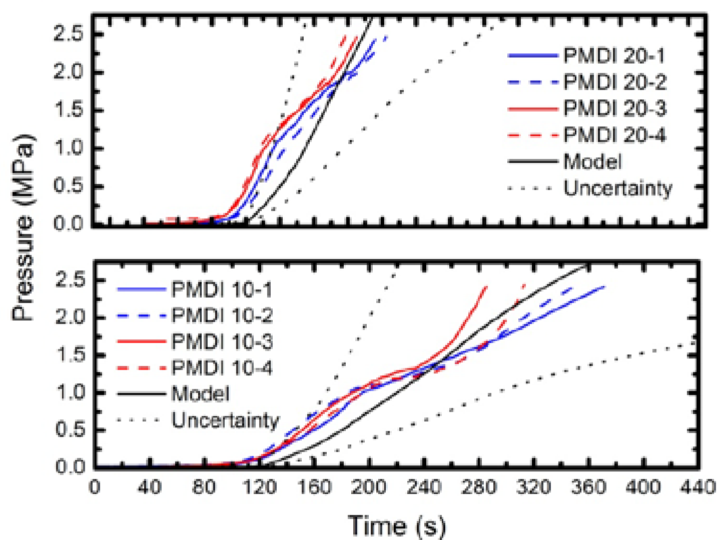
Sandia National Laboratories

Model and Experimental Comparison Examining Density Effects

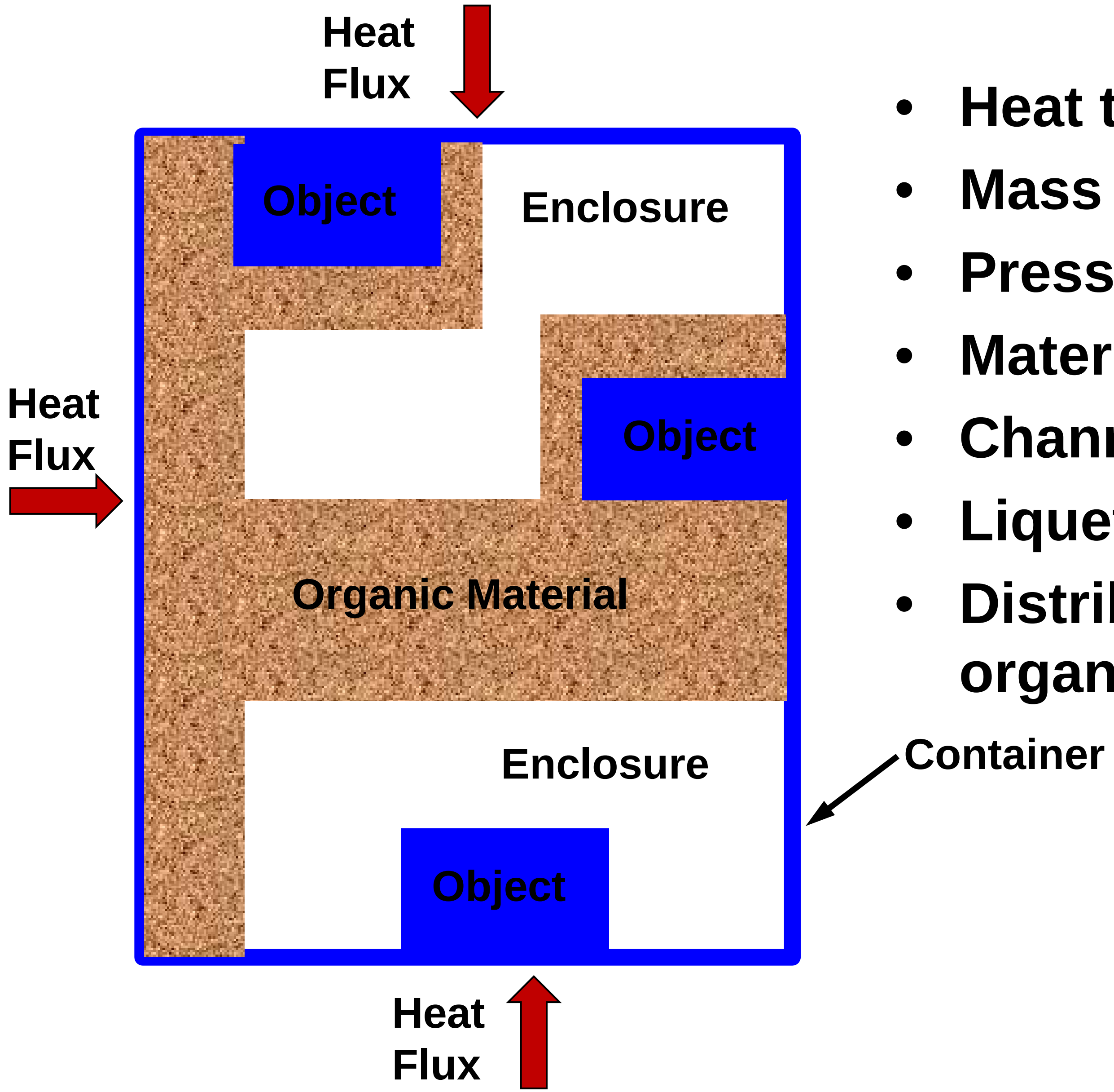
TDI



PMDI



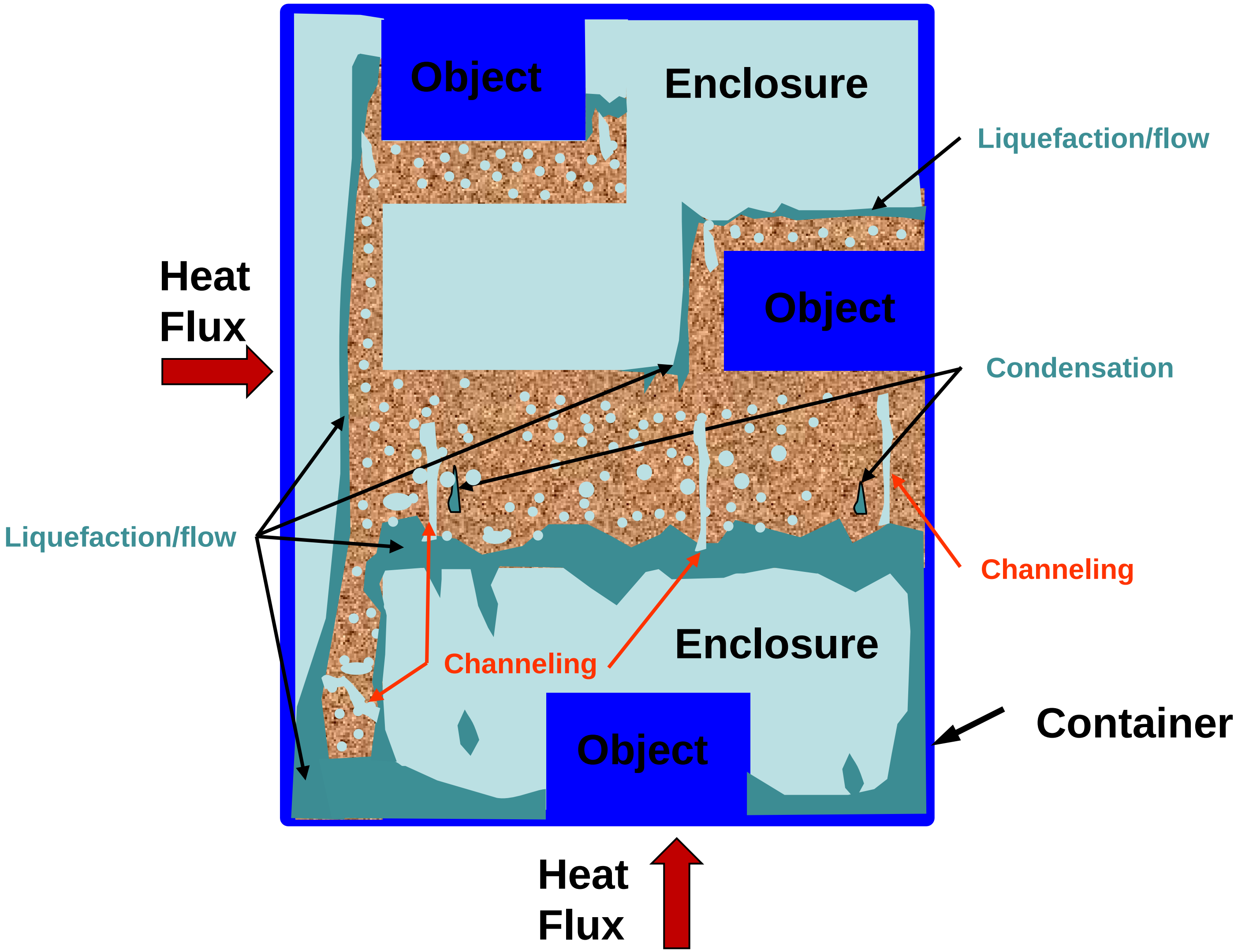
Organic Material Problem of Interest



- Heat transfer
- Mass transfer
- Pressurization
- Material relocation
- Channeling
- Liquefaction
- Distribution of organics in liquid/gas

Sandia National Laboratories

Organic Material Problem of Interest



Experimental and Modeling Efforts

- **Objective: Hierarchal approach with incremental improvements to modeling and experimental capabilities**
- **Approach:**
  - Modeling:
    - Provide today's capability with enhancements as appropriate
    - Develop a plan for future capabilities to be developed incrementally with increasing complexity
    - Implement new code capability, verify, validate
    - Assess feasibility of approach
    - Modify path foward
  - Experimentally
    - Use 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

Near Term Approach: Porous Media Capability coupled with Fluid Region

- **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
  - Saturation
  - Darcy flow
  - Generalize reaction capability
- **Interface with fluid region**

Mass and Species Porous Media Equations

Condensed Phase

Mass Conservation

$$\frac{\partial \bar{\rho}}{\partial t} = -\dot{\omega}'''_{fg}$$

Species Conservation

$$\frac{\partial \left(\bar{\rho} Y_i \right)}{\partial t} = \dot{\omega}'''_{fi} - \dot{\omega}'''_{di}$$

Gas Phase

Mass Conservation

$$\frac{\partial \left(\bar{\varphi} \rho_g \right)}{\partial t} = \nabla \cdot \left(\frac{\rho_g \bar{K}}{\mu_g} \left(\nabla P + \rho_g \vec{g} \right) \right) + \dot{\omega}'''_{fg}$$

Species Conservation

$$\frac{\partial \left(\bar{\varphi} \rho_g Y_j \right)}{\partial t} = \nabla \cdot \left(\frac{\rho_g Y_j \bar{K}}{\mu_g} \left(\nabla P + \rho_g \vec{g} \right) \right) + \nabla \cdot \left(\bar{\varphi} \rho_g D \nabla Y_j \right) + \dot{\omega}'''_{s,fj} - \dot{\omega}'''_{s,dj} + \dot{\omega}'''_{g,fj} - \dot{\omega}'''_{g,dj}$$

Condensed and Gas Phase Energy and Momentum Equations

Energy Conservation Condensed Phase

$$\frac{\partial\left(\bar{\rho}\bar{h}\right)}{\partial t} = \nabla\cdot\bar{k}\nabla T + \sum_{k=1}^{K} \dot{Q}'''_{s,k} + \sum_{i=1}^{M}\left(\dot{\omega}'''_{fi} - \dot{\omega}'''_{di}\right)h_i - h_{cv}\left(T - T_g\right)$$

Energy Conservation Gas Phase

$$\frac{\partial\left(\bar{\psi}\rho_g\bar{h}_g\right)}{\partial t} = \nabla\cdot\left(\frac{\rho_g\bar{h}_g\bar{K}}{\mu_g}\left(\nabla P + \rho_g\vec{g}\right)\right) + \nabla\cdot\left(\bar{\psi}\rho_g D\nabla\bar{h}_g\right)$$

$$+\sum_{l=1}^{L}\dot{Q}'''_{g,l} + \sum_{j=1}^{N}\left(\dot{\omega}'''_{s,fj} - \dot{\omega}'''_{s,dj}\right)h^{*}_{g,j} + h_{cv}\left(T - T_g\right)$$

Heterogeneous Reactions

Stoichiometry of heterogeneous reaction k

$$1\ \text{kg}\ A_k + \sum_{j=1}^{N} \nu'_{j,k}\ \text{kg gas}\ j \rightarrow \nu_{B,k}\ \text{kg}\ B_k + \sum_{j=1}^{N} \nu''_{j,k}\ \text{kg gas}\ j \qquad \nu_{B,k} = \frac{\rho_{B_k}}{\rho_{A_k}}$$

Destruction rate of condensed-phase species A_k

$$\dot{\omega}'''_{dA_k} = \left(\frac{\bar{\rho} Y_{A_k}}{\left(\bar{\rho} Y_{A_k}\right)_\Sigma} \right)^{n_k} \left(\bar{\rho} Y_{A_k}\right)_\Sigma Z_k \exp\left(-\frac{E_k}{RT} \right) \qquad (\text{for } n_{O_2,k} = 0)$$

$$\dot{\omega}'''_{dA_k} = \left(\frac{\bar{\rho} Y_{A_k}}{\left(\bar{\rho} Y_{A_k}\right)_\Sigma} \right)^{n_k} \left(\bar{\rho} Y_{A_k}\right)_\Sigma \left[\left(1 + Y_{O_2}\right)^{n_{O_2,k}} - 1 \right] Z_k \exp\left(-\frac{E_k}{RT} \right) \qquad (\text{for } n_{O_2,k} \neq 0)$$

Formation rate of condensed-phase species B_k

$$\dot{\omega}'''_{fB_k} = \nu_{B,k} \dot{\omega}'''_{dA_k} = \frac{\rho_{B_k}}{\rho_{A_k}} \dot{\omega}'''_{dA_k}$$

Conversion rate of condensed-phase mass to gas-phase mass

$$\dot{\omega}'''_{fg_k} = \left(1 - \nu_{B,k}\right) \dot{\omega}'''_{dA_k} = \left(1 - \frac{\rho_{B_k}}{\rho_{A_k}}\right) \dot{\omega}'''_{dA_k}$$

Net formation rate and destruction rate of gaseous species *j* from reaction *k*

$$\dot{\omega}'''_{s,fj,k} = \dot{\omega}'''_{fg_k} y_{s,j,k} \qquad \dot{\omega}'''_{s,dj,k} = -\dot{\omega}'''_{fg_k} y_{s,j,k}$$

Heat of reaction

$$\dot{Q}'''_{s,k} = -\dot{\omega}'''_{dA_k} \Delta H_k$$

Homogeneous Reactions

Stoichiometry of homogeneous reaction

$$1\ \text{kg}\ A_\lambda - y_{g,B_\lambda,\lambda}\ \text{kg}\ B_\lambda \rightarrow \sum_{j=1}^{N} \max(y_{g,j,\lambda},0)\ \text{kg gas}\ j$$

Destruction rate of gas-phase species A_λ

$$\dot{\omega}'''_{dA_\lambda} = \bar{y}\,[A_\lambda]^{p_\lambda}\,[B_\lambda]^{q_\lambda}\,T^{b_\lambda} Z_\lambda \exp\left(-\frac{E_\lambda}{RT_g}\right)$$

Net formation rate and destruction rate of gaseous species *j* by homogeneous gaseous reaction

$$\dot{\omega}'''_{g,fj,\lambda} = \dot{\omega}'''_{dA_\lambda}\, y_{g,j,\lambda}$$

$$\dot{\omega}'''_{g,dj,\lambda} = -\dot{\omega}'''_{dA_\lambda}\, y_{g,j,\lambda}$$

Heat of reaction:

$$\dot{Q}'''_{g,\lambda} = -\dot{\omega}'''_{dA_\lambda}\, \Delta H_\lambda$$

Path Forward

- **Porous media approach coupled with fluid region**
  - Two phase: gas/solid
  - Three phase: gas/liquid/solid
  - Material expansion
- **Front tracking methods**
  - Decomposition front with gas domain formation
  - Liquefaction and flow
  - Vapor/Liquid Equilibrium (approximations?)
- **Coupling to structural mechanics**

Path Forward

- **Potential Concerns**
  - Experimental data
    - Can we measure properties that we need?
  - Numerical Issues
    - Galerkin finite element approach
    - Required time step vs. real time run requirements
  - Gas phase ignition
  - Approach does not resolve fluid flow
- **Mitigation**
  - Assess capability along the way
  - Utilize additional codes as appropriate
  - Develop modeling approaches to work around numerical issues
  - Collaborate with industry, academia, etc.
  - Additional experiments, instrumentation, etc.

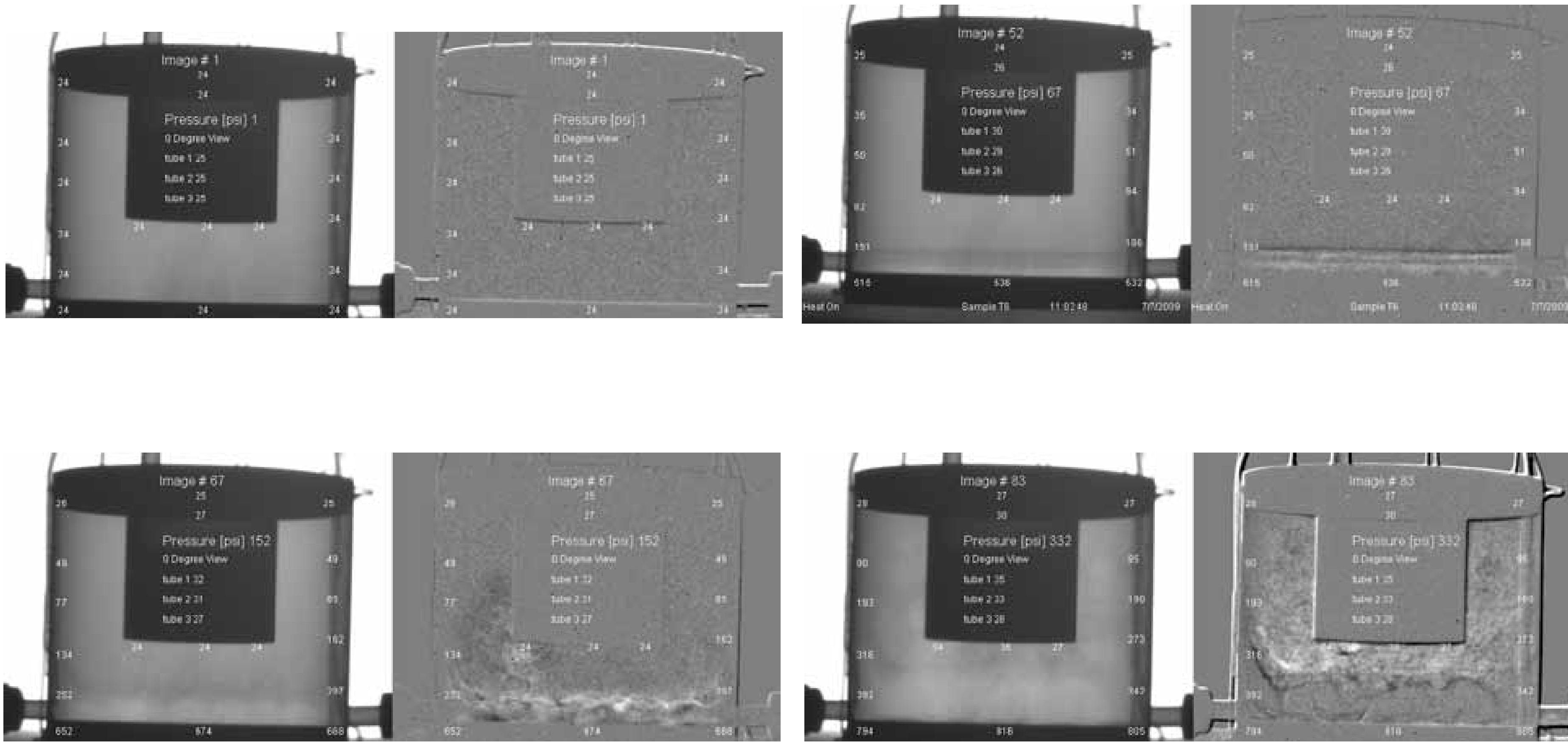
Summary

- Difficult multi-physics problems with applications in large systems
- An initial approach has been proposed and is being implemented and tested
- Approach will have to be assessed along the way with the end goal in mind
- Concerns and mitigation strategies

Questions

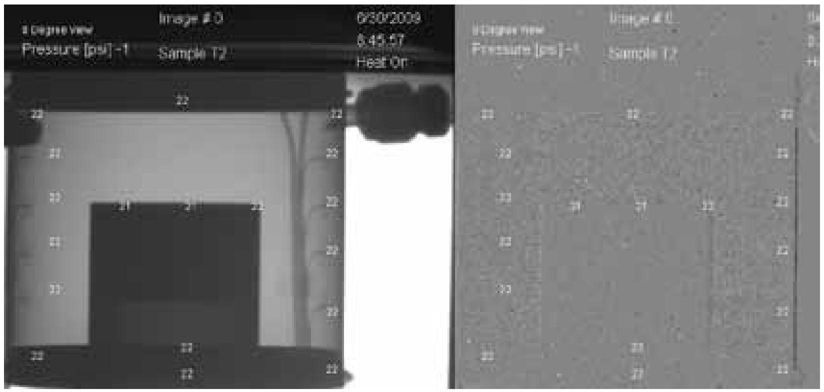
Channeling, liquefaction, and flow were more obvious in inverted orientation

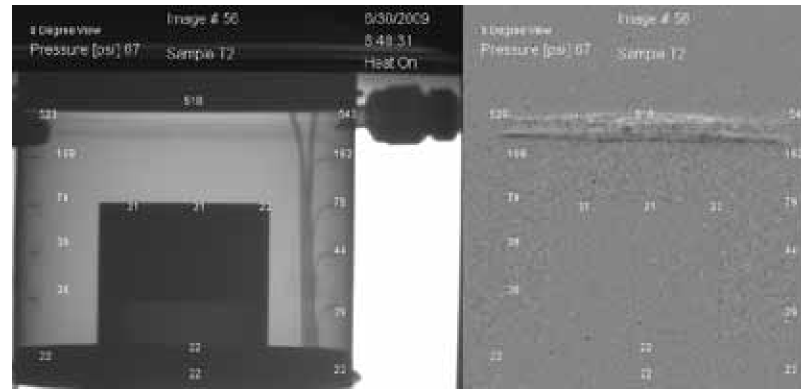
TDI-based polyurethane (14 lb/ft^3): ramp 200 K/min to 1173 K

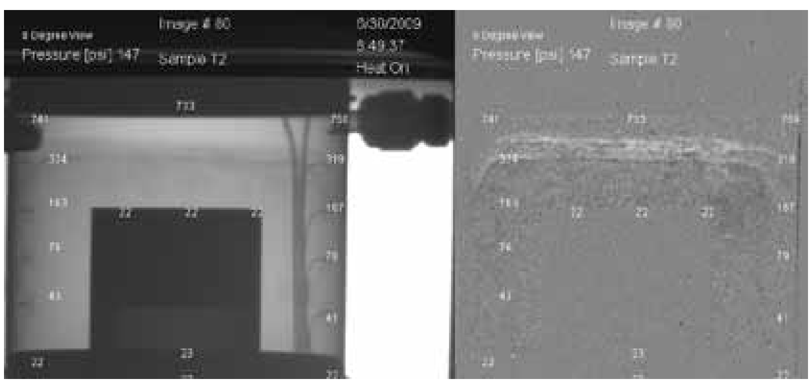


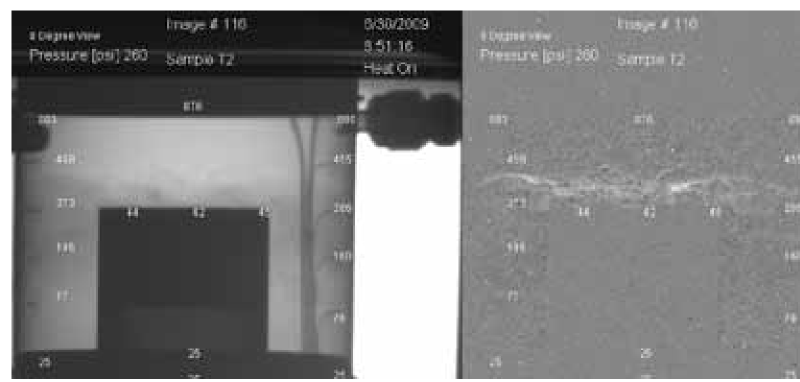
X-ray imaging provided insight into physical behavior of foam during experiments

TDI (toluene diisocyanate)-based polyurethane (14 lb/ft^3): ramp 200 K/min to 1173 K









Thermal Properties

Volume Fraction/Mass Fraction relation:

$$X_i = \bar{\rho}\,\frac{Y_i}{\rho_i} \qquad X_i = Volume\ Fraction \qquad Y_i = Mass\ Fraction$$

Average Condensed Phase Bulk Density:

$$\bar{\rho} = \sum_{i=1}^{M} X_i \rho_i \quad \textbf{or} \quad \bar{\rho} = \left(\sum_{i=1}^{M} \frac{Y_i}{\rho_i}\right)^{-1}$$

Species Condensed Phase Bulk Density {i.e. (1-ψ)ρ}

$$\rho_i(T) = \rho_{0,i}\left(\frac{T}{T_r}\right)^{n_{r,i}} \quad \textit{or other temperature dependence}$$

Average Porosity:

$$\bar{\psi} = \sum X_i \psi_i \qquad \psi_i(T) = 1 - \frac{\rho_i(T)}{\rho_{s0,i}} \qquad \rho_{s0,i}\ \textit{is density of solid nonporous species, i}$$

Average Condensed Phase Conductivity:

$$\bar{k} = \sum_{i=1}^{M} X_i k_i \qquad k_i(T) = k_{s,i}(T) + k_{r,i}(T) = k_{0,i}\left(\frac{T}{T_r}\right)^{n_{k,i}} + \gamma_i \sigma T^3$$

Average Condensed Phase Specific Heat:

$$\bar{c} = \sum_{i=1}^{M} Y_i c_i$$

$$\left.\bar{h}^0\right|_{t=0} = \sum_{i=1}^{M} \left(Y_{i0} h_{i0}\right)$$