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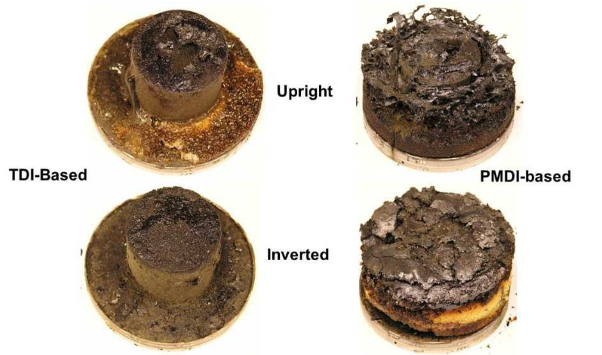

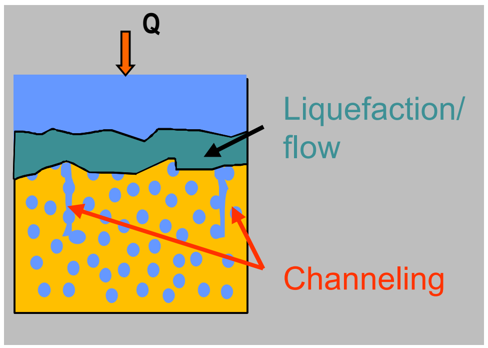

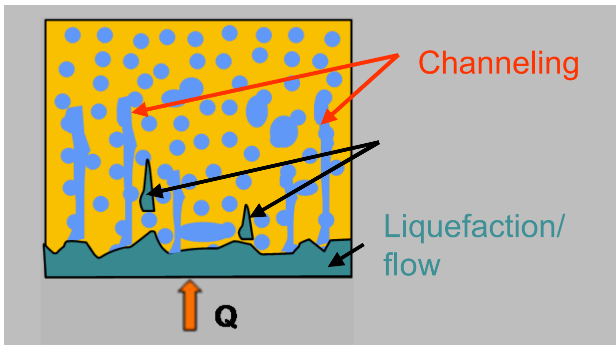

Interface Tracking For Modeling Thermal Decomposition of Polymer Foams

Victor E. Brunini

Ryan Keedy, Sarah Scott, David Noble, Amanda Dodd

U.S. DEPARTMENT OF ENERGY
NNSA National Nuclear Security Administration

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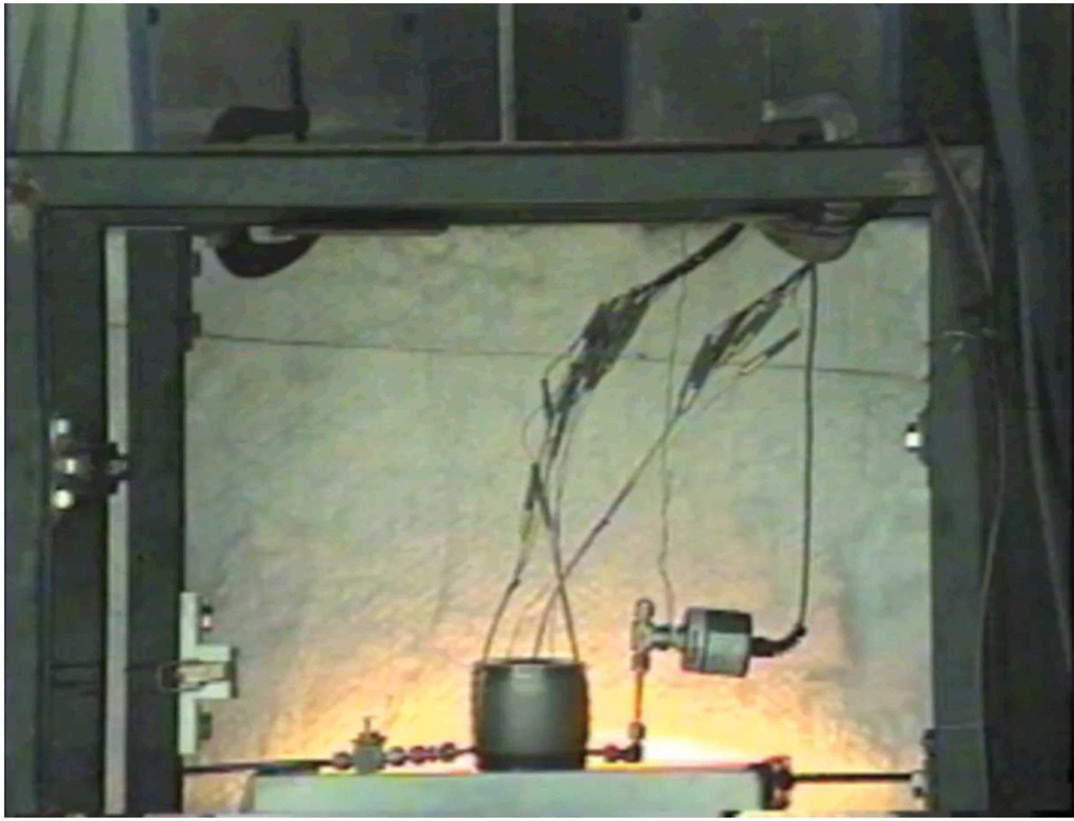
Outline

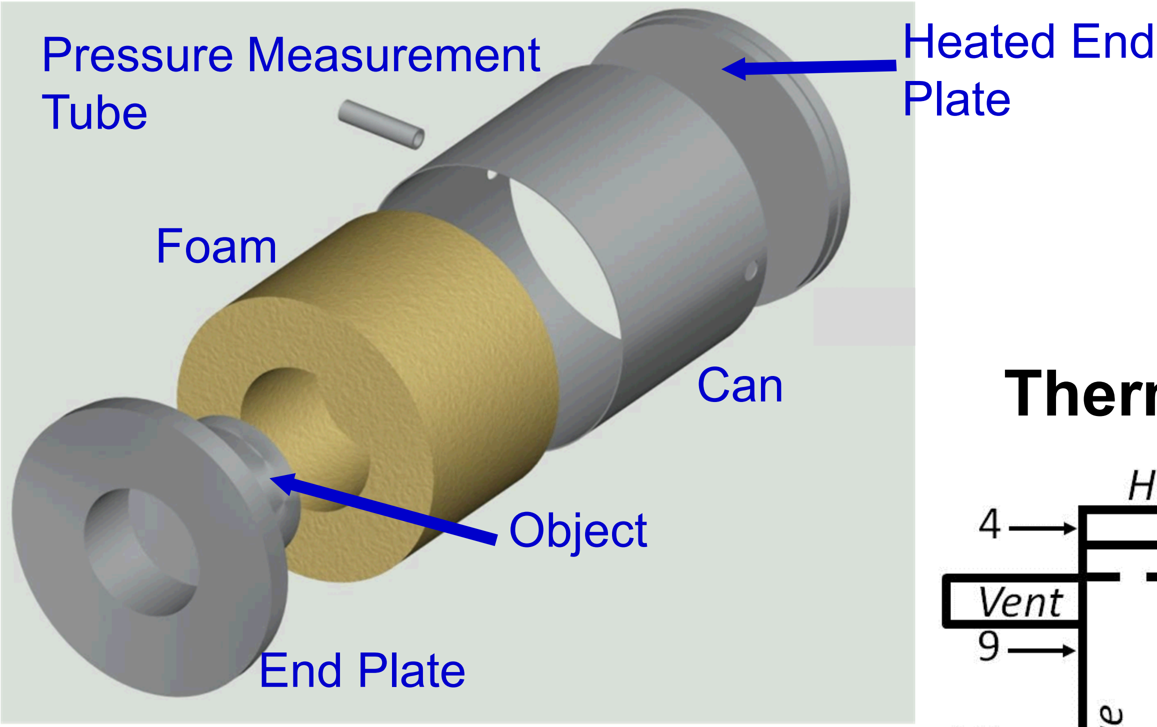
1. Motivation
2. Background and experimental understanding
3. Modeling approach
4. Preliminary model results
5. Conclusions + Future work

Foam Behavior in Fire Environments

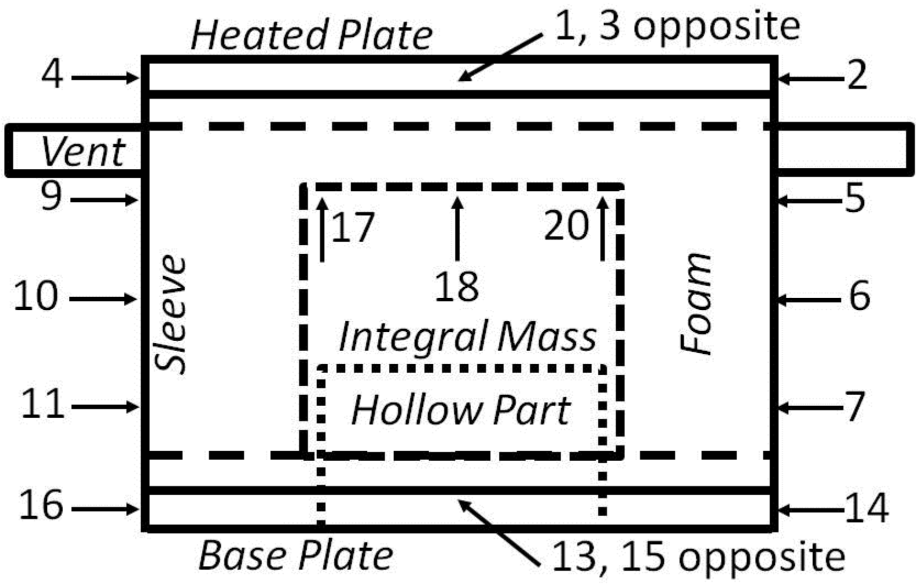
- Polymer foams provide thermal, mechanical, & electrical isolation in engineered systems
- In a fire foam decomposes and loses effectiveness as insulator
- Modeling techniques also applicable to other problems like ablation, carbon composite fires, etc.



Foam in a Can (FIC) Geometry

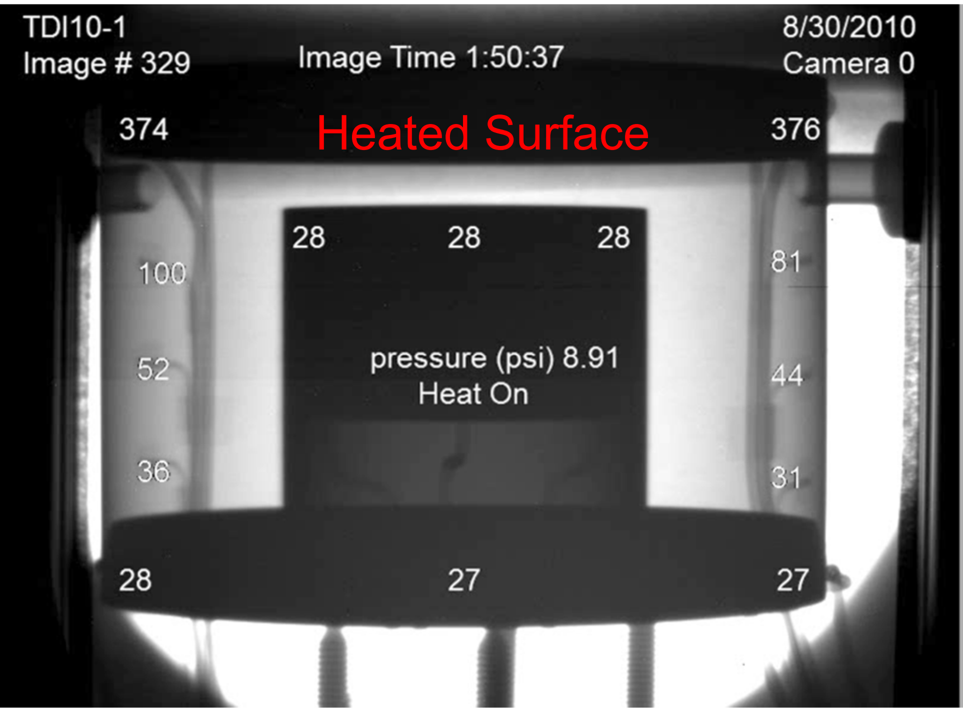


Thermocouple Locations

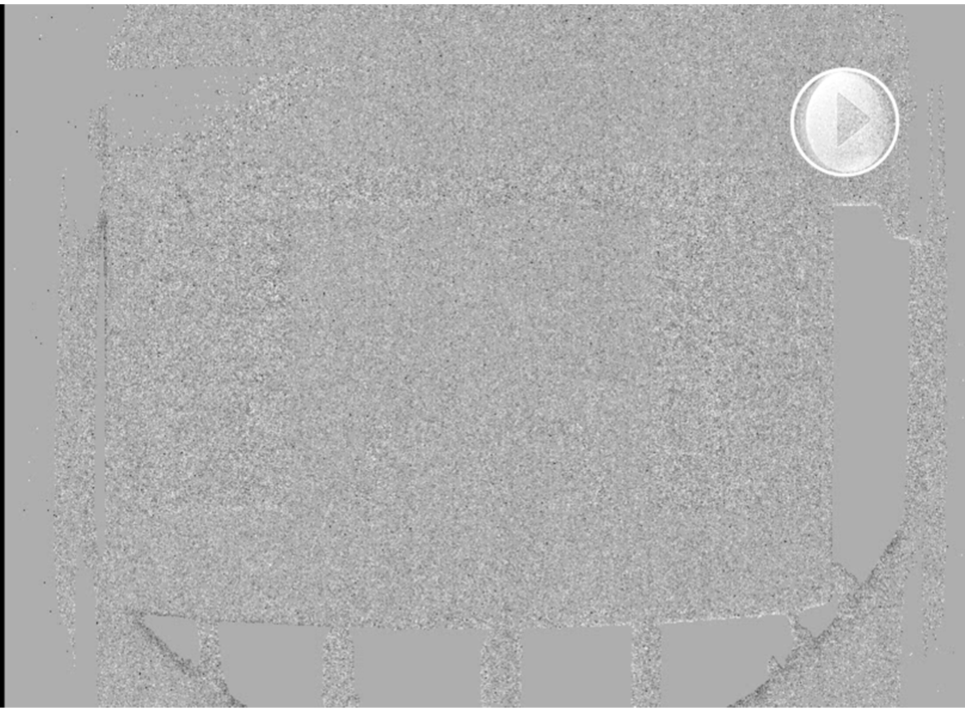


X-ray Video Captures Foam Decomposition Front

X-ray



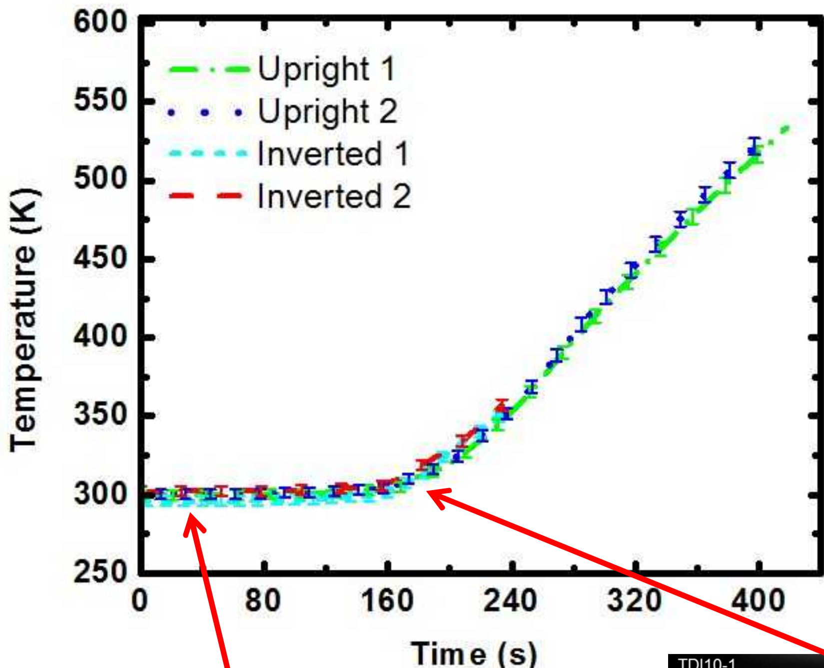
X-ray Frame Difference

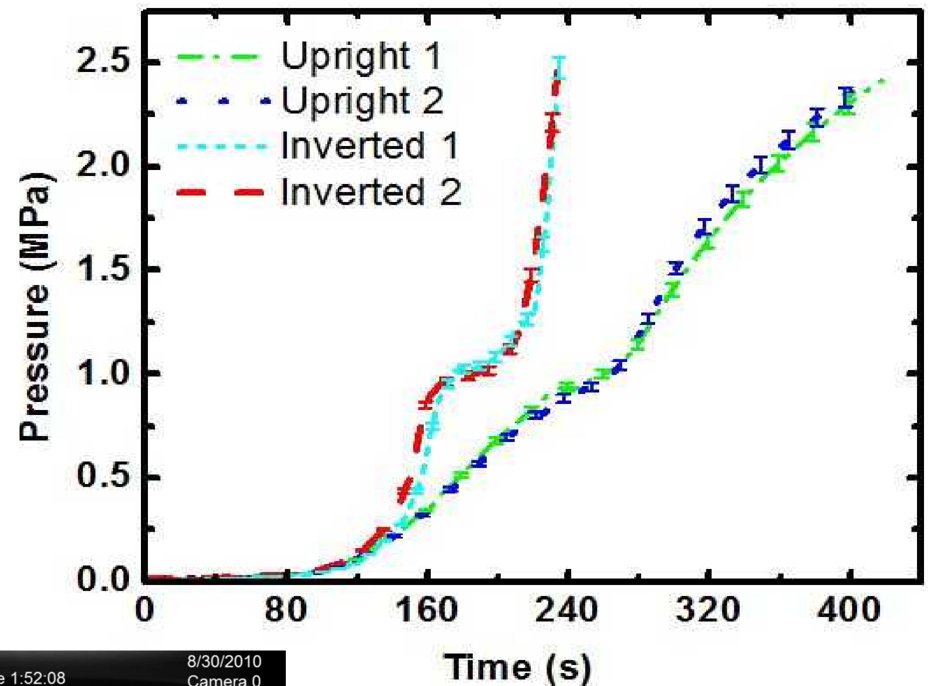


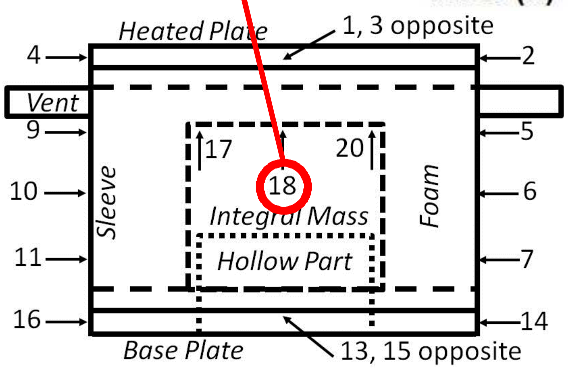
Upright 160 kg/m^3 TDI polyurethane foam
Heated at 150C/minute

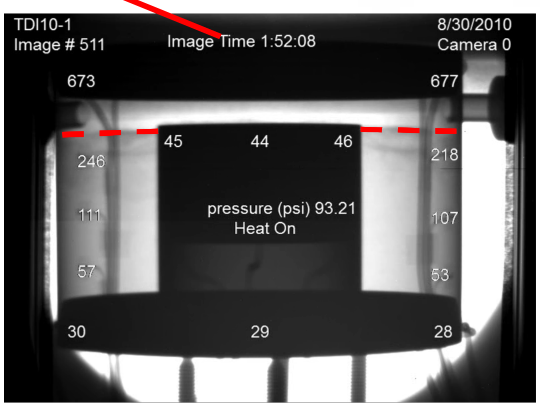
Experimental data courtesy of Ken Erickson

Orientation and Front Regression Important for Pressure and Temperature Response



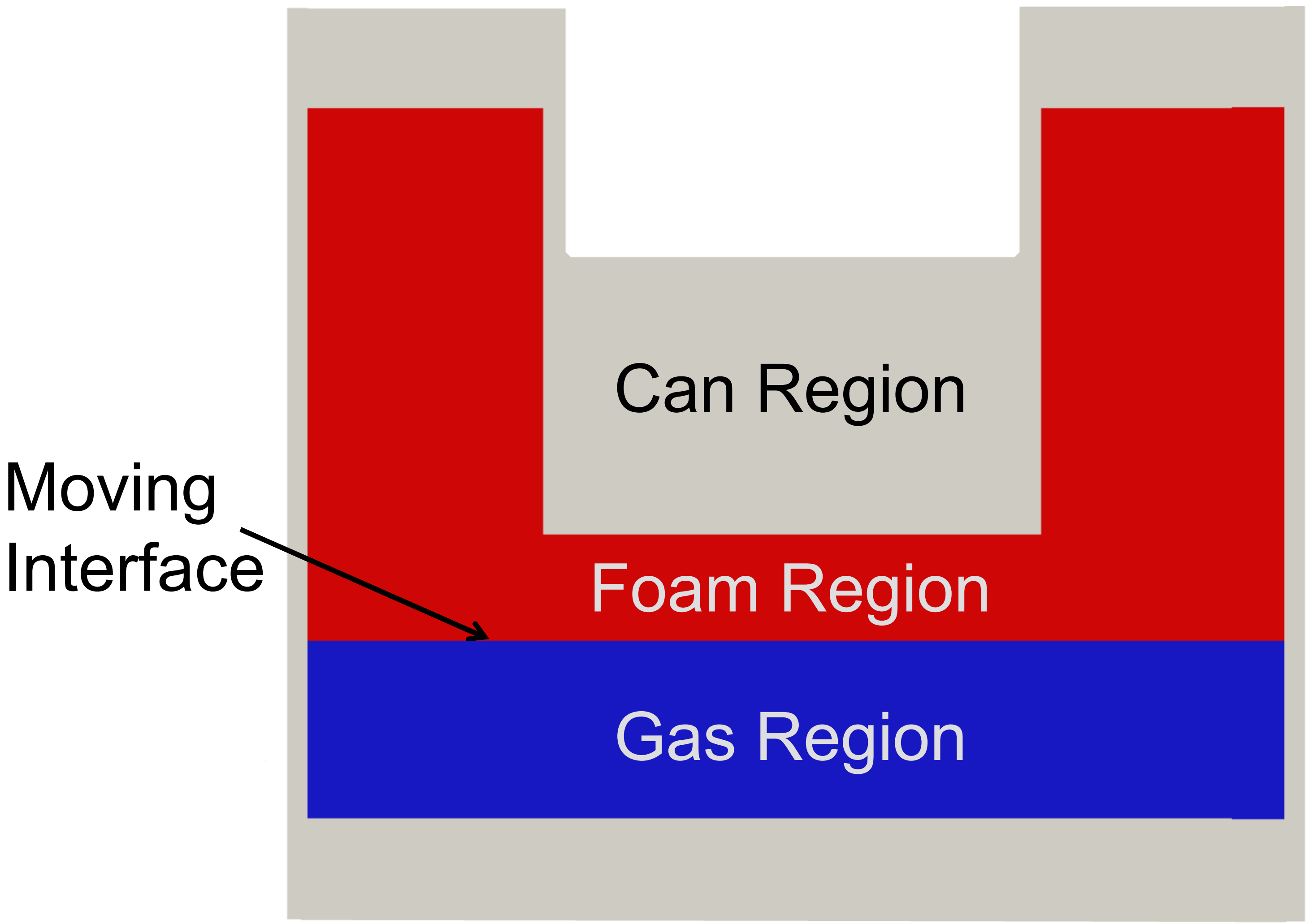






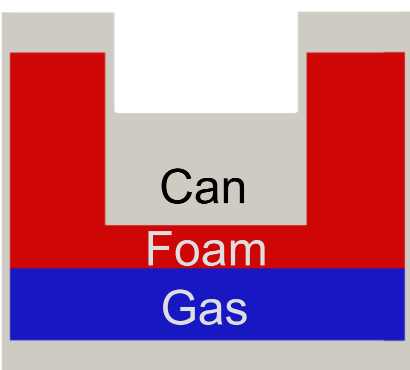
Experimental data courtesy of Ken Erickson

Model Domain Split Into 3 Regions



Modeled Physics

- **Gas Region**
  - Continuity
  - Momentum
  - Species
  - Energy
  - Enclosure radiation
- **Can Region**
  - Energy

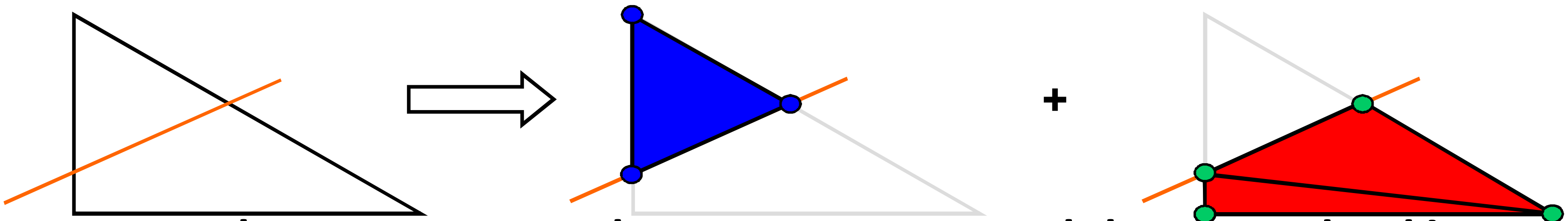


- **Foam Region**
  - Gas Phase
    - Darcy Mass Balance
    - Species
    - Energy
  - Solid Phase
    - Energy
    - Mass balance
    - Species

- All solved using SIERRA Multiphysics Module – Aria, implicit finite element code.
- Gas region uses control volume finite element method (CVFEM), remainder is Galerkin FEM.

Interface Motion

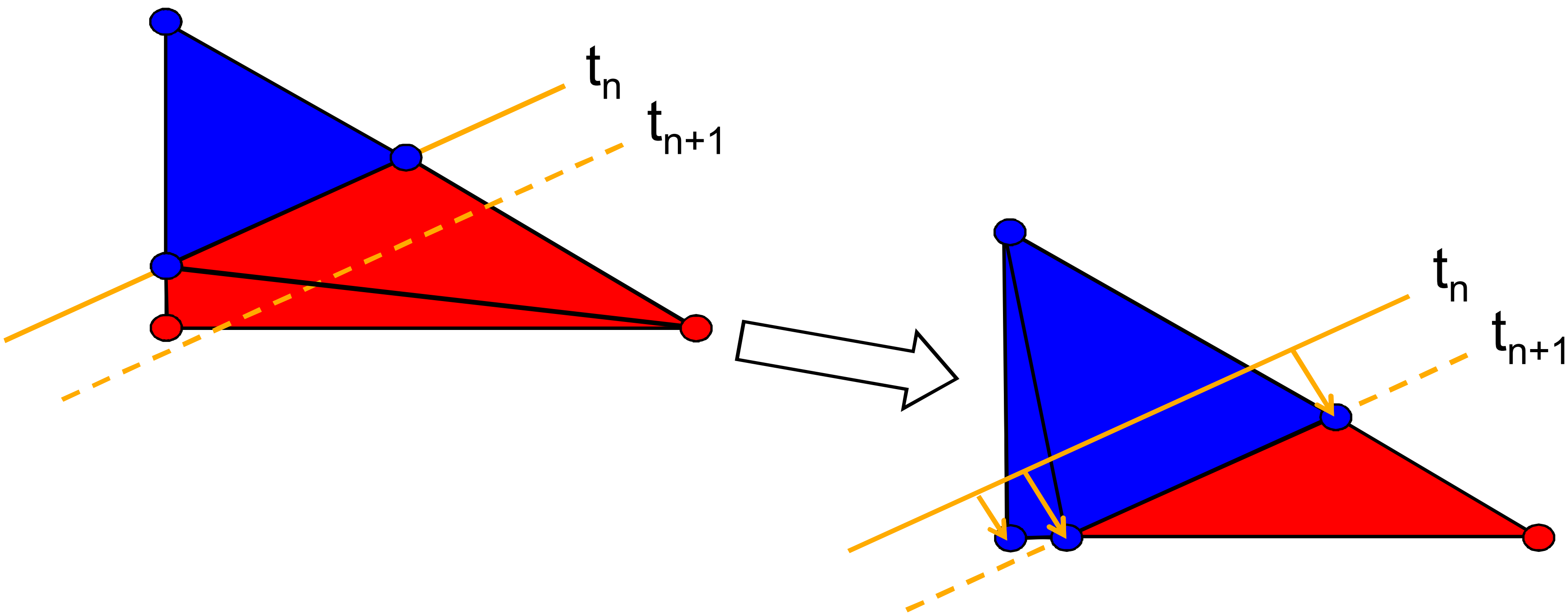
- Conformal Decomposition Finite Element Method (CDFEM)[1]



- No changes to element assembly needed!
- Supports different physics on either side of interface.
- Convert Foam -> Gas as it decomposes
  - Interface tracks 99% mass fraction isosurface of decomposition product

1. Noble et al, IJNMF 63 (2010)

A note on prolongation



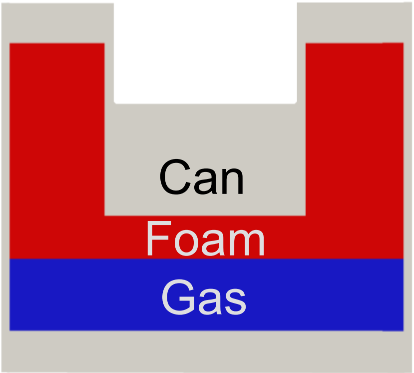
- At each time step newly created nodes and nodes that have moved or changed phase prolong their field values from the nearest interface location at the last time step.
- Time derivatives are adjusted appropriately using an ALE approach.[1]

1. Kramer, R.M.J. and Noble, D.R., IJNME 100(2014)

How can we solve this robustly and efficiently?

1. Fully monolithic Newton iteration
   - Excellent nonlinear convergence… if linear solves are successful
   - Poor scalability
2. Segregated solution scheme
   - How to split up equations?
   - Smaller matrices with fewer off-diagonal terms
   - Nonlinear convergence more challenging – Lots of trial + error to find usable set of equation systems

Segregated Solution Scheme



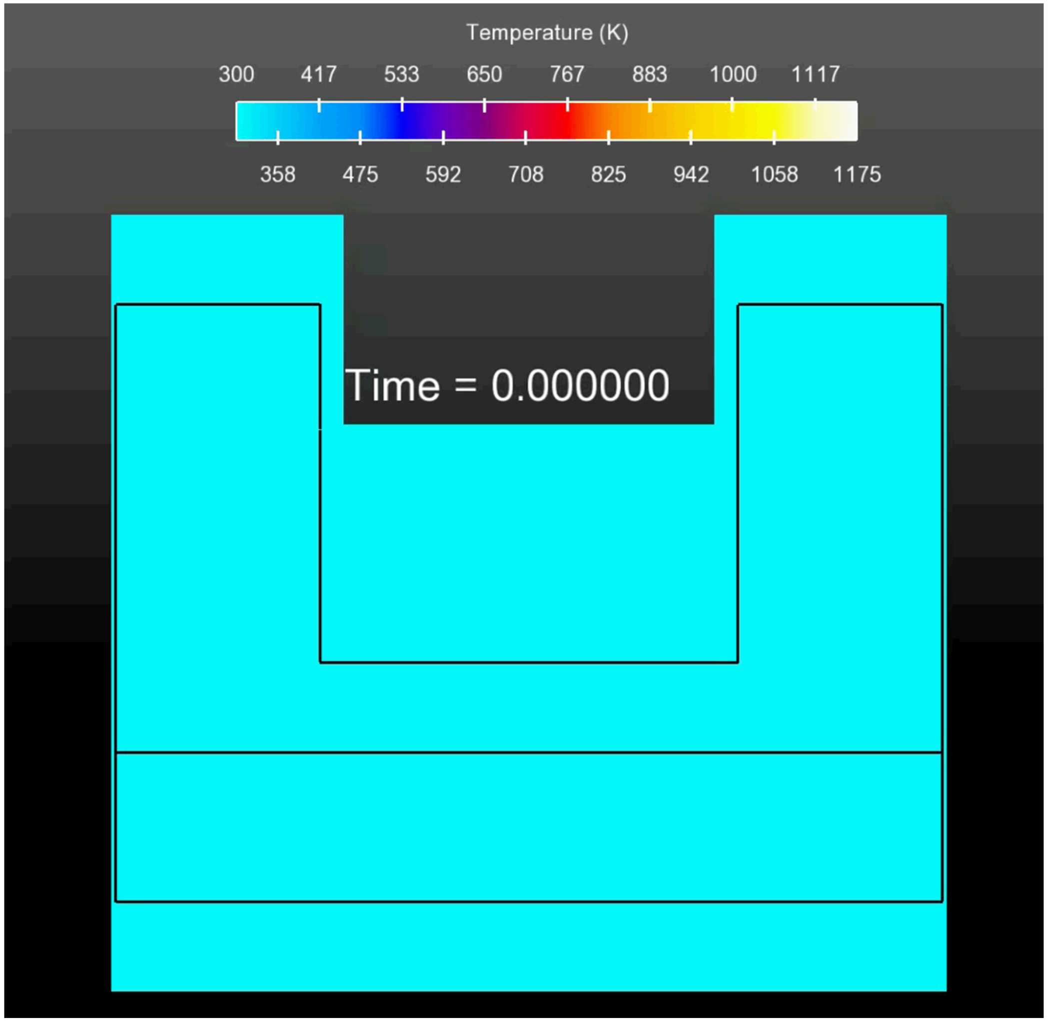
- Interface moves at the start of each time step

5 equation systems:

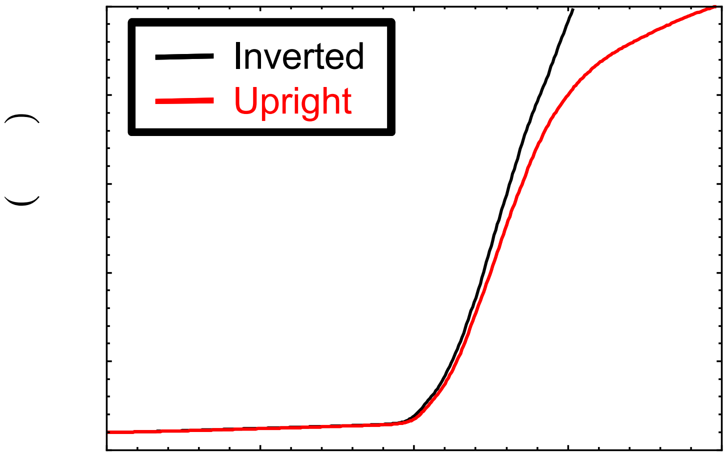
1. Solid Phase Mass Balance and Species
2. Continuity, Momentum, Darcy Mass Balance
3. Energy, Gas Phase Energy, Solid Phase Energy, Enclosure Radiation
4. Energy
5. Species, Gas Phase Species

- Loop until all equation system residuals < tolerance
  - Run 1-3 Newton iterations per equation system in each outer iteration.
- Essential to use same gas density from solution of 2 in solution of 3, 5.

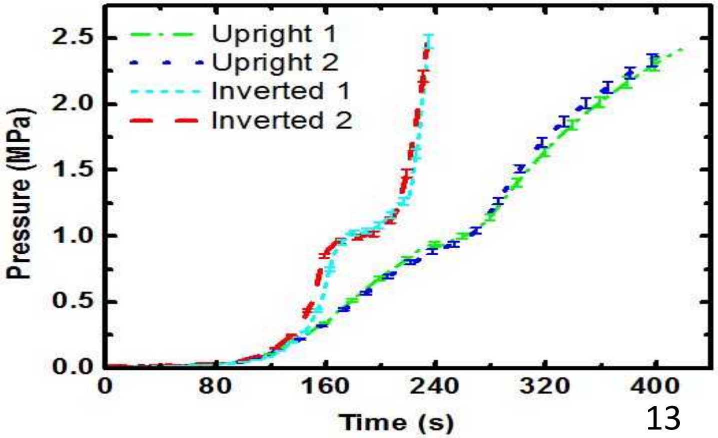
Model Captures Pressure Difference Between Upright and Inverted



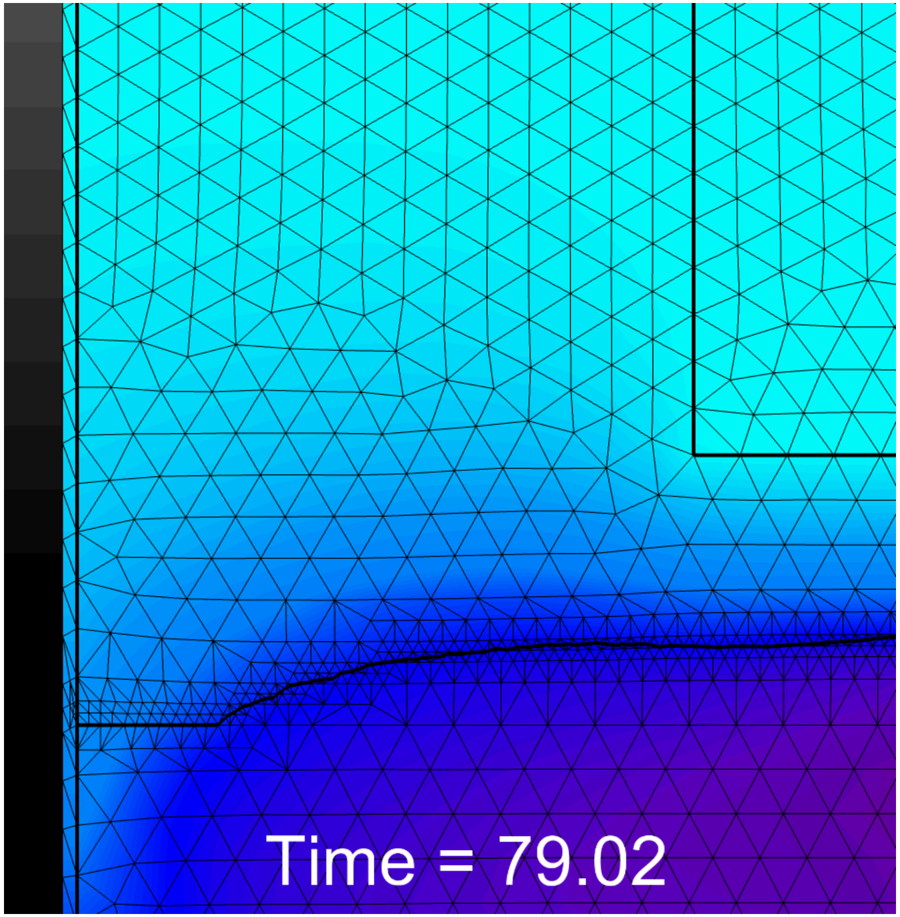
Model

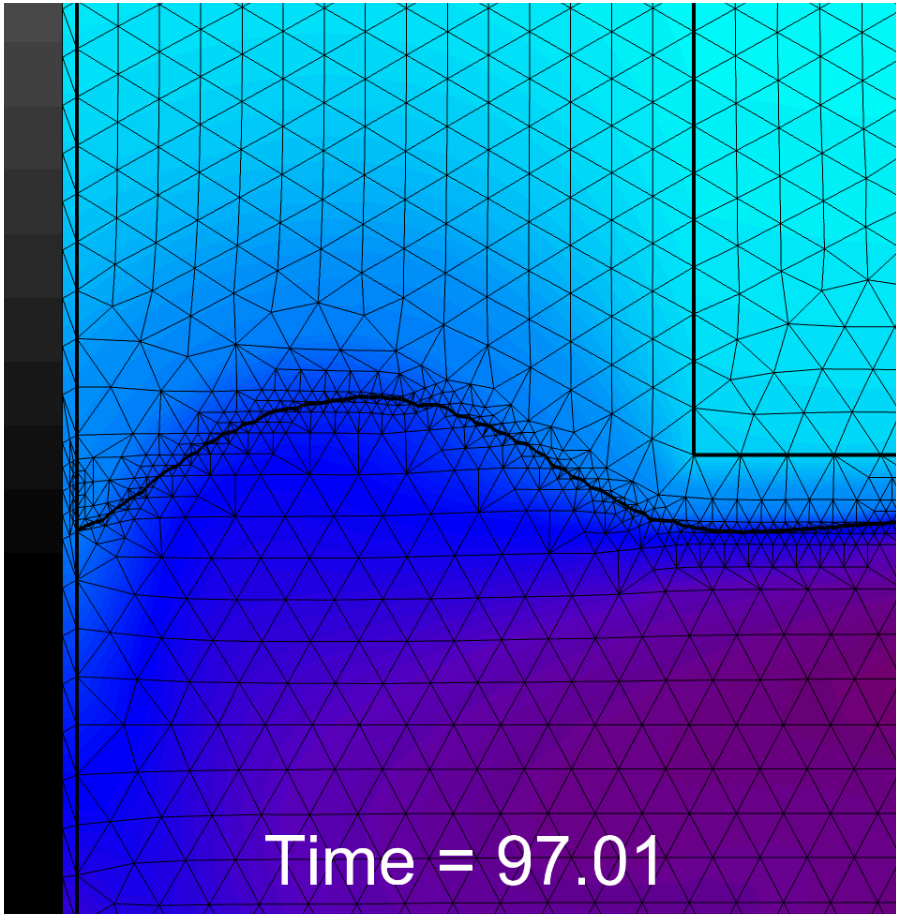


Experiment

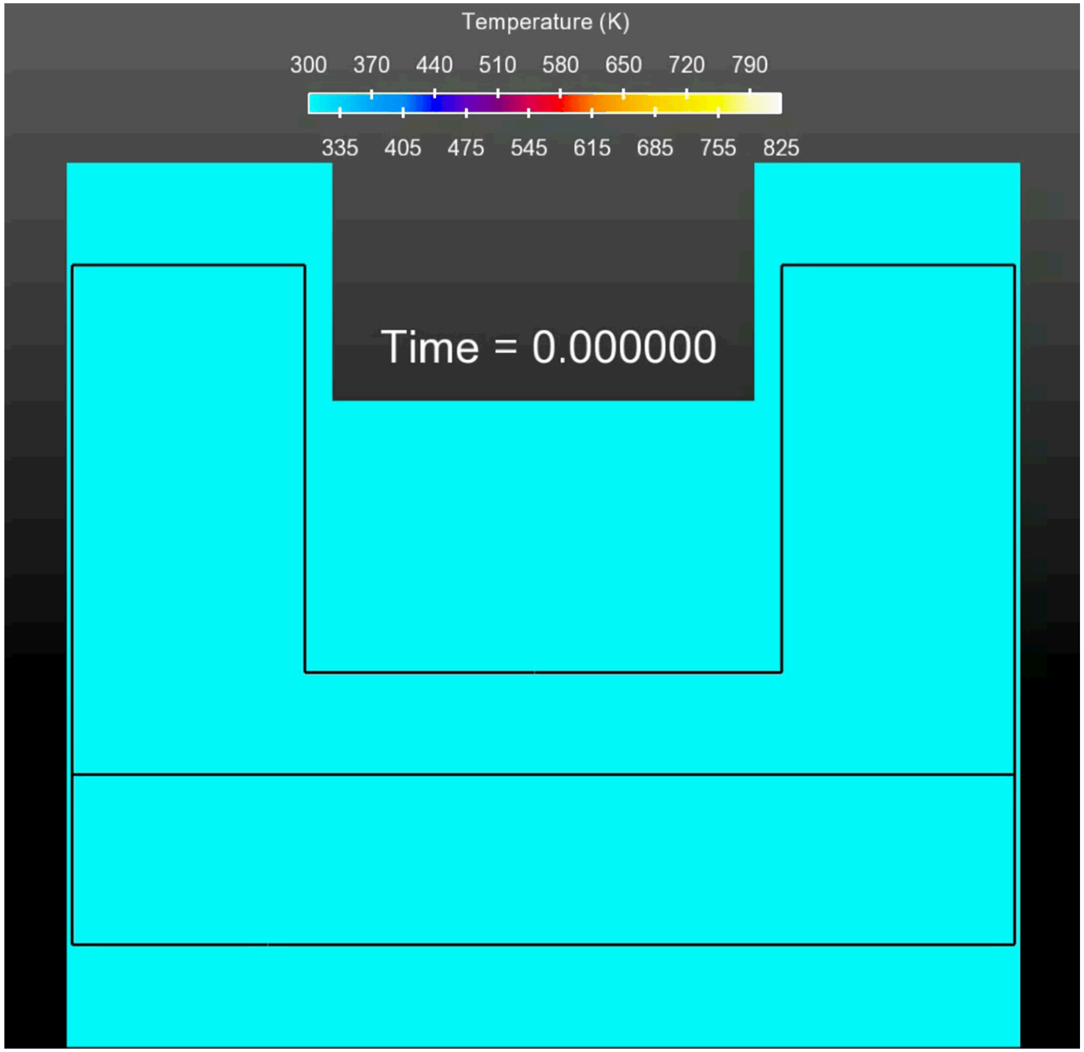


Adaptivity Improves Interface Decomposition





Adaptivity Improves Interface Decomposition



Conclusions and Future Work

- CDFEM is attractive for interface capturing in multiphysics simulations
  - Different equations/fields on either side of interface
  - Standard element and boundary condition assembly everywhere

- 3D
- Adaptivity robustness
- Incorporating liquefaction and flow of foam.

Backup Slides

Modeling Heat Transfer to Components and Pressurization in Dynamic Geometries

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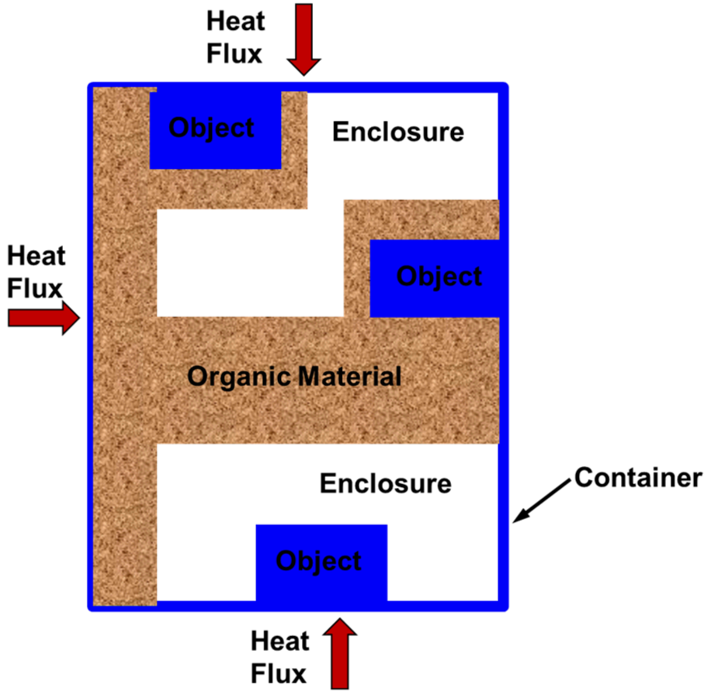
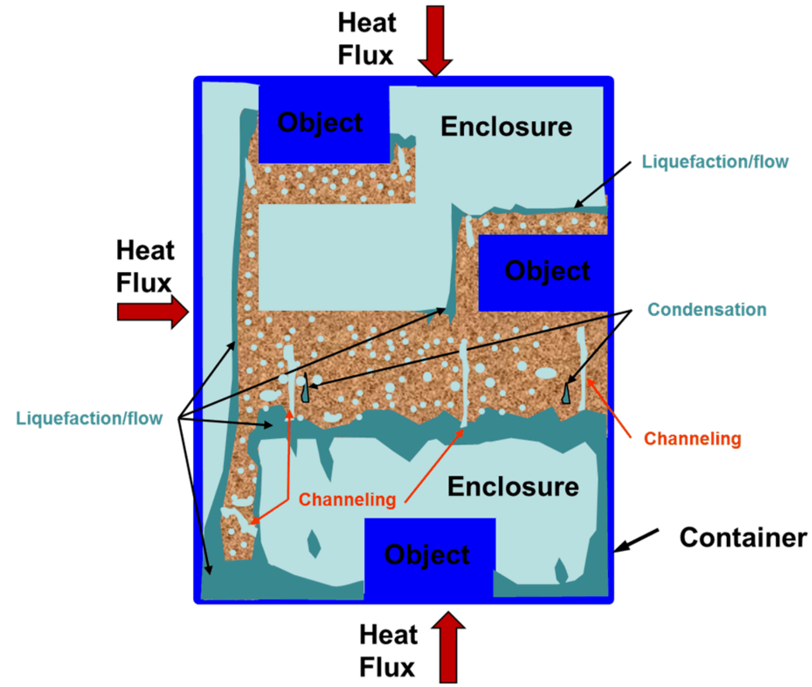
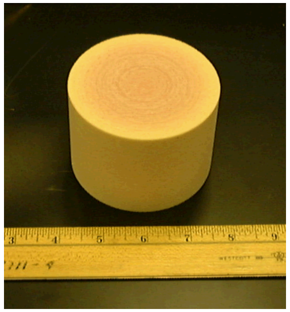
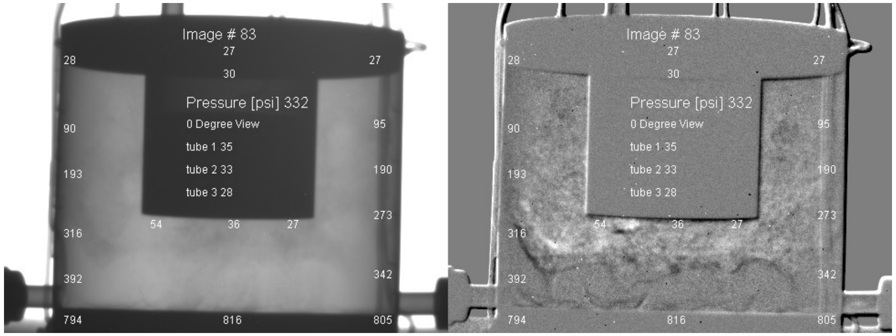
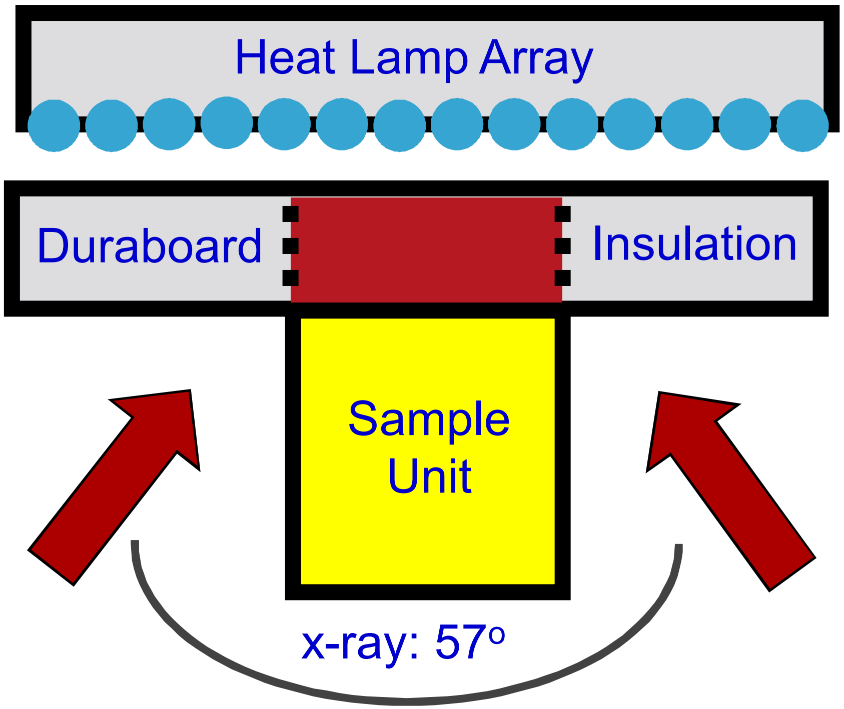




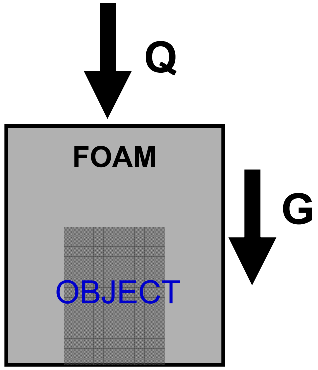




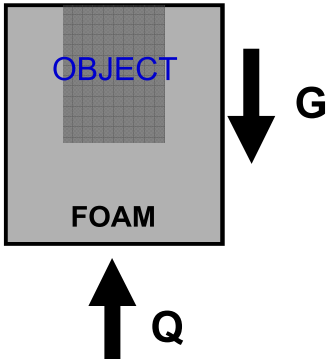
FIC Experimental Setup



Experiments Repeated in Different Orientations



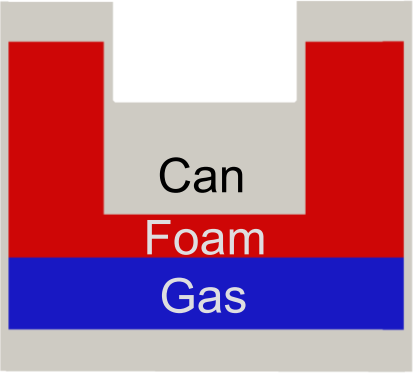
Upright – 0°



Inverted – 180°

Coupled Heat Transfer Between Foam and Can

- Foam-Can Interface
  - Heat transfer between can and both solid and gas phases



Foam

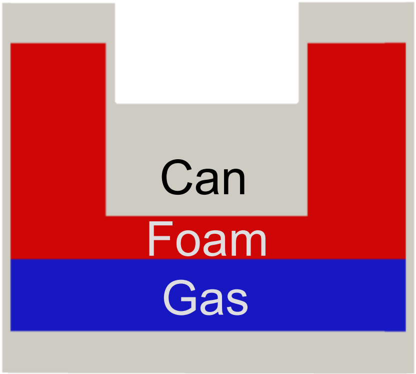
$$T_{\text{solid}} = T_{\text{can}}$$
$$T_{\text{gas}} = T_{\text{can}}$$

Can

$$\vec{q} \cdot \hat{n} = (\vec{q}_{\text{solid}} + \vec{q}_{\text{gas}}) \cdot \hat{n} + \alpha (T_{\text{can}} - T_{\text{solid}})$$

Coupled Heat Transfer Between Gas and Can

- Gas-Can Interface
  - Heat transfer between gas and can



Gas

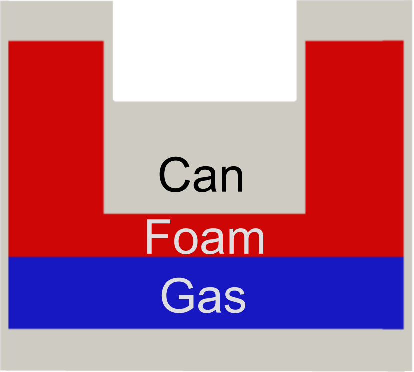
$$T_{\text{gas}} = T_{\text{can}}$$

Can

$$\vec{q}_{\text{can}} \cdot \hat{n} = \vec{q}_{\text{gas}} \cdot \hat{n} + \alpha(T_{\text{can}} - T_{\text{gas}})$$

Coupled Flow Between Foam and Gas

- Foam-Gas Interface
  - Coupled gas flow, species transport, and energy transport



Gas

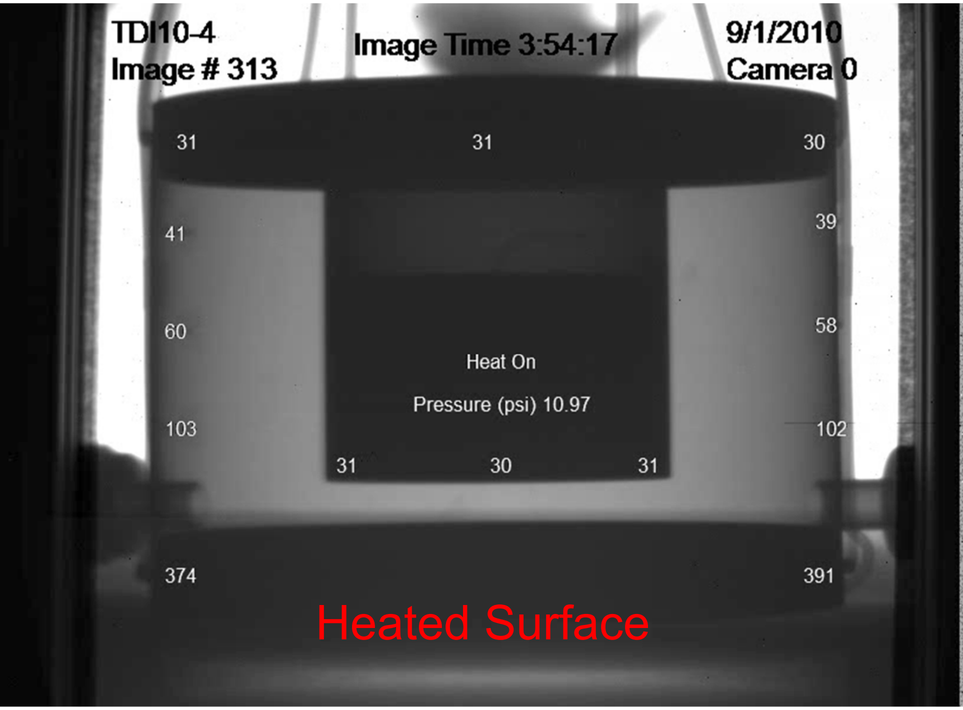
$$\vec{J}_{\text{gas}} \cdot \hat{n} = \vec{J}^{\text{foam}}_{\text{gas}} \cdot \hat{n} + \alpha(X_{\text{gas}} - X_{\text{foam}})$$

Foam

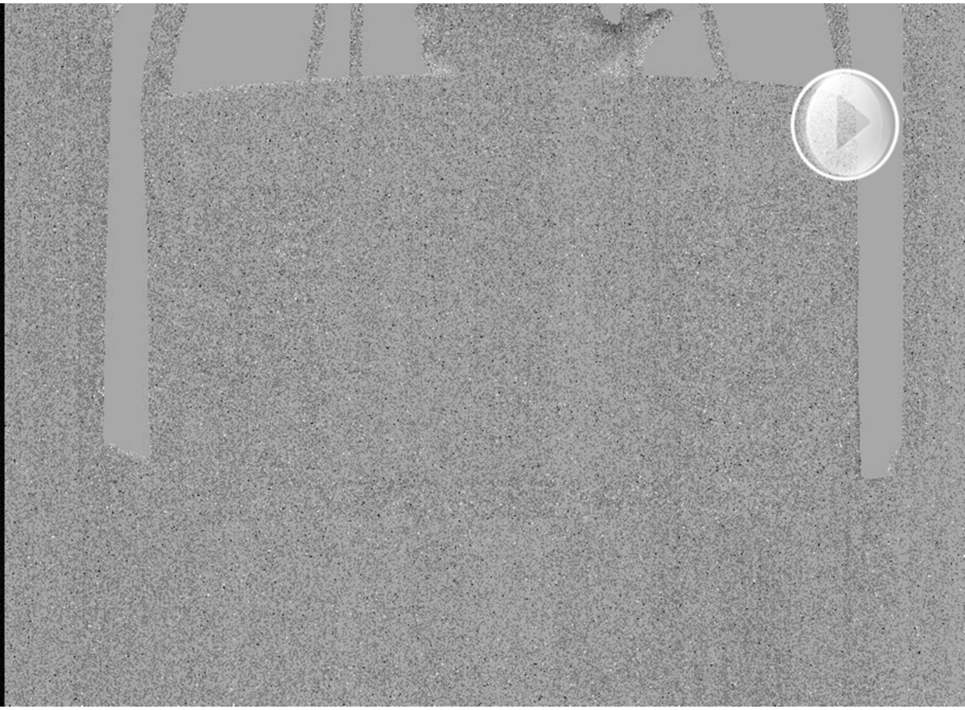
$$\vec{J}^{\text{foam}}_{\text{gas}} \cdot \hat{n} = \vec{J}_{\text{gas}} \cdot \hat{n} + \alpha(X_{\text{foam}} - X_{\text{gas}})$$

X-ray Video Captures Foam Decomposition Front

X-ray



X-ray Frame Difference



Inverted 160 kg/m^3 TDI polyurethane foam
Heated at 150C/minute

Decomposition Front Motion Controls Radiative Heat Transport