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Sandia National Laboratories

Uncertainty Quantification for Experimental and Model Results of Pyrolyzing and Pressurizing Polyurethane Foam at Varying Heating Rates

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

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Motivation

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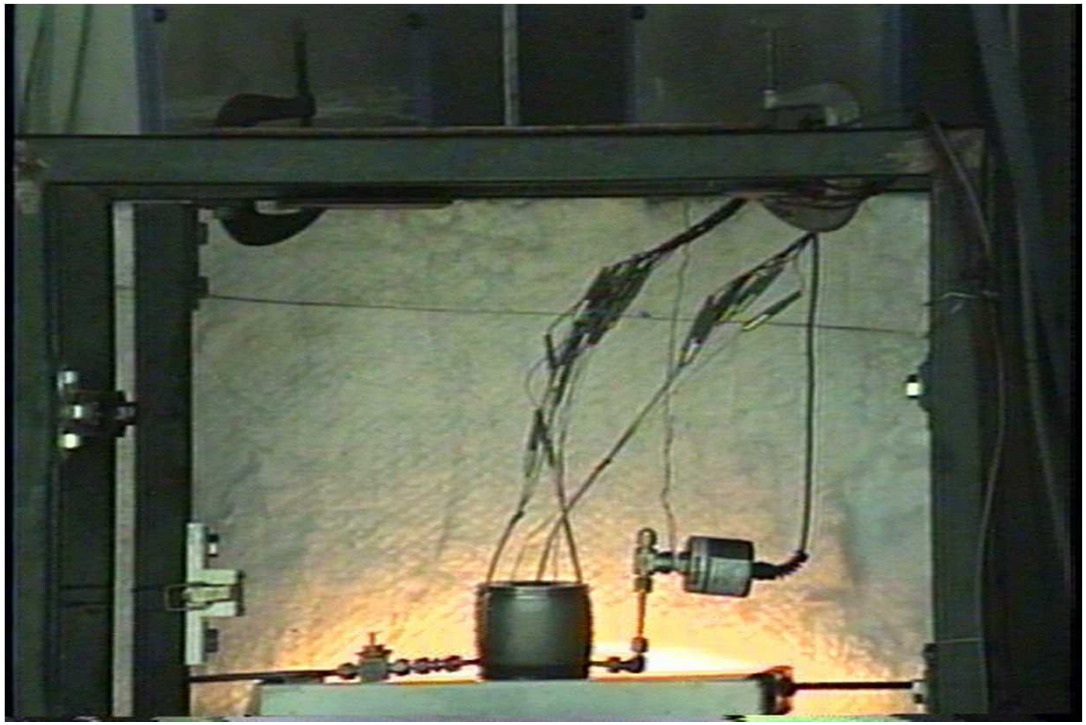
- Electronic devices need protection from mechanical and thermal shocks
  - Foams, ex PMDI polyurethane
- Foams pyrolyze at low temperatures
  - Fire environment
  - In sealed systems, can cause pressurization
- Need a computer simulation to model heat transfer and pressurization
  - Medium scale experiments for validation

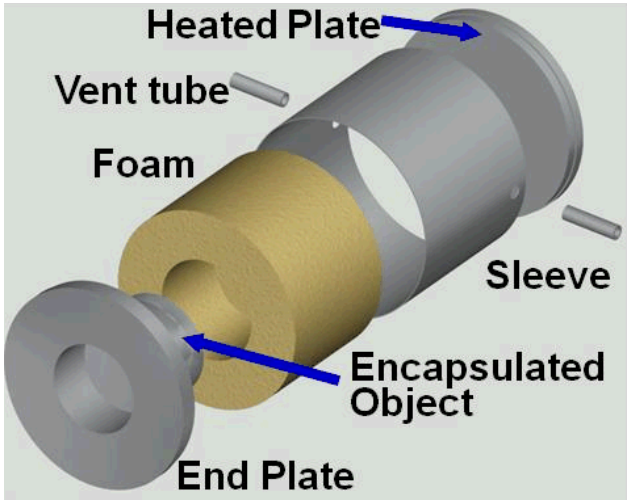
Foam in a Can



Removable Epoxy Foam heated to 900 C at a rate of 200 C/min

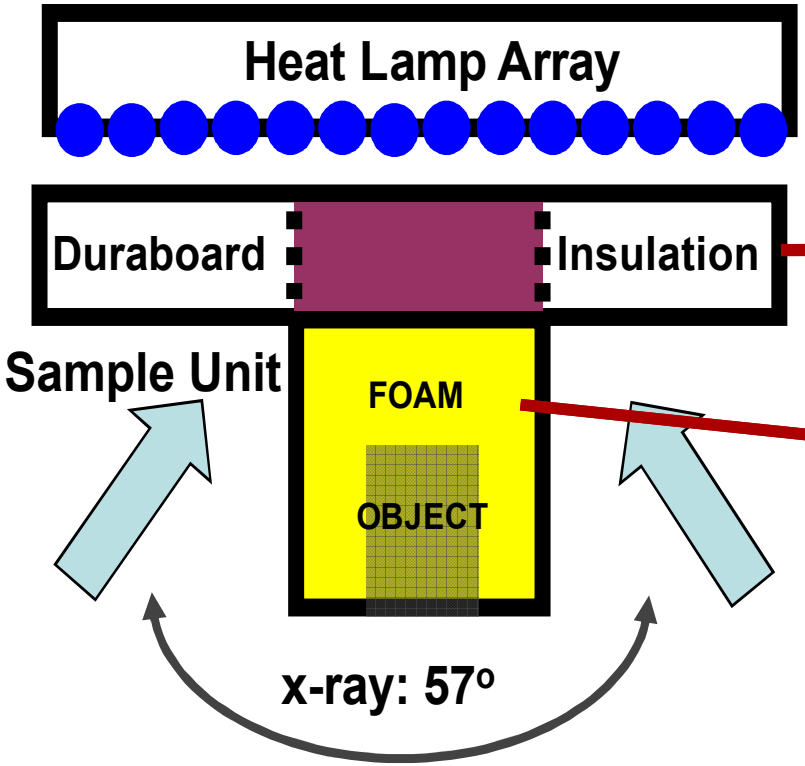
- Medium Scale Experiment
  - Foam in a Can (FIC)

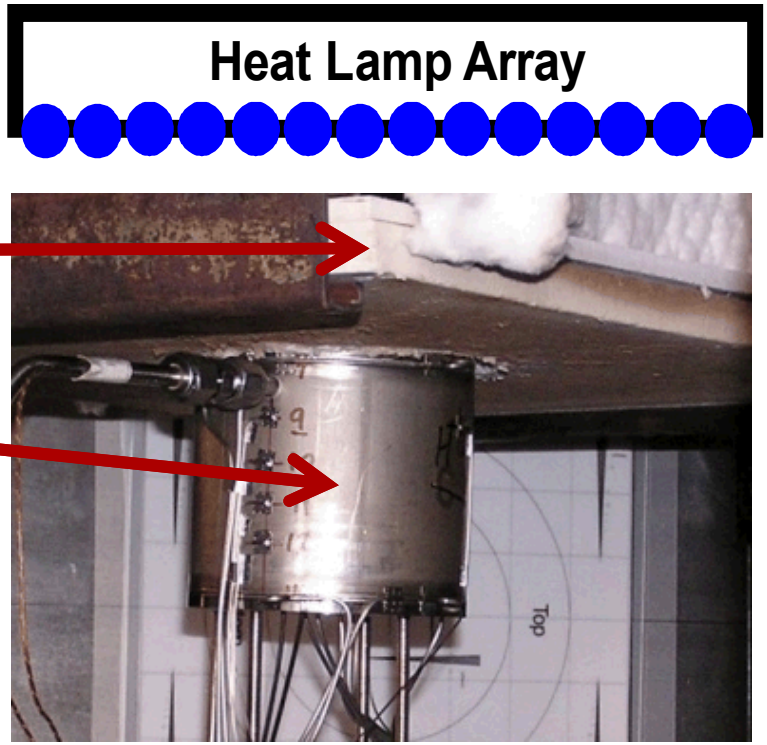
Foam in a Can Experiment



- Data Set:
  - 320 kg/m^3 PMDI polyurethane foam (rigid, closed cell)
  - Heated to 800 C at a rate of 150 C/min and 50 C/min.
  - 16 sets collects, representative data is shown
- Can dimensions are approximately
  - Diameters: 9 cm
  - Length: 6.5 cm
  - Wall Thickness: 0.5 mm

Foam in a Can Experiment

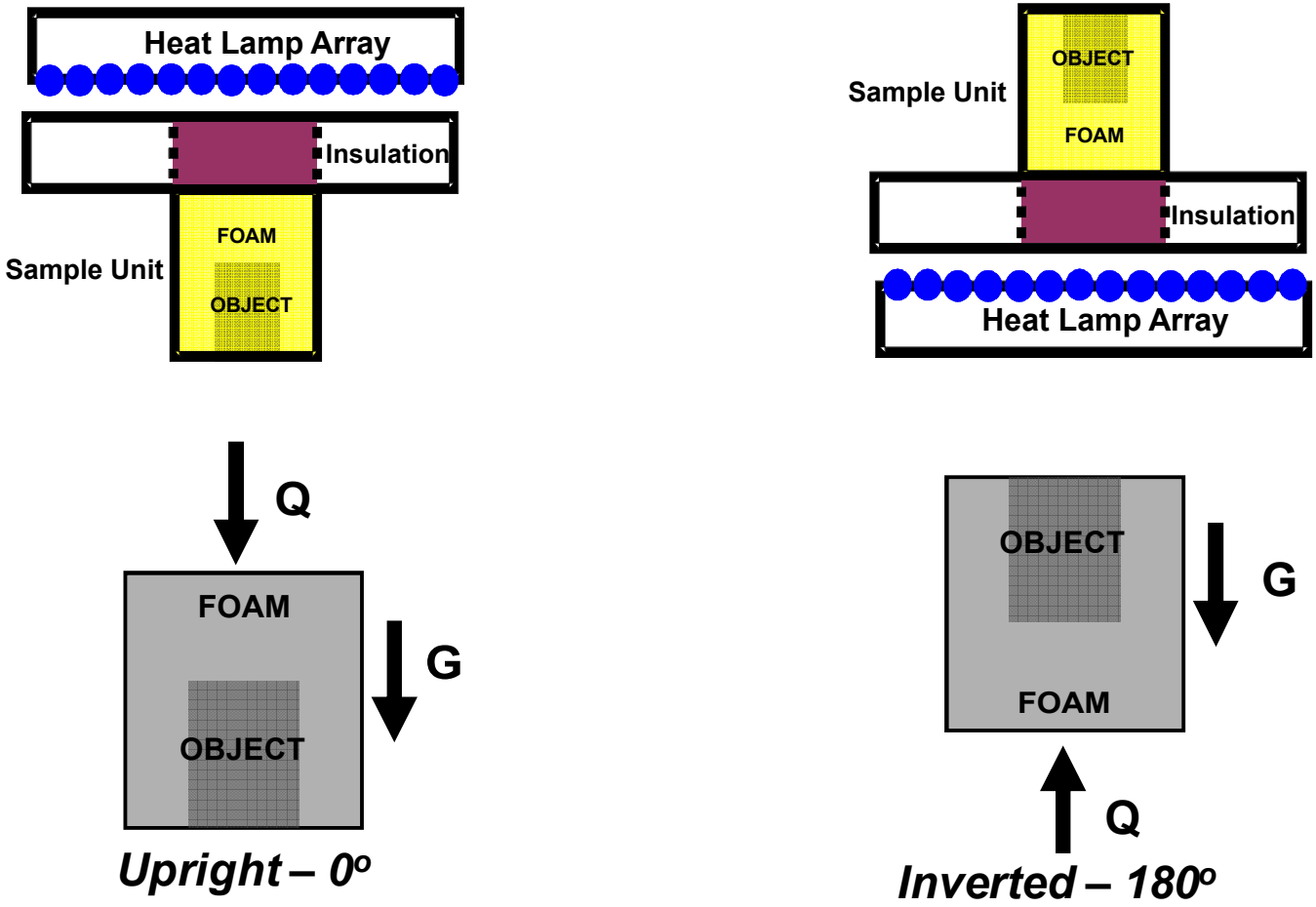




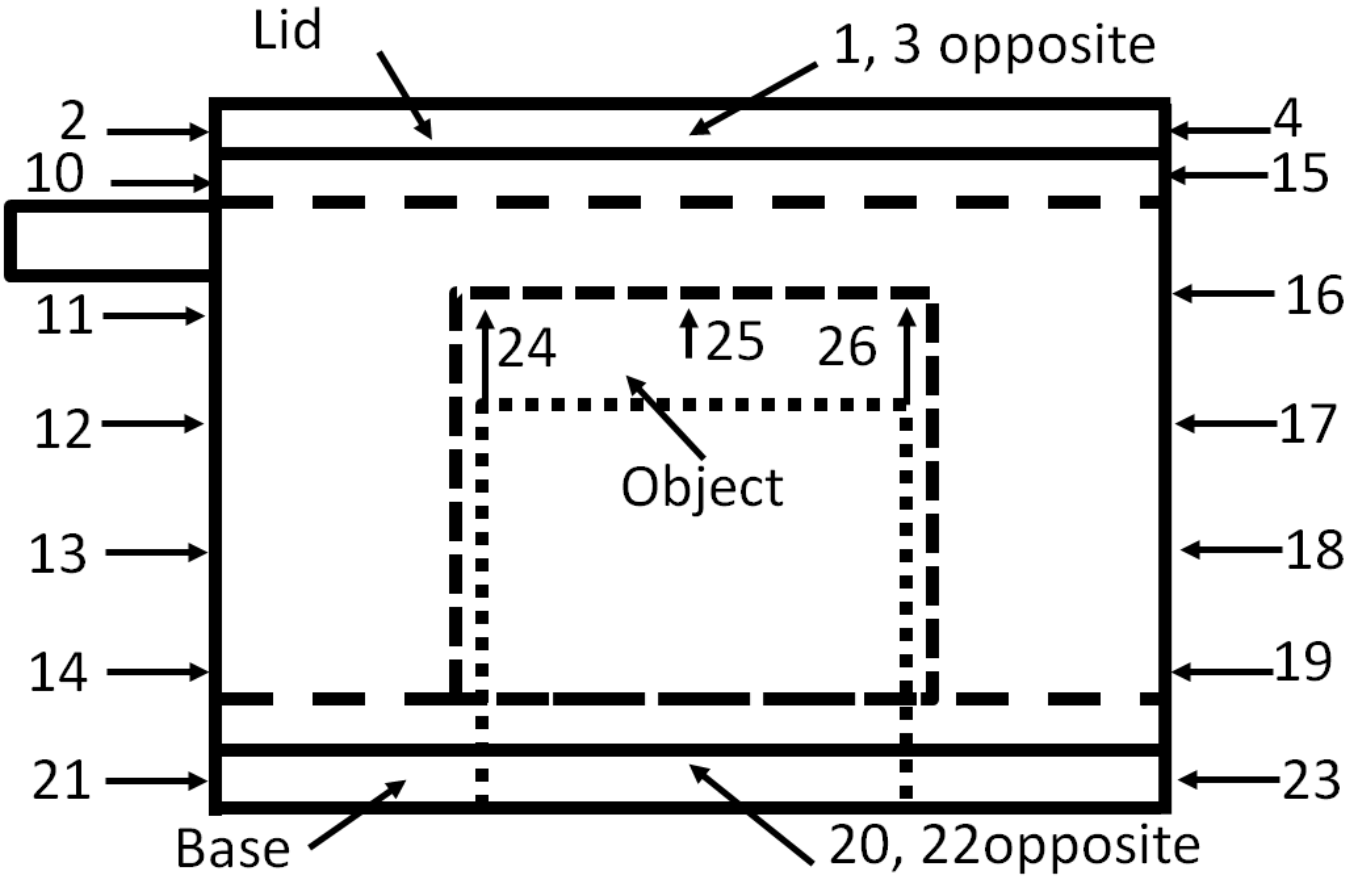
- Monitor pressure inside the can
  - X-Rays to view can interior
  - Experiments run to breach

Foam in a Can Experiment

- Experiment conducted in upright and inverted orientations
  - Material bulk movement towards or away from heat source



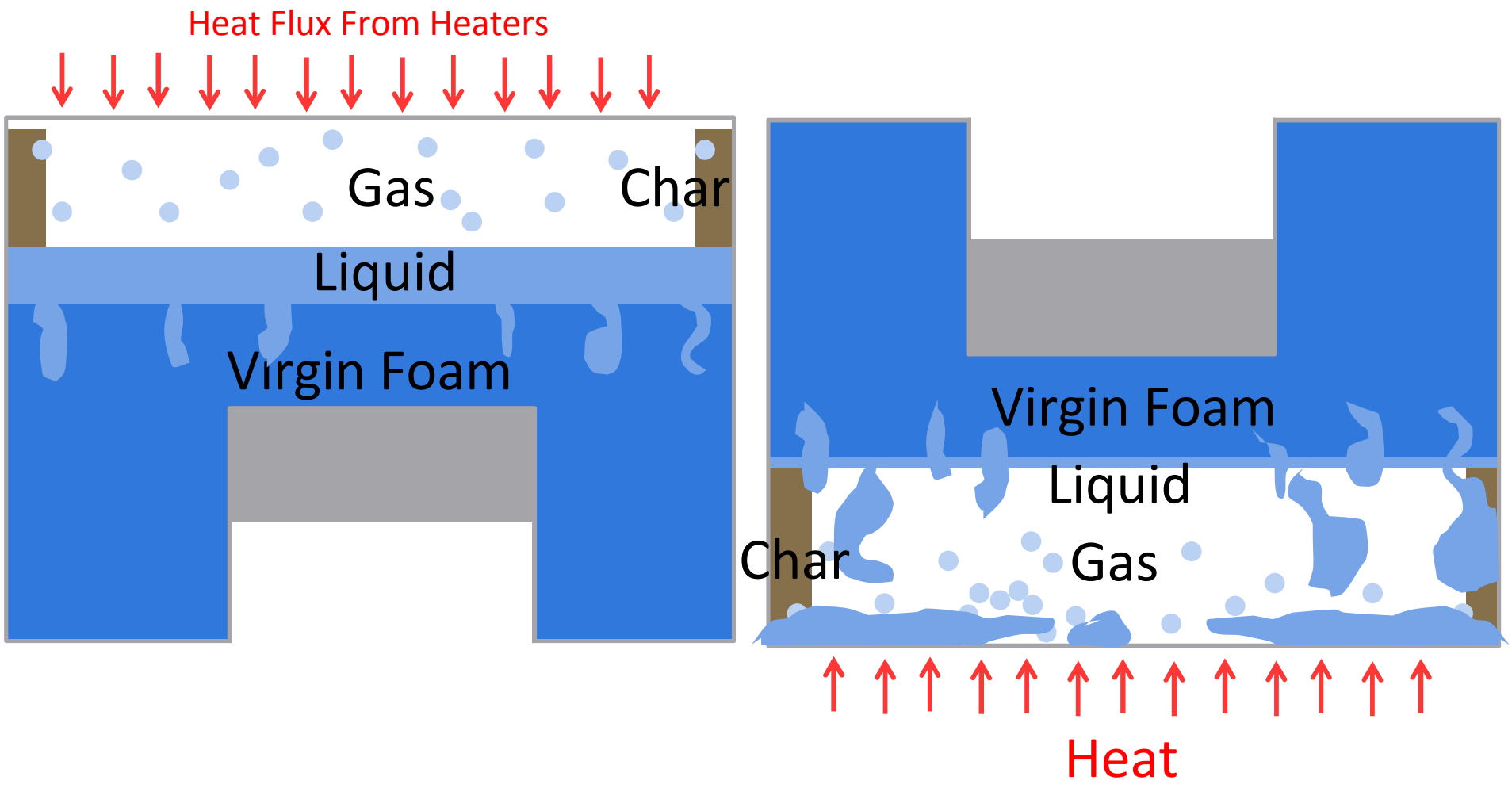
Foam in a Can Experiment



Temperature is monitored on the top, along the sides, and on the bottom of the can as well as on an embedded object.

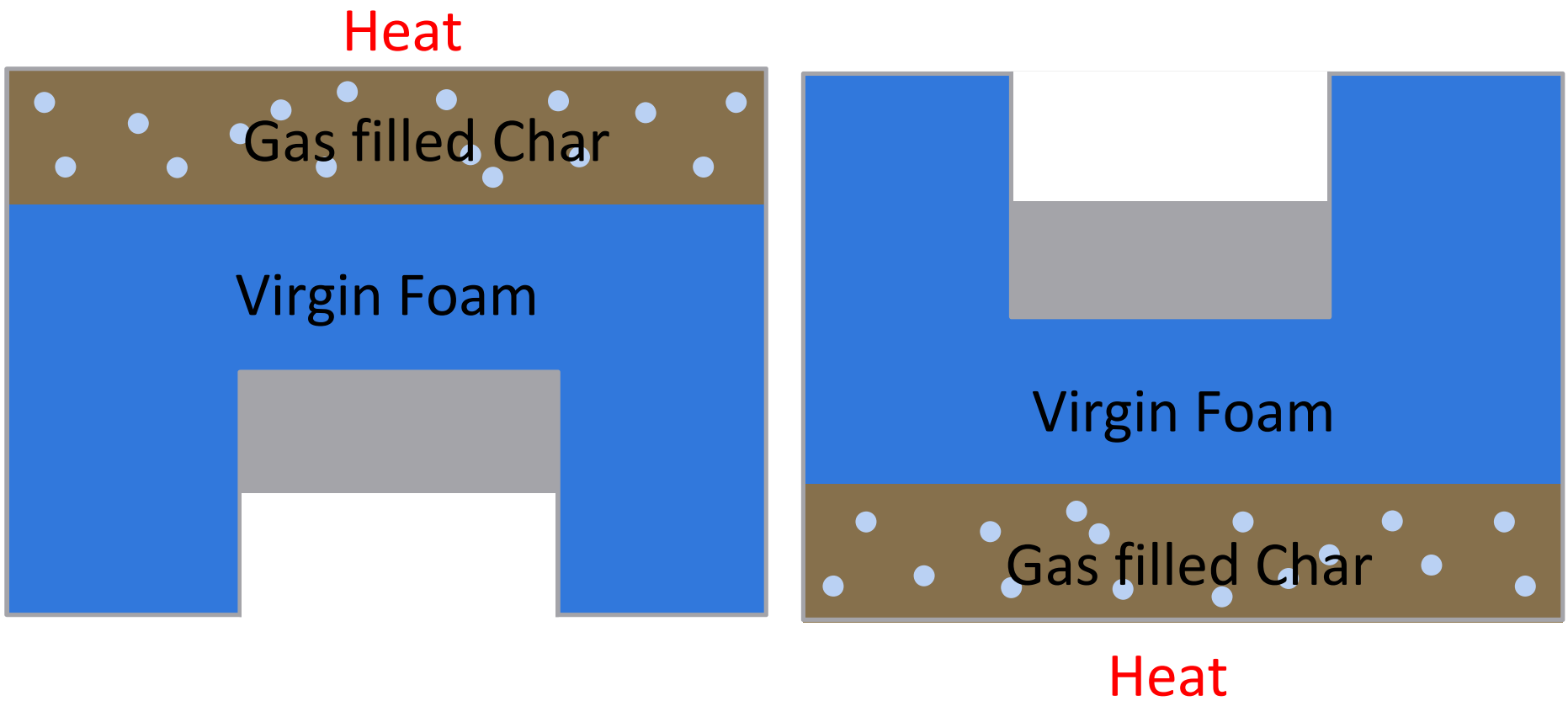
Decomposing Foam

Virgin Material + Heat → Decomposition Products (solids, liquids, gases)

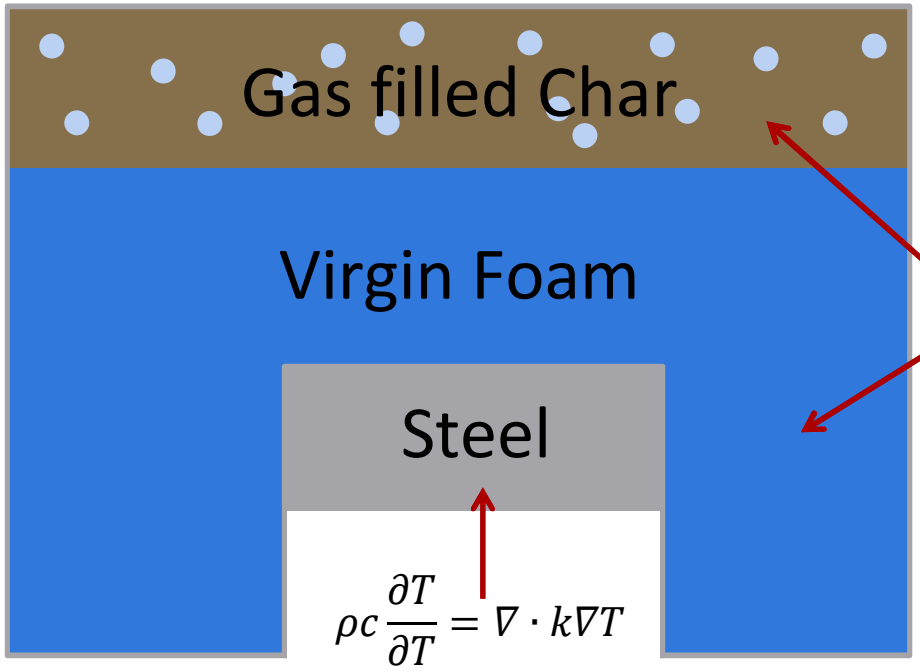


Model

Virgin Material + Heat → Decomposition Products (solids, gases)



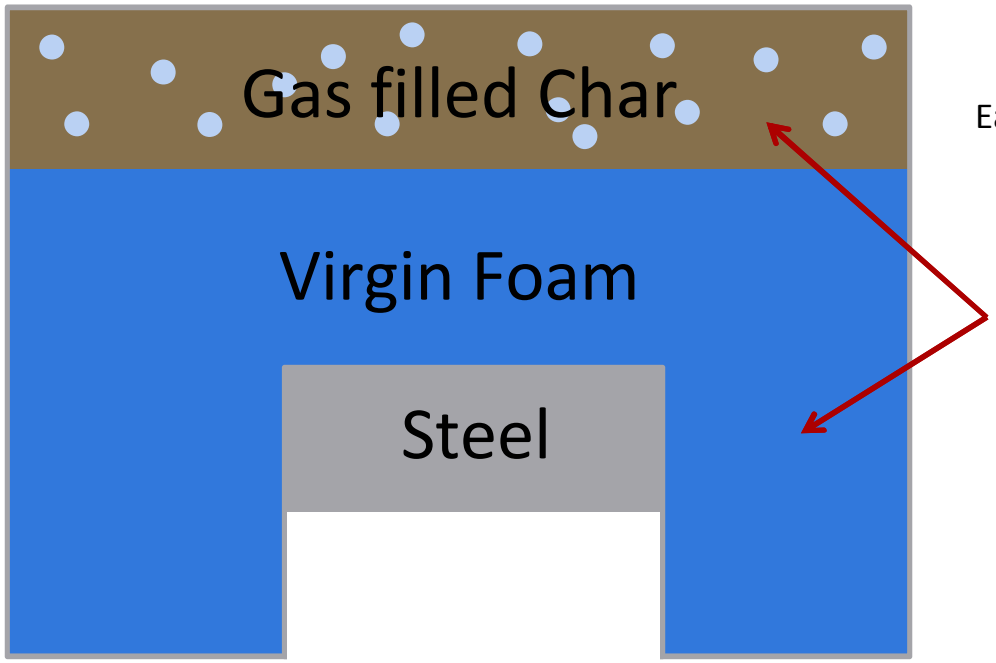
Current Model – Heat Transfer



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

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

Current Model – Pyrolysis



A polymer is composed of A_i moieties

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

Each of the A_i moieties will decompose by different mechanisms to form B_{ij} products at a rate of r_i

$$A_i \overset{r_i}{\rightarrow} \xi_{i1} B_{i1} + \xi_{i2} B_{i2} + \cdots + \xi_{in} B_{in}$$

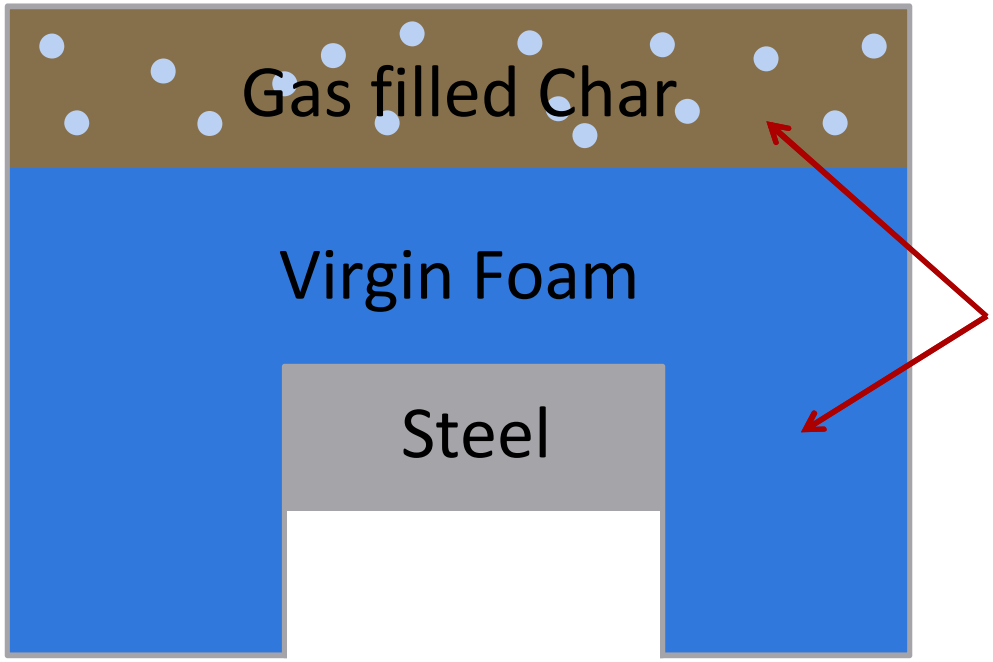
The rate is modeled as an Arrhenius type reaction (k_i) and the mass fraction of unreacted moieties A_i (w_{A_i})

$$\frac{dw_{A_i}}{dt} = -k_i w_{A_i} = -r_i \qquad k_i = k_i^0 e^{\frac{-E_a}{RT}}$$

The production of B_{ij} products is also controlled by this rate.

$$\frac{d\bar{\rho}_{B_{ij}}}{dt} = \rho_B^0 \frac{\xi_{ij} w_i^0}{\bar{M}_{B_{ij}}} k_i w_{A_i}$$

Current Model – Pressurization



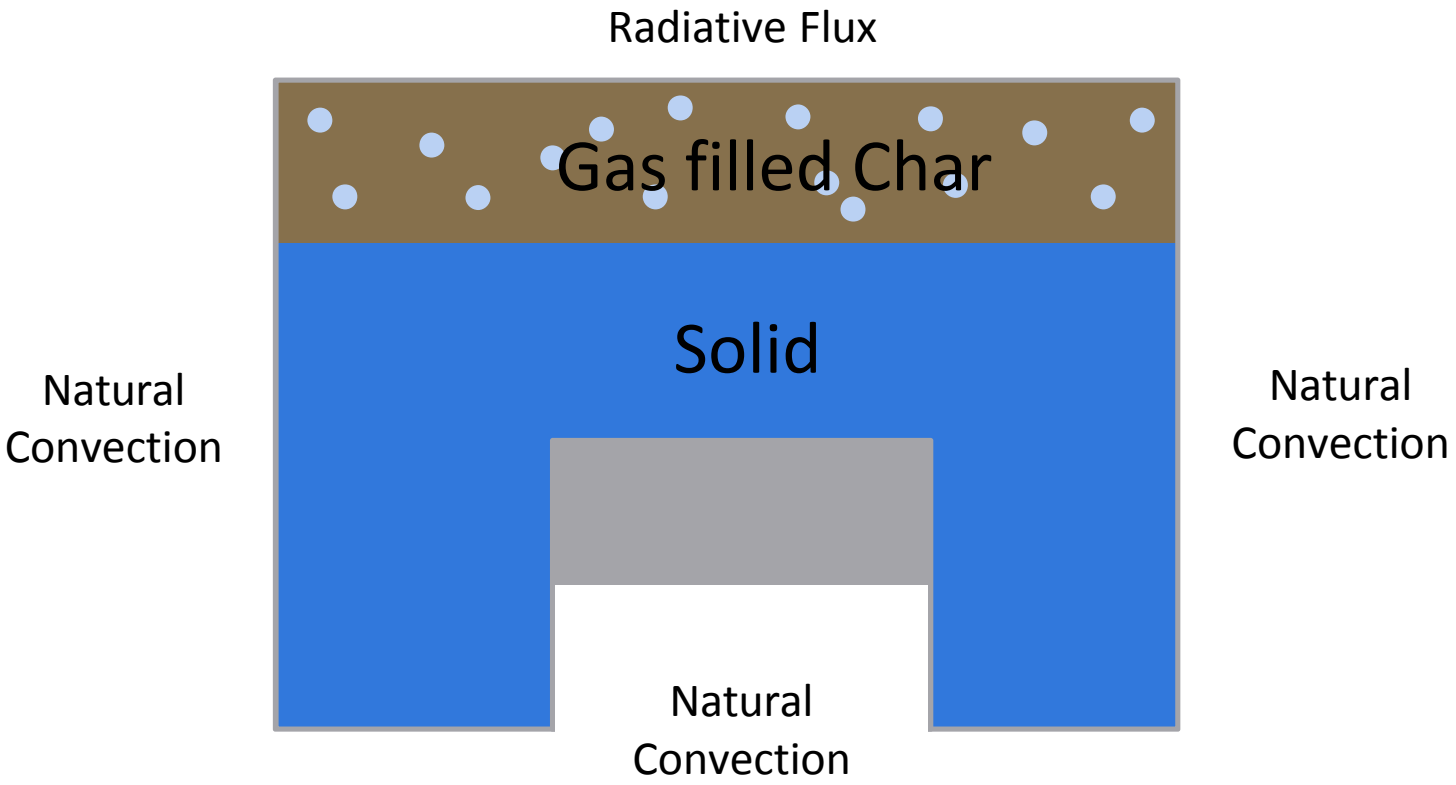
$$p = \frac{n_g R}{\int_{V_g} \frac{1}{T} dV_g} = \frac{n_g R}{\int_{V_g} \frac{1}{T} dV_{fv} + \int_{V_B^0} \frac{1}{T} dV_B^0}$$

Moles of Gas

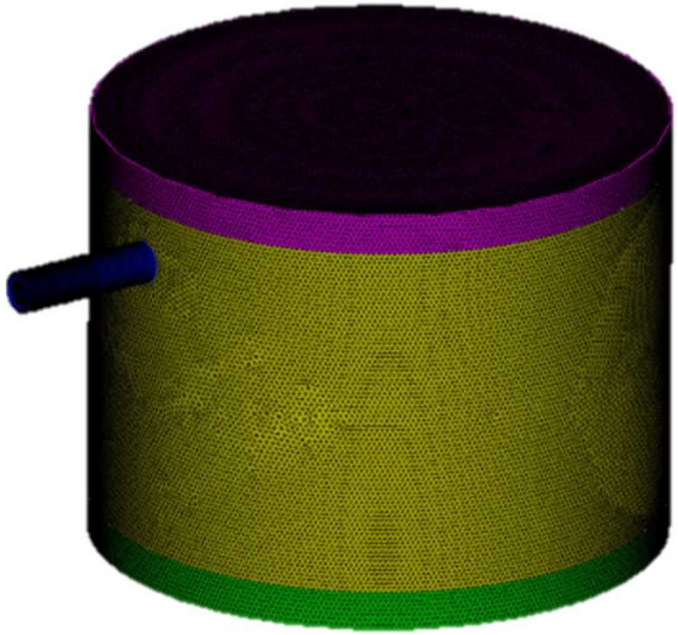
Free volume divided by temperature

Gas Volume reacted area and pore space

Current Model – Boundary Conditions



Finite Element Model



- Sierra Thermal/Fluids Code
- 3D heat transfer

Uncertainty Quantification: Mean Value

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Input parameter	σ_i
Foam Conductivity	0.1
Foam Specific Heat	0.1
Foam Density	0.01
Foam Activation Energy	0.02
Far Field Temperature	0.05
Steel Conductivity	0.1
Steel Specific Heat	0.1
Steel Emissivity	0.1
Convective heat transfer coefficient	0.2
Temperature of heated surface	0.01

Uncertainty Quantification

A vector of N input parameters $\bar{P}$ produces a vector of M response predictions, $\bar{R}$. Each parameter is perturbed and the sensitivity is estimated by central difference.

$$\frac{\partial R_j}{\partial P_i} \approx \frac{R_j(\bar{P} + \delta P_i) - R_j(\bar{P} - \delta P_i)}{2\delta P_i}$$

The variance for the system response considering all the parameter uncertainties is estimated

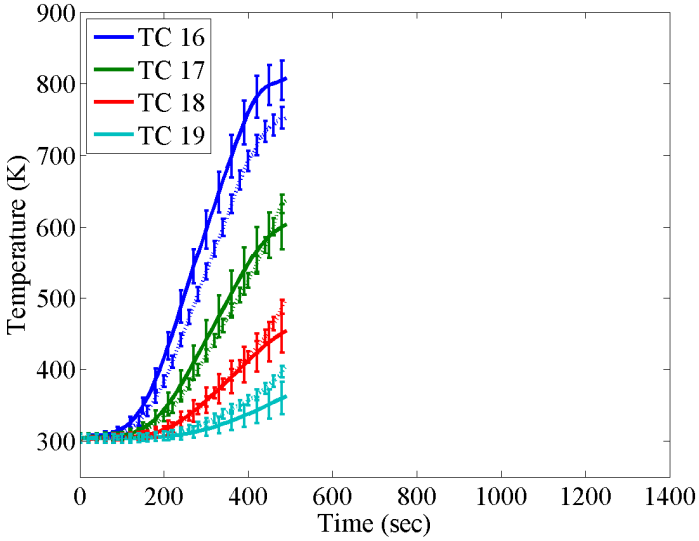
$$\sigma_{R_j}^2 = \sum_{i=1}^{N} \left(\frac{\partial R_j}{\partial P_i} \sigma_i \right)^2$$

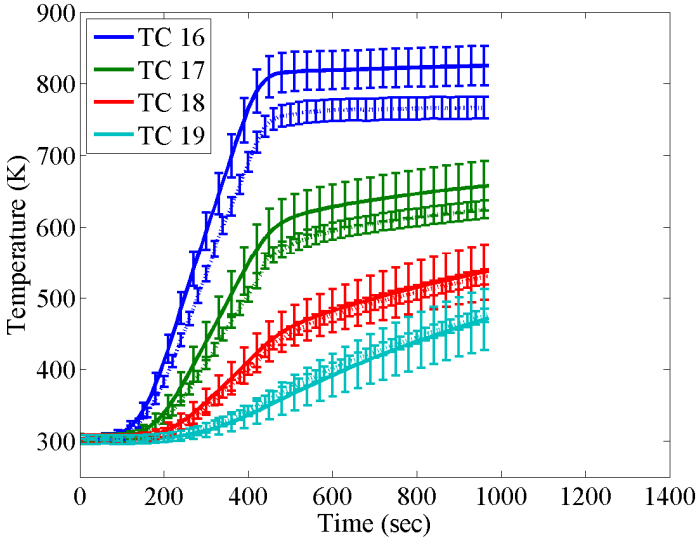
The importance measures the relative contribution of each parameter to the variance

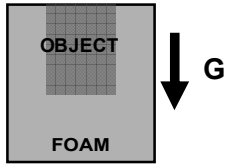
$$I_{ij} = \left(\frac{\partial R_j}{\partial P_i} \frac{\sigma_i}{\sigma_{R_j}} \right)^2$$

Results: Temperature

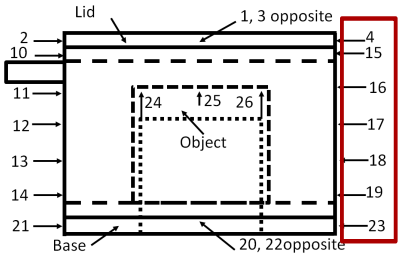
150 C/min

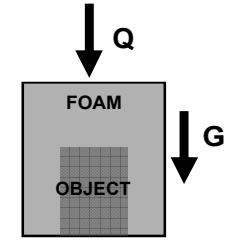






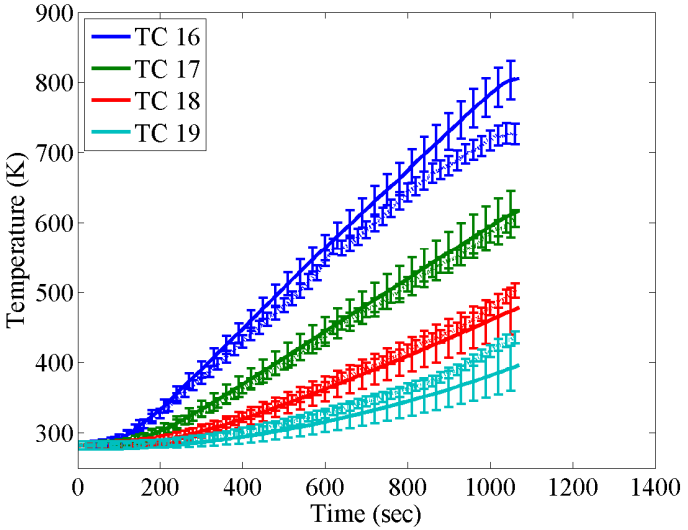
Inverted – 180º

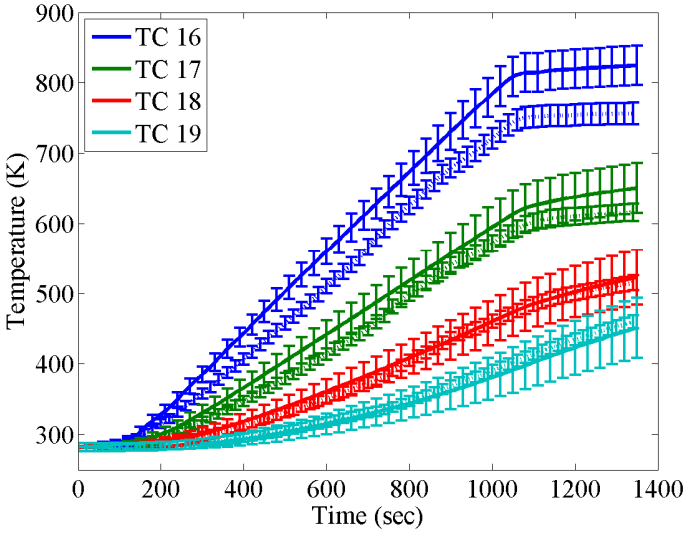




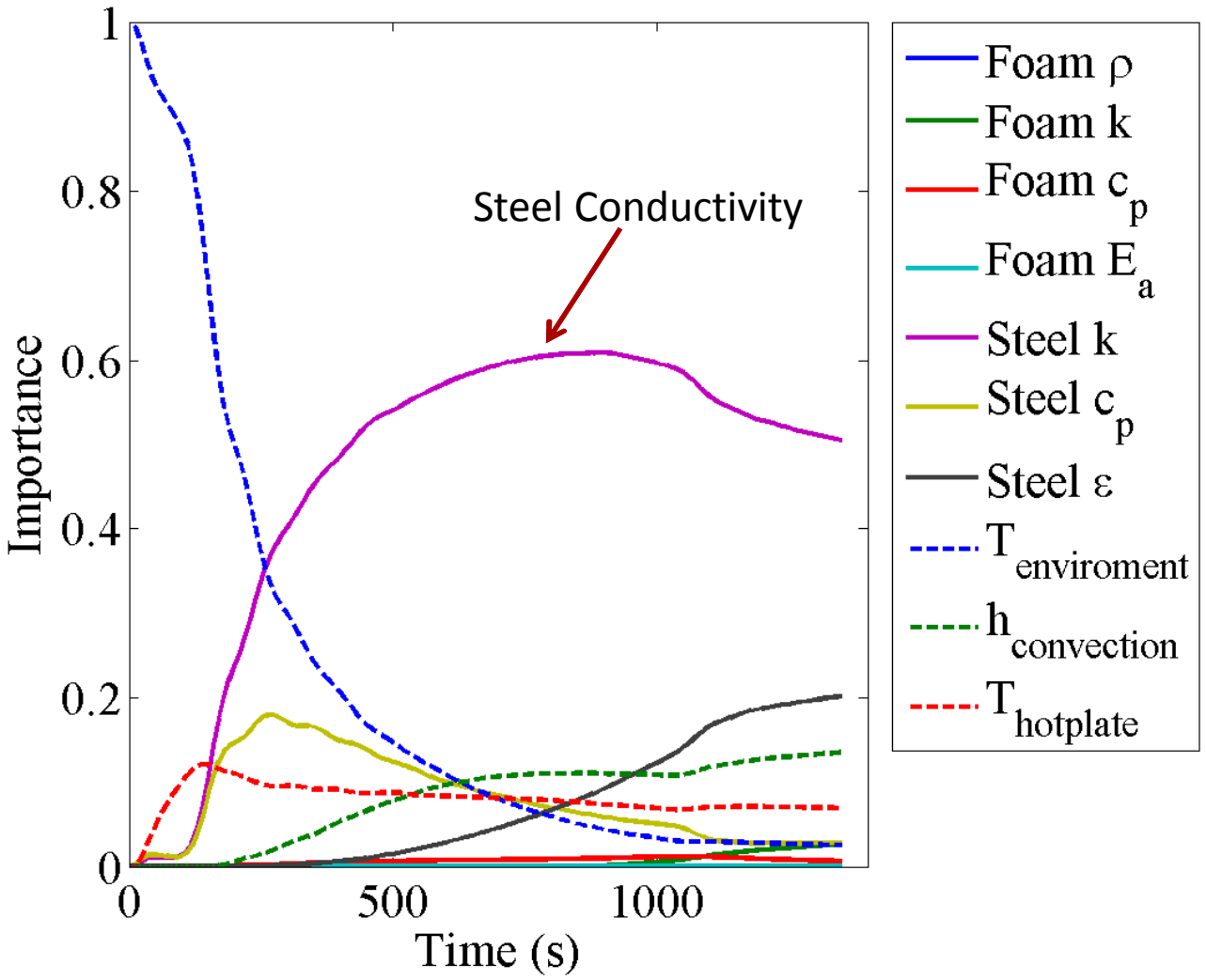
Upright – 0º

50 C/min

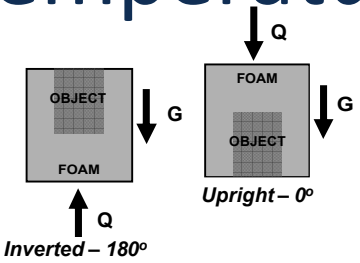




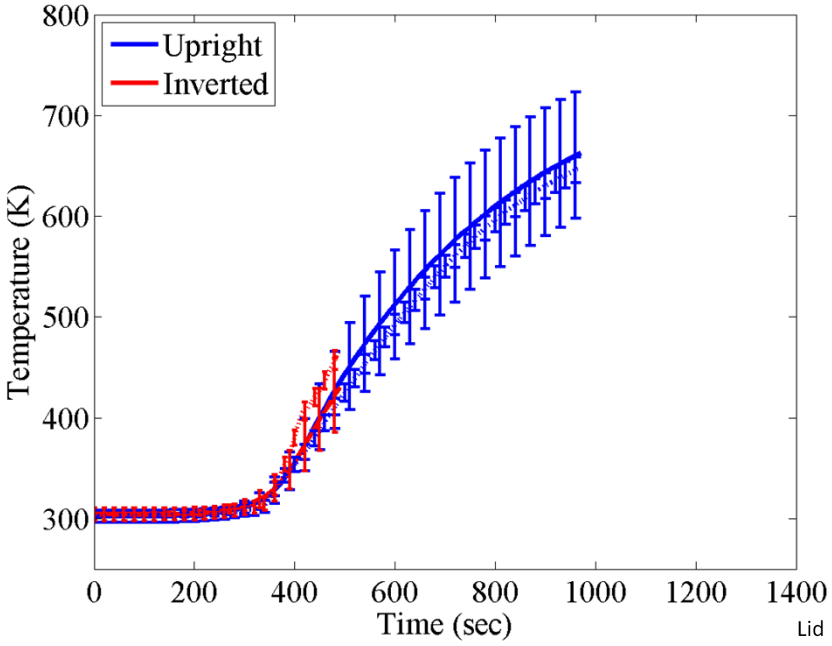
Sensitivity for Side Wall Temperature



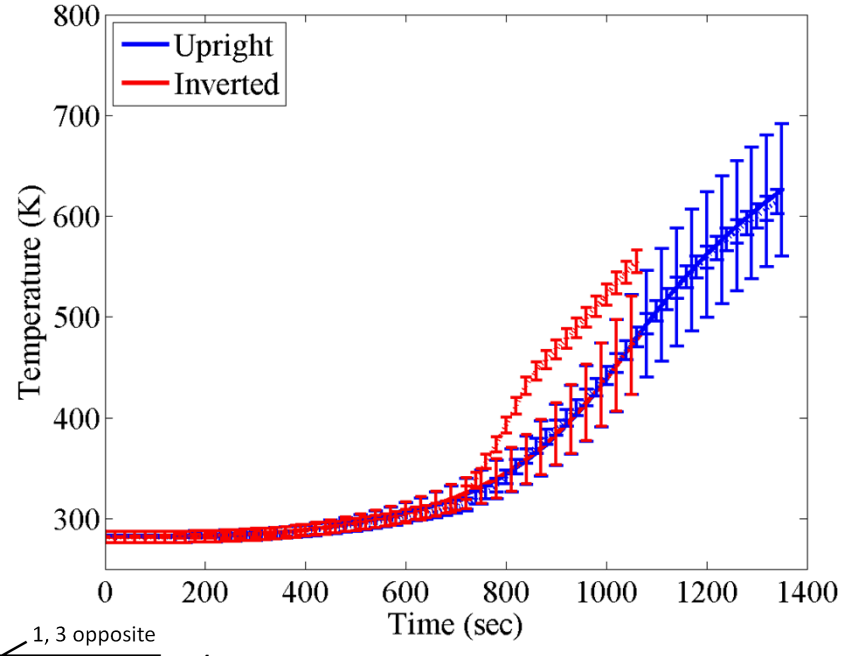
Results: Object Temperature

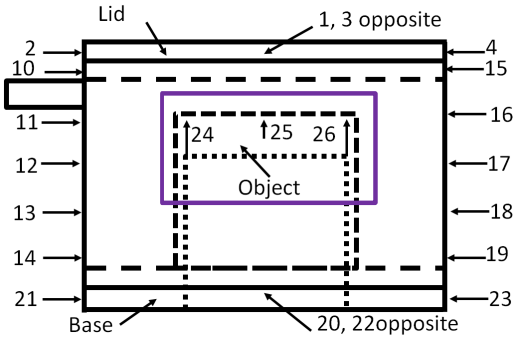


150 C/min

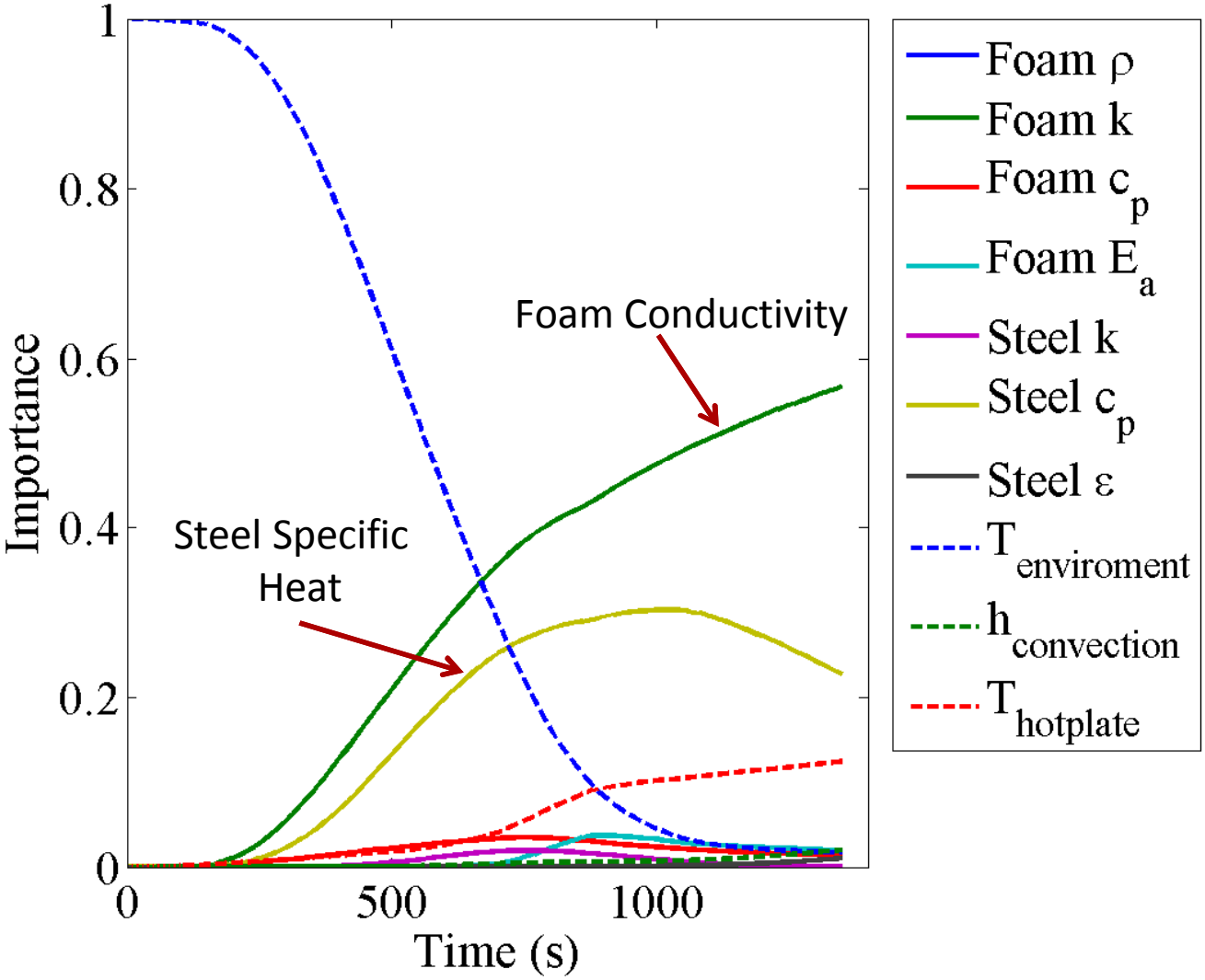


50 C/min

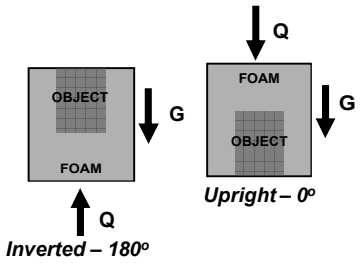




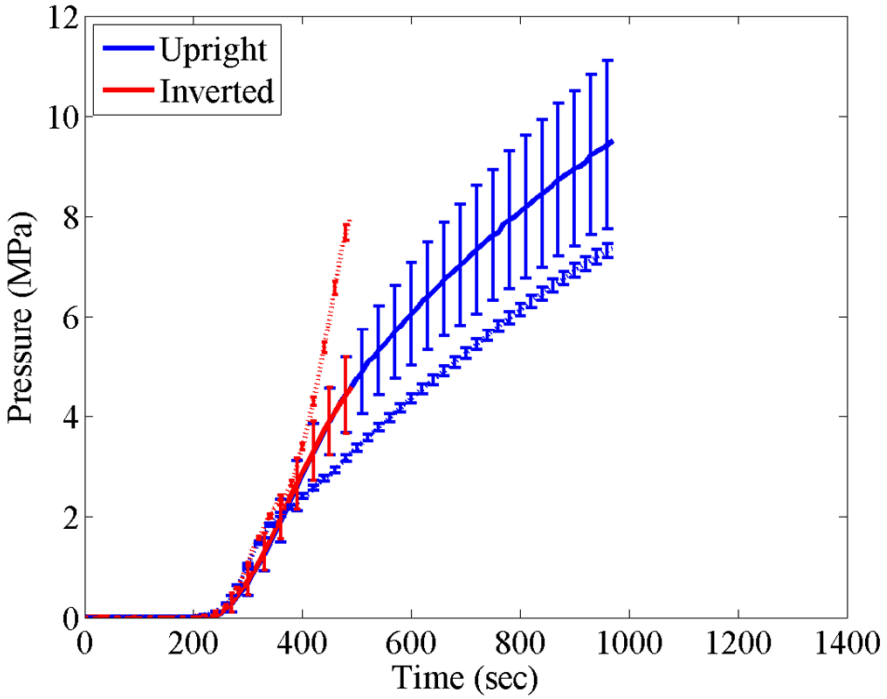
Sensitivity for Object Temperature



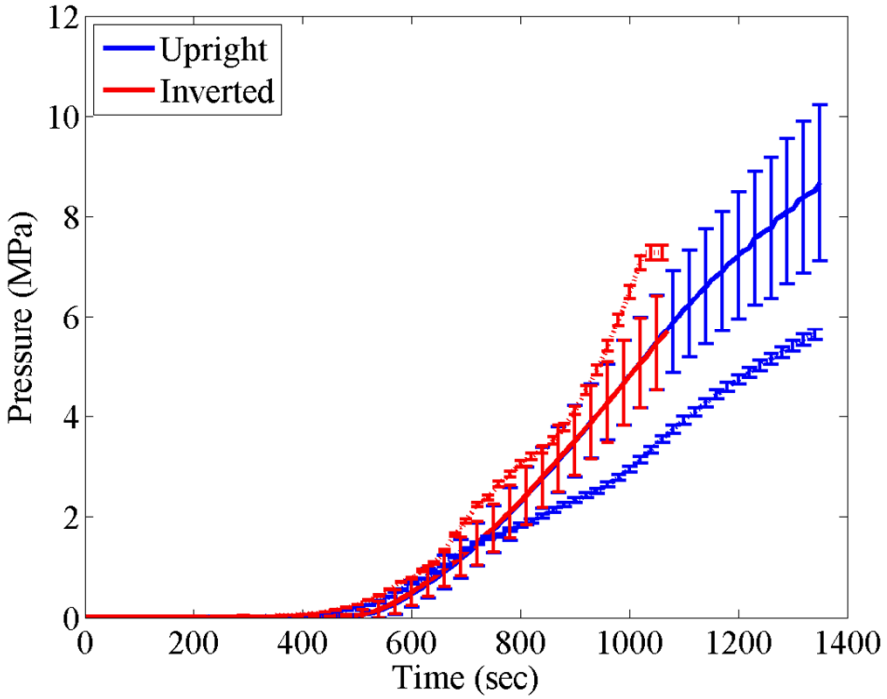
Results: Pressure



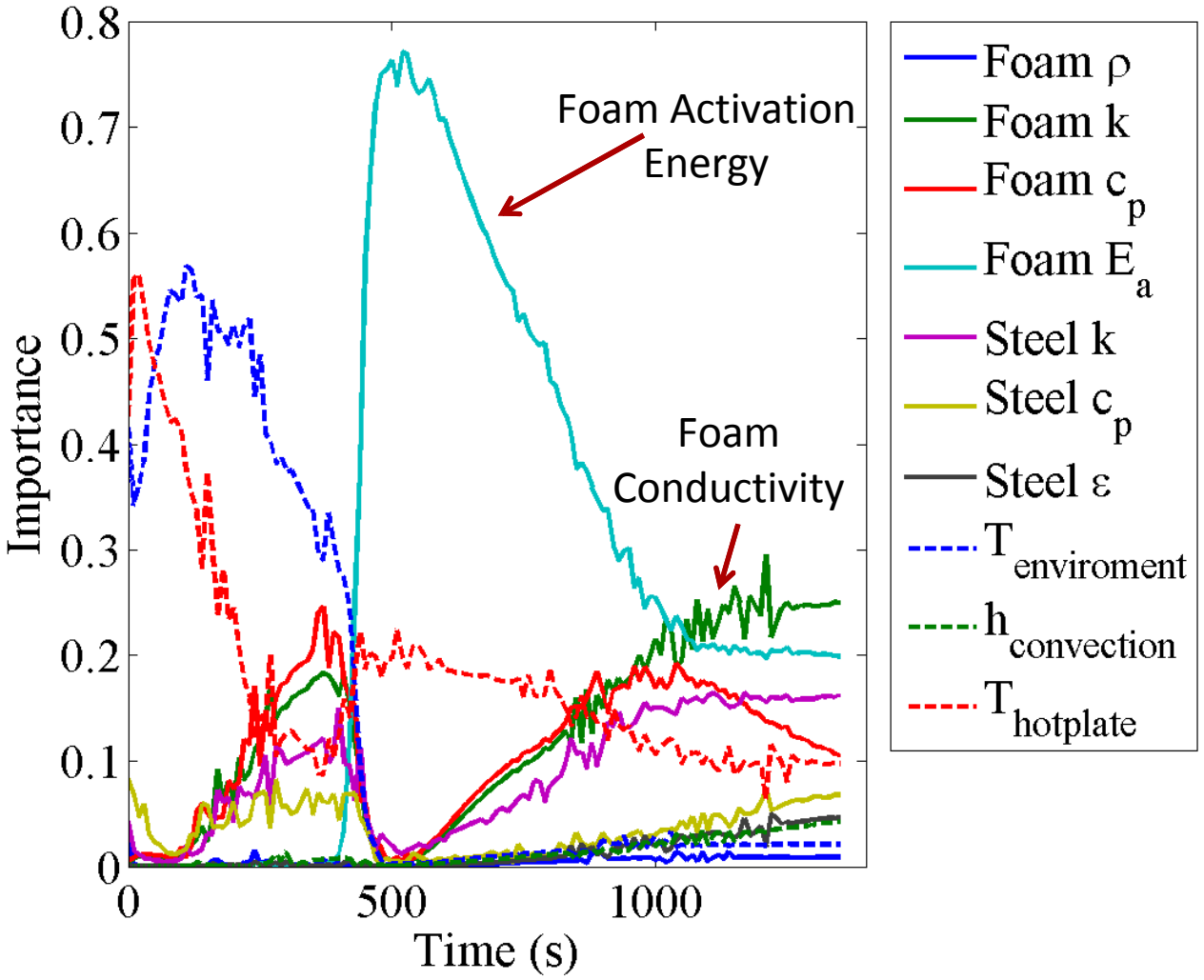
150 C/min



50 C/min



Sensitivity for Pressure



Modeled Physics

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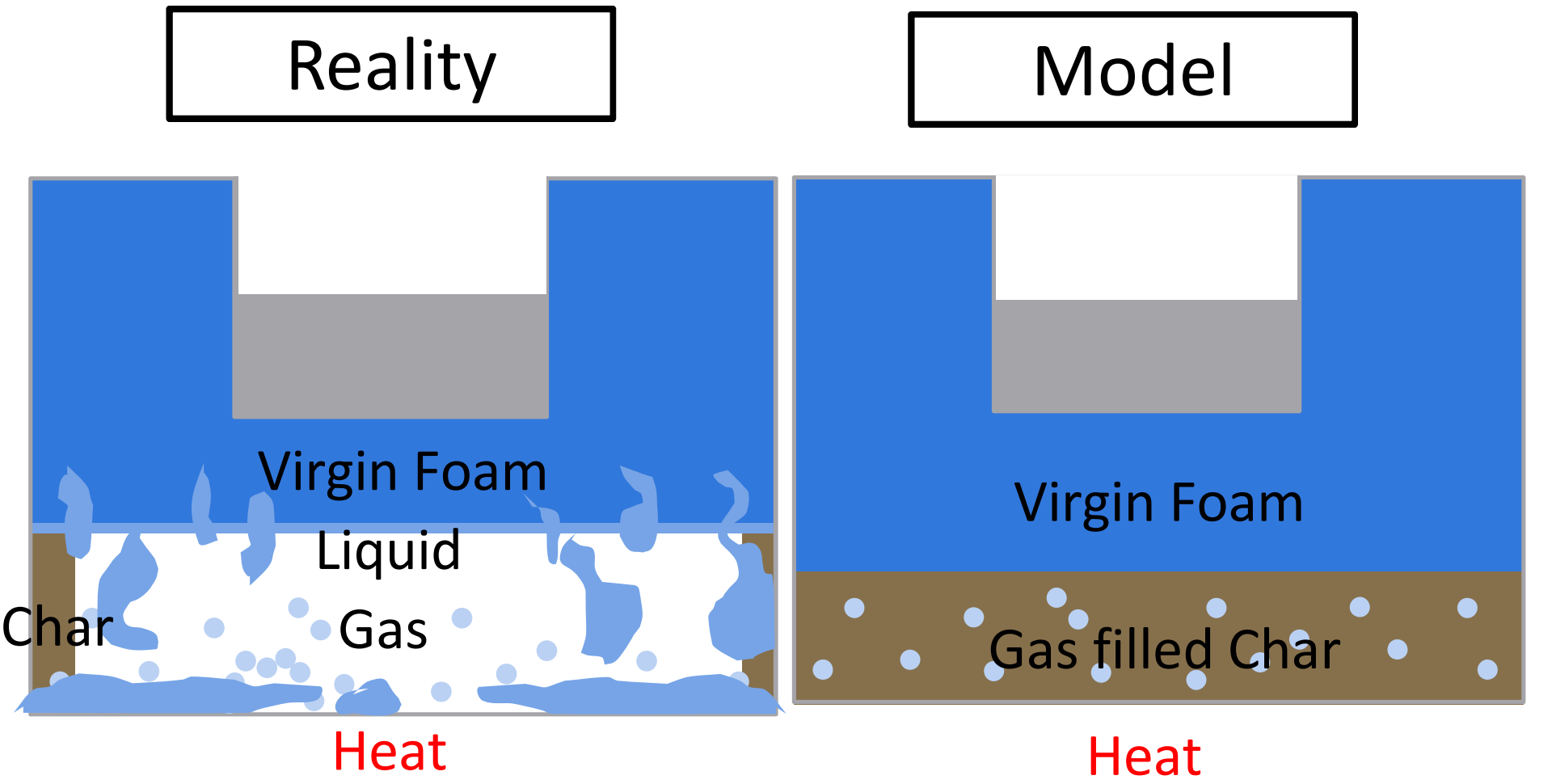
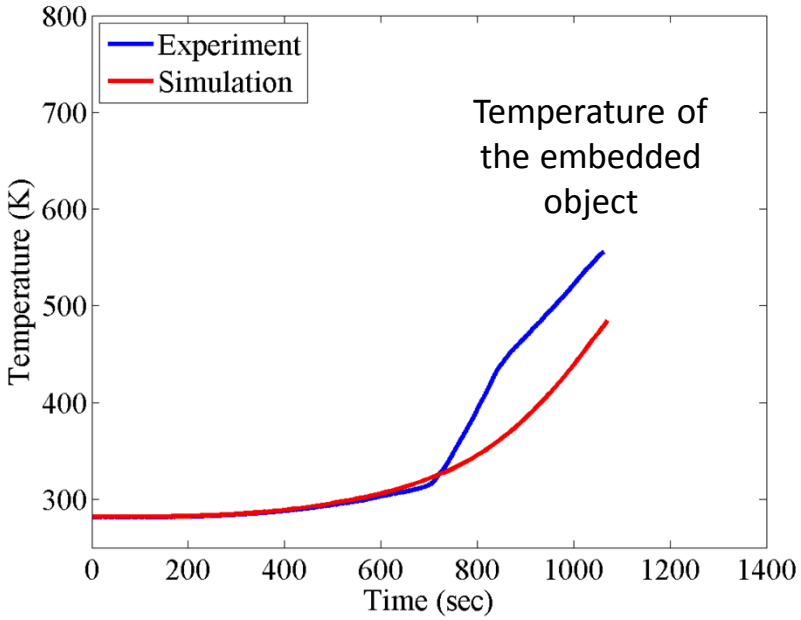


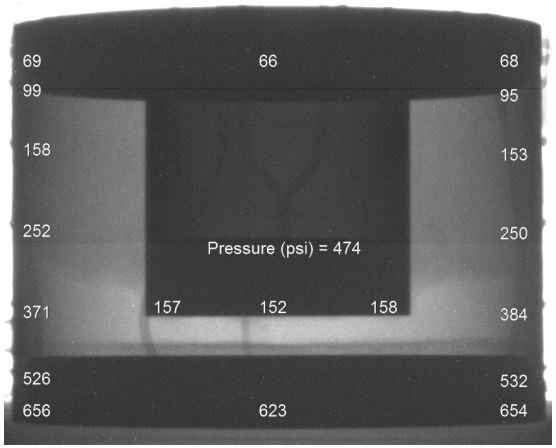
Unmodeled Physics: Radiation

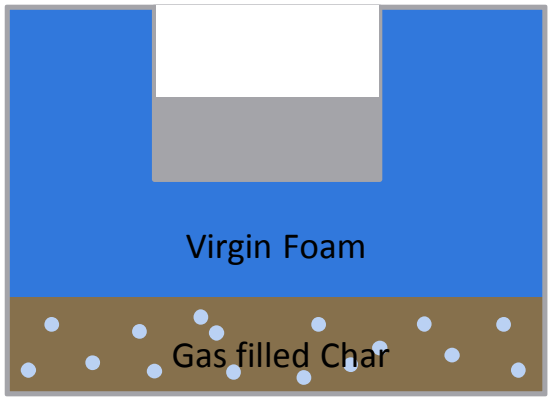


- Current model assumes a structured char is left behind in the reacted space.
  - Heat transfer through reacted space accounted for using conduction with diffuse approximation for optically thick material

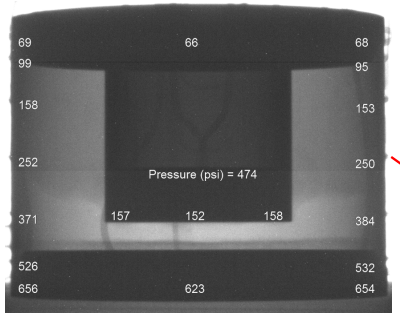
$$\rho c \frac{\partial T}{\partial T} = \nabla \cdot (k + k_e)\nabla T + \sum_i \rho r_i(-\Delta H_i) \qquad k_e = \frac{16\sigma}{3(a+\sigma_s)} T^3$$

- Alternative: Radiation Enclosure





Unmodeled Physics: Liquids



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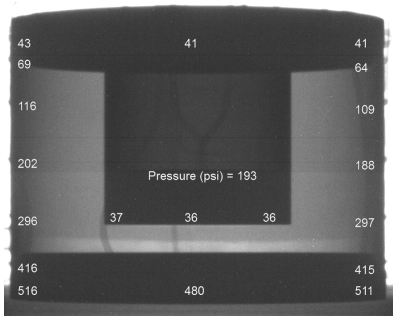

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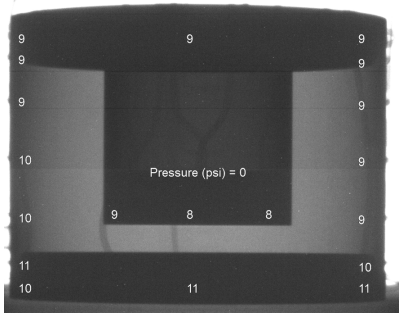

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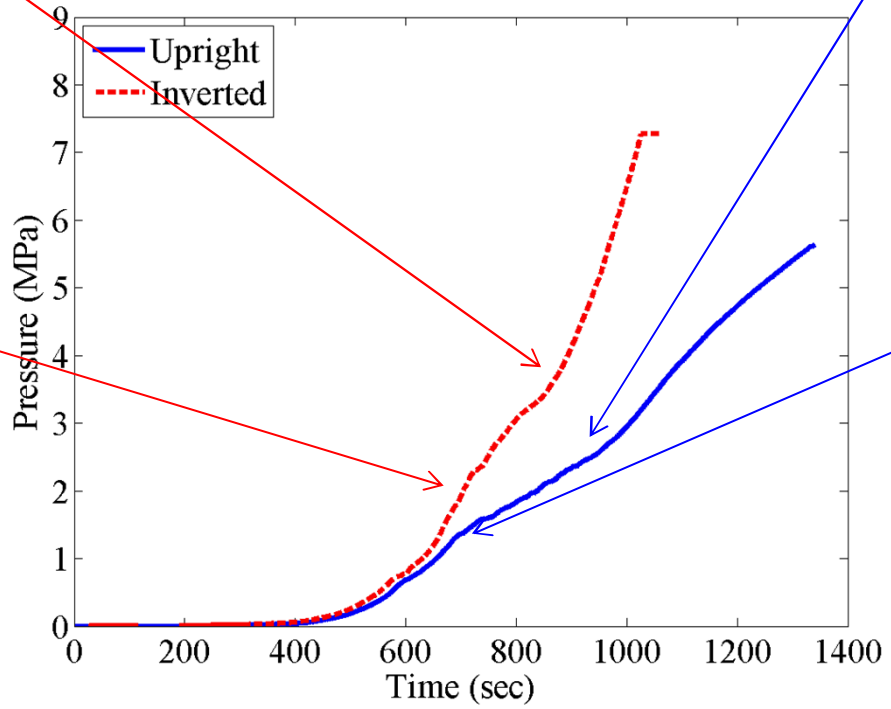

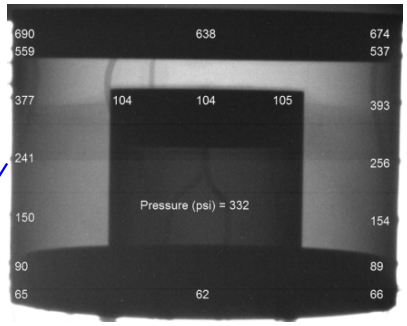

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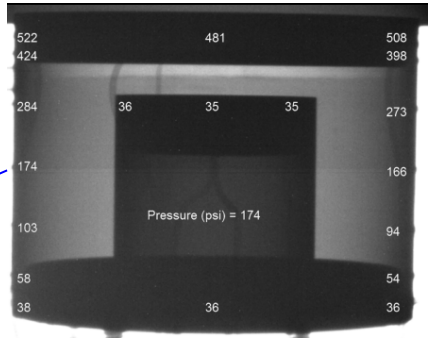

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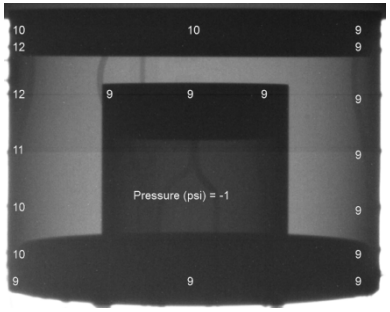

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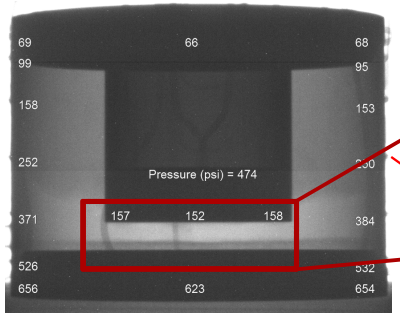
Unmodeled Physics: Liquids



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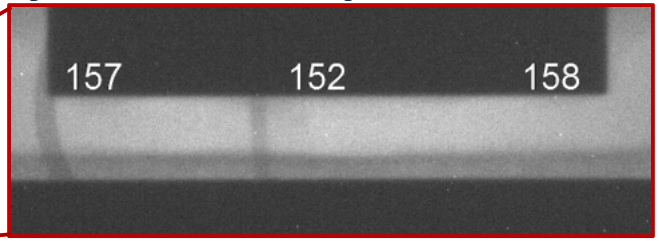

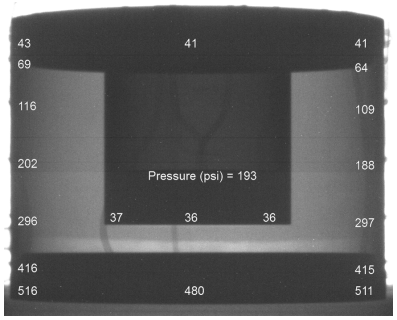

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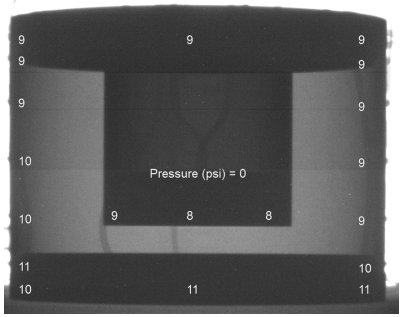

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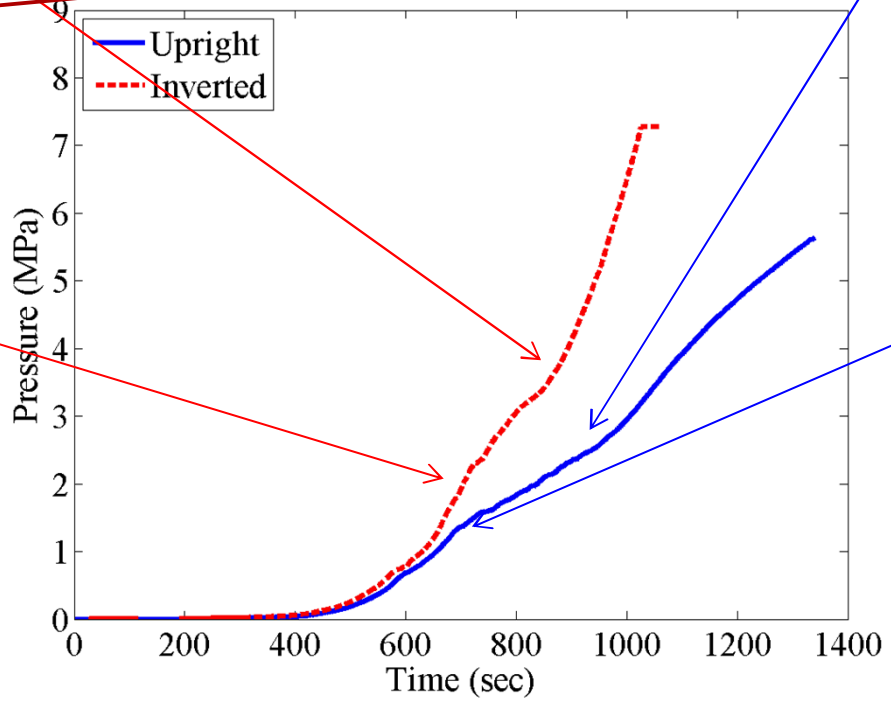

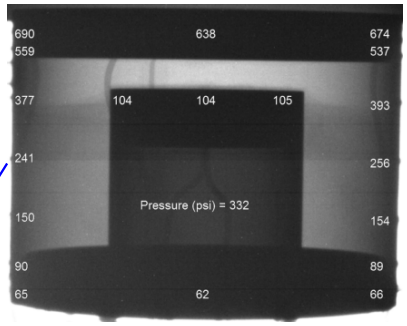

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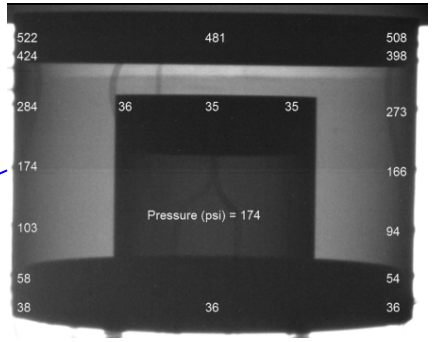

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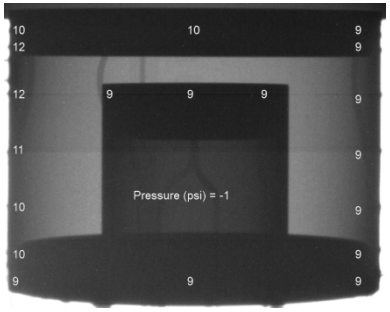

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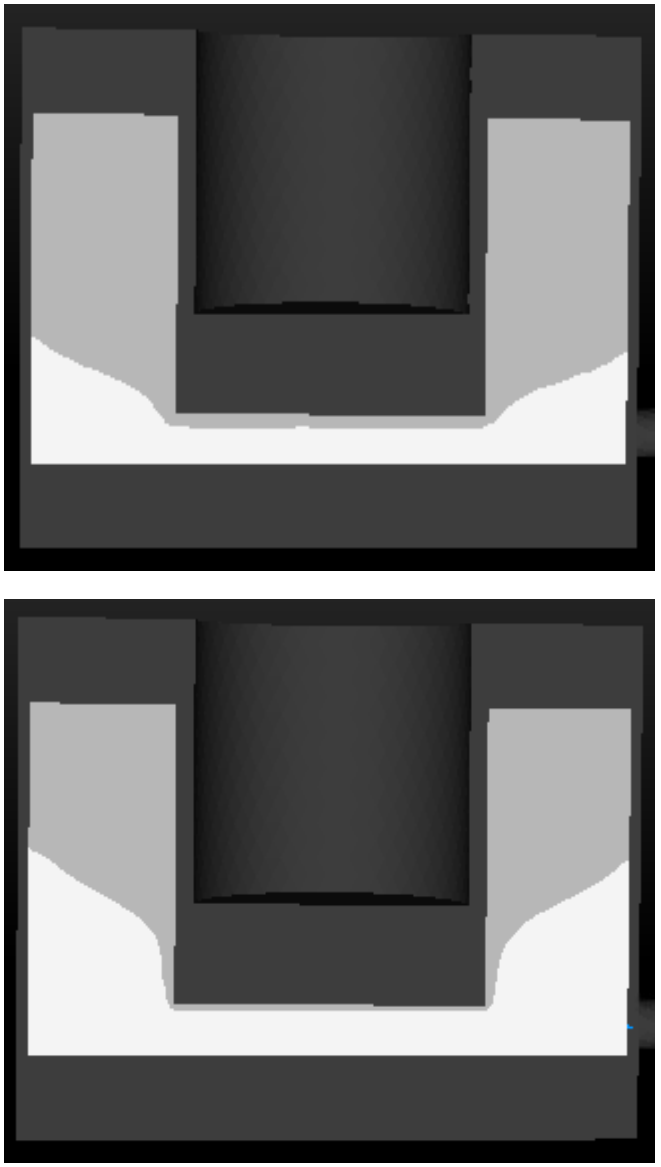
Future Work

- Address radiation and liquefaction
  - CDFEM – Front tracking
  - Liquefaction
  - Radiation enclosures behind the front
- Vapor-Liquid Equilibrium



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QUESTIONS?

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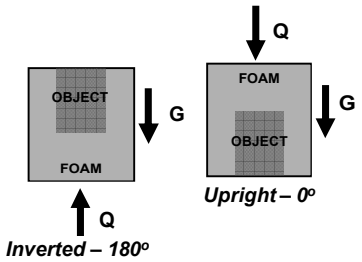
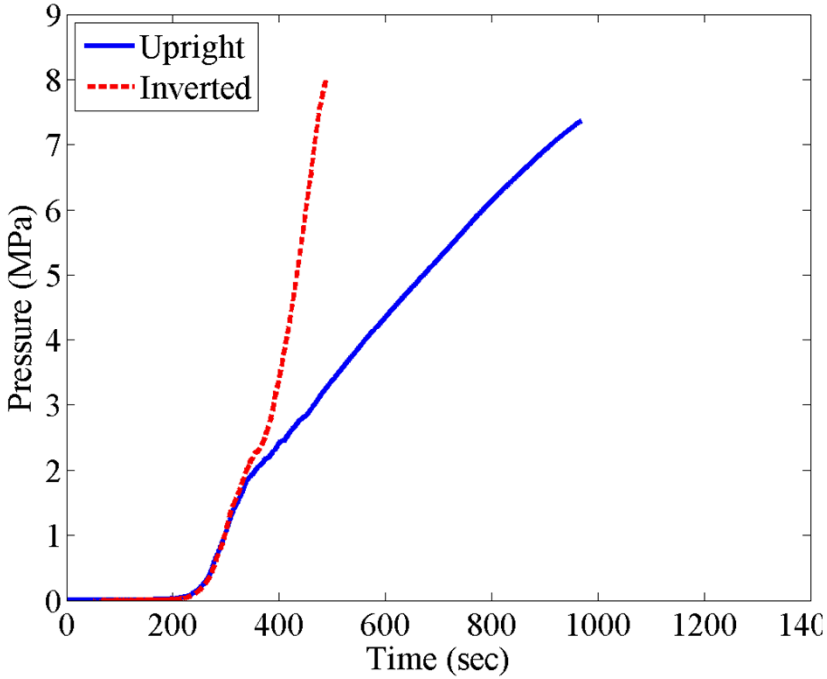
BACKUP SLIDES

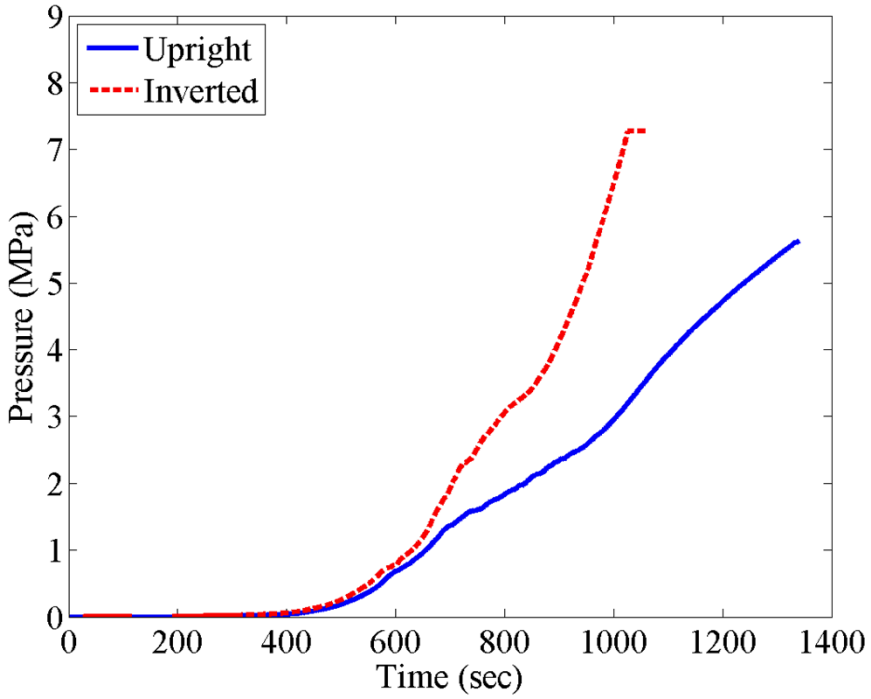
Experimental Results: Pressure



150 C/min

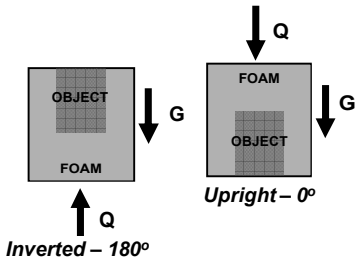


50 C/min

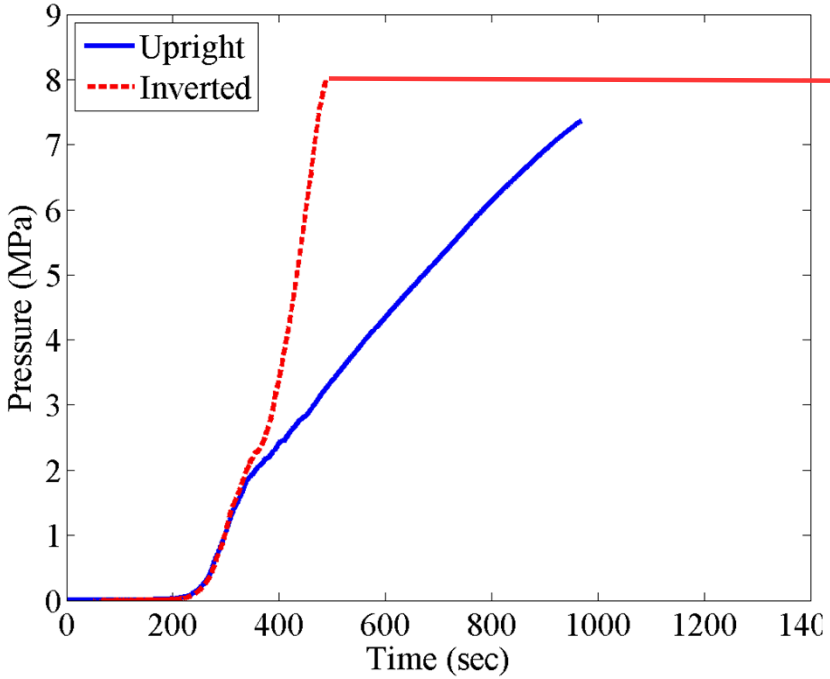


Inverted cans have a steeper pressure increase than upright

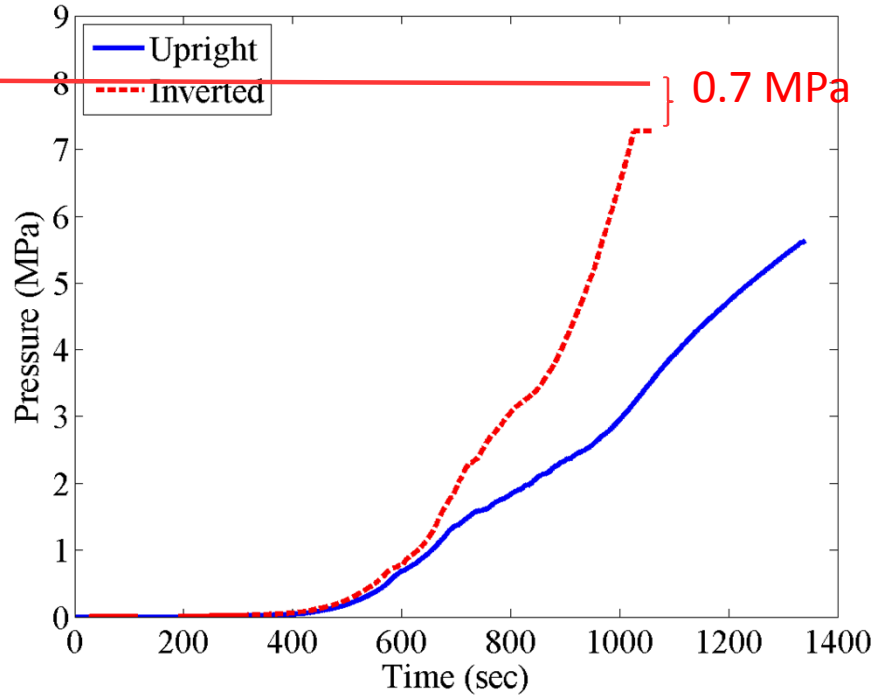
Experimental Results: Pressure



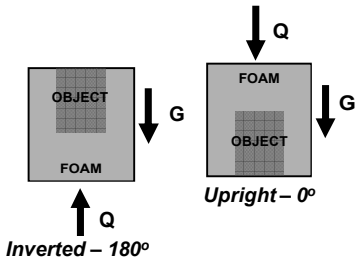
150 C/min



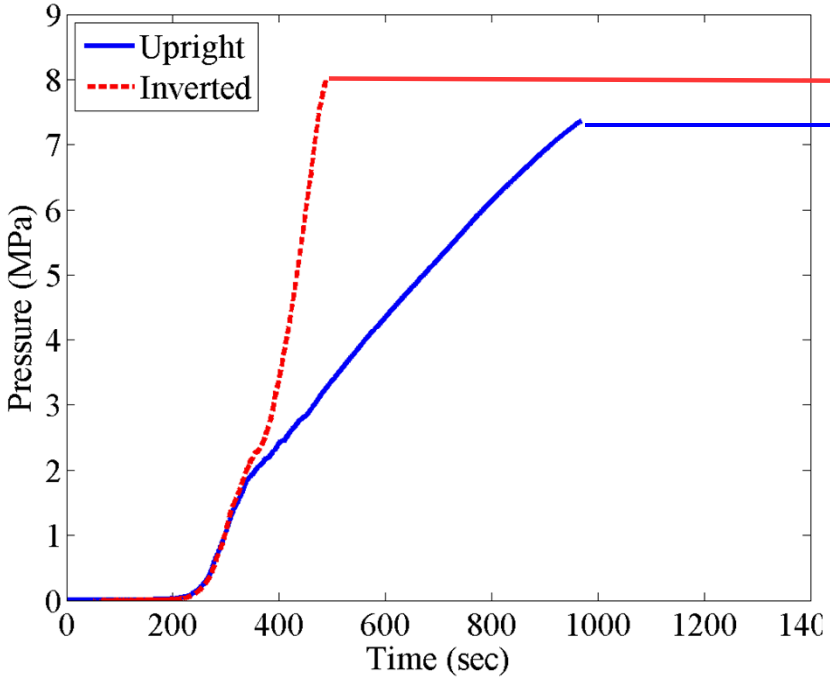
50 C/min



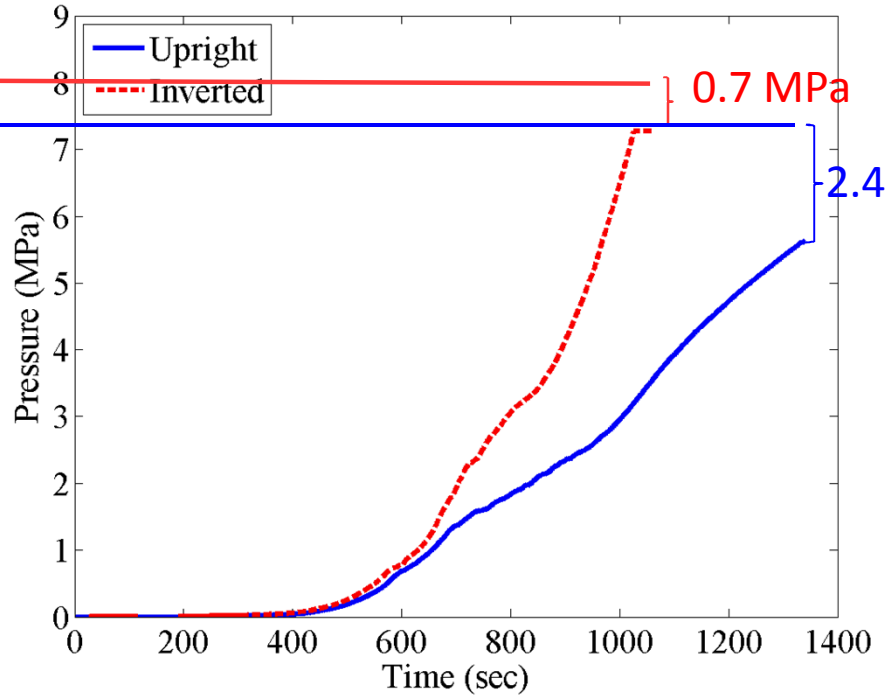
Experimental Results: Pressure



150 C/min



50 C/min



Experimental Results: Temperature

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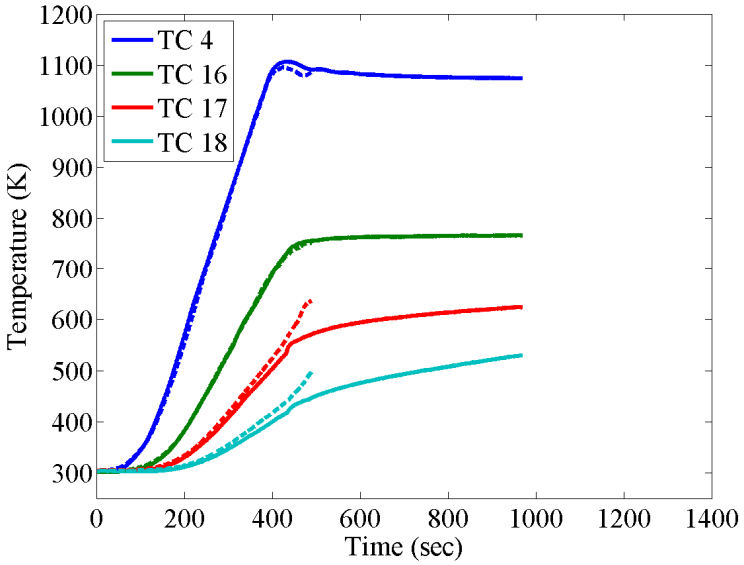
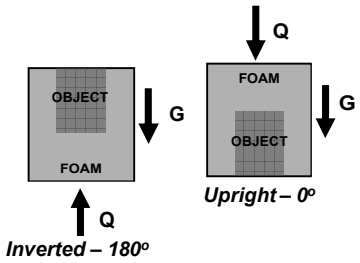
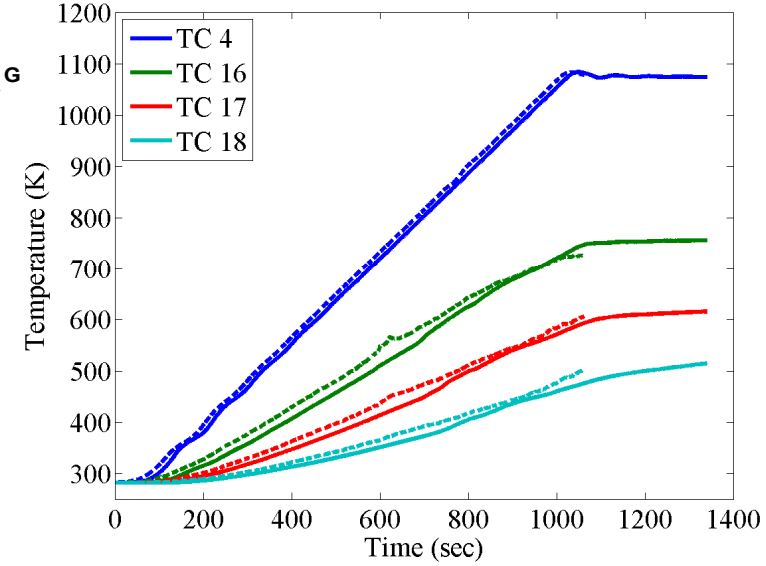
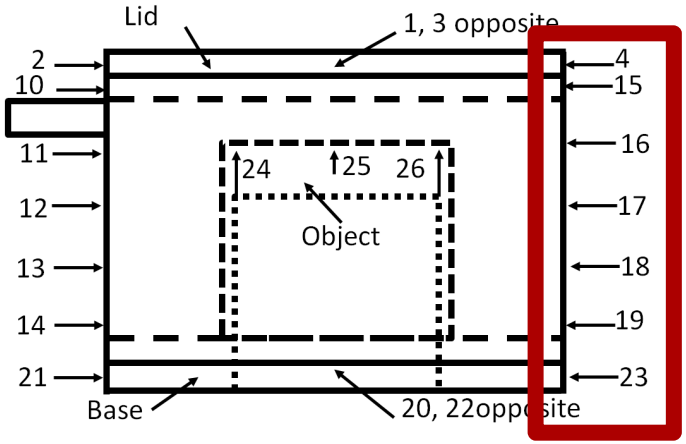
150 C/min





50 C/min





Experimental Results: Temperature

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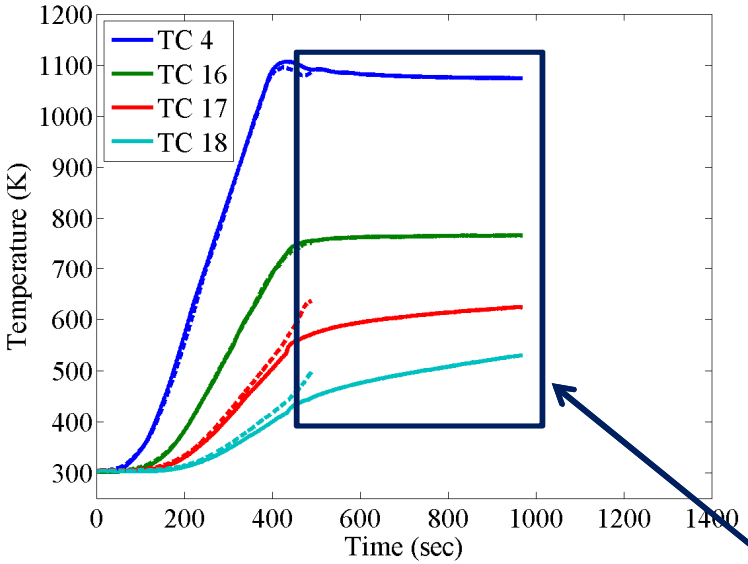
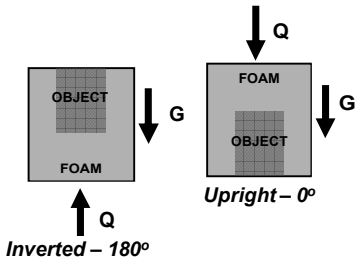
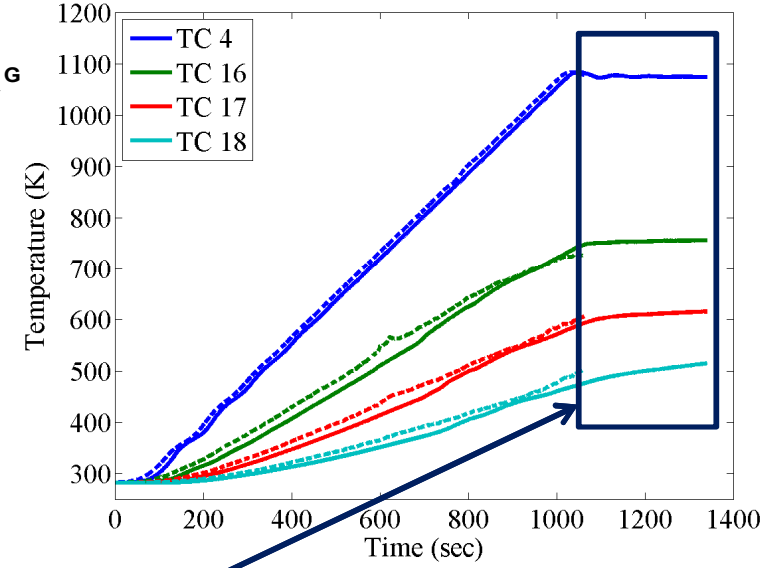
150 C/min





50 C/min



Temperature Plateau

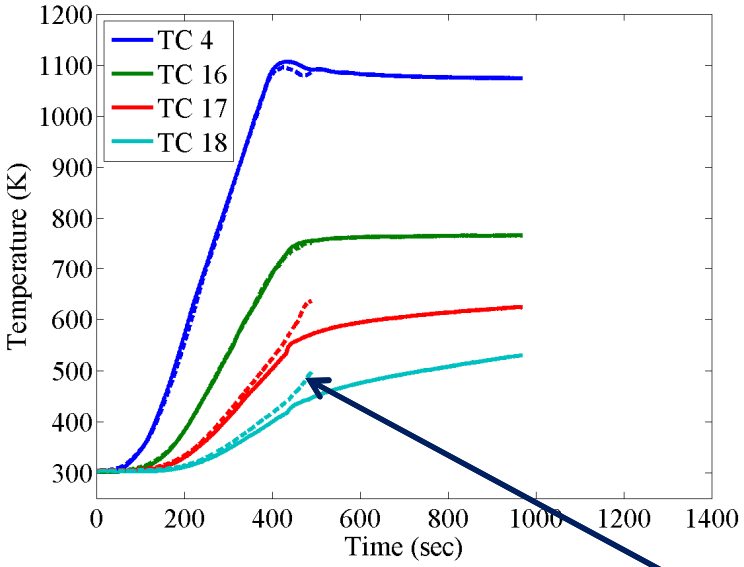
Upright

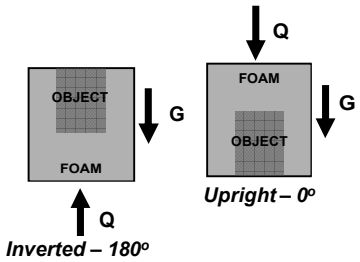
150 C/min 55% of test

50 C/min 22% of test

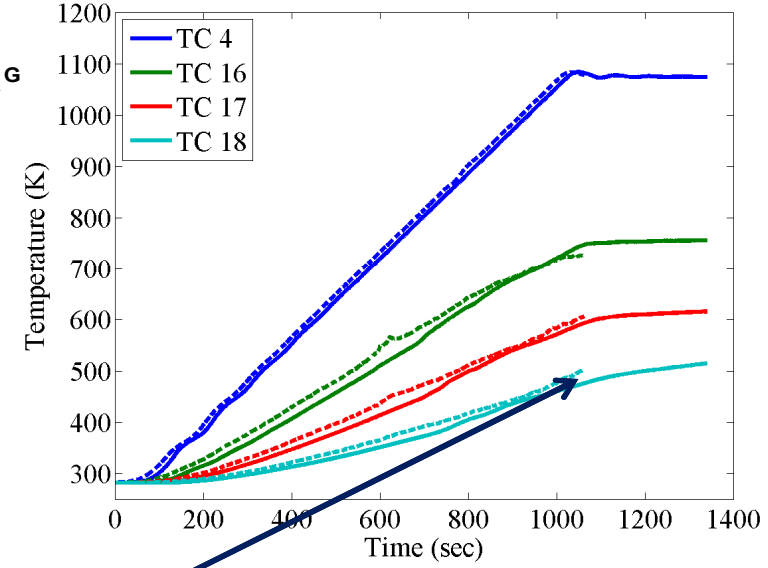
Experimental Results: Temperature

150 C/min





50 C/min



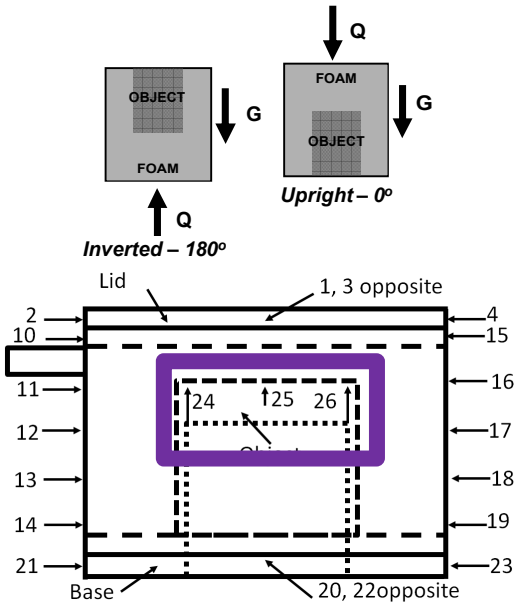
Inverted

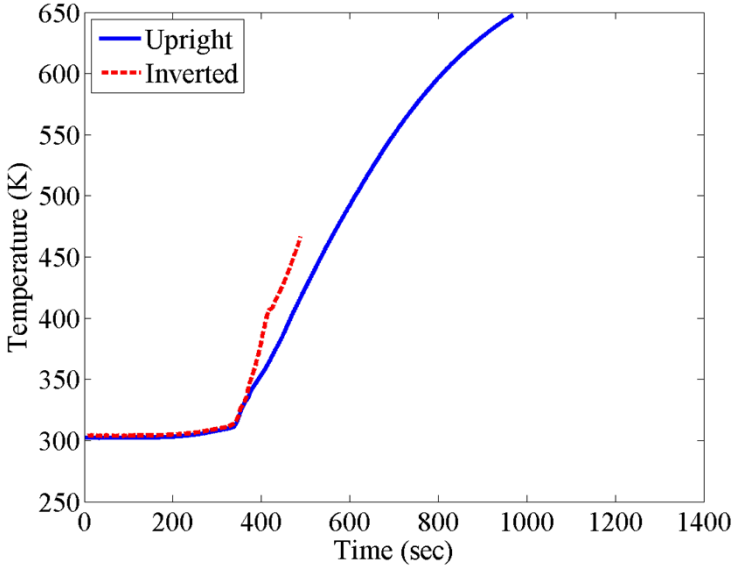
Breach occurs when hold temperature is reached

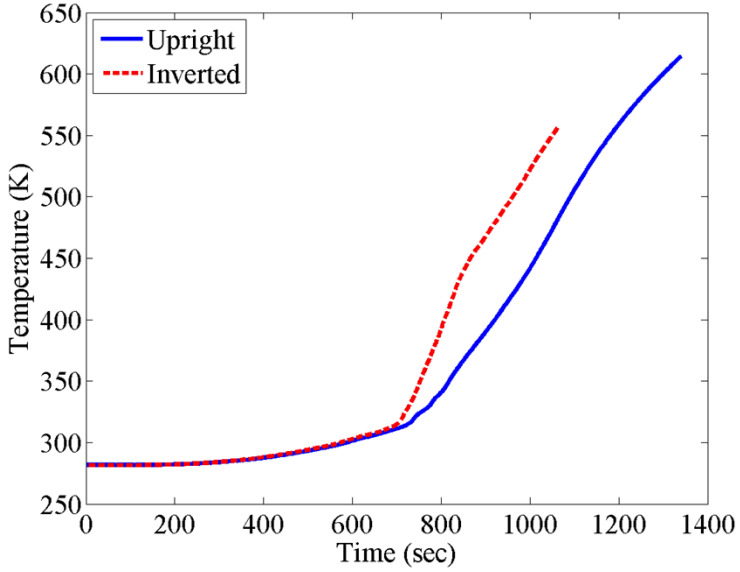
Experimental Results: Temperature

150 C/min

50 C/min







Experimental Results: Temperature

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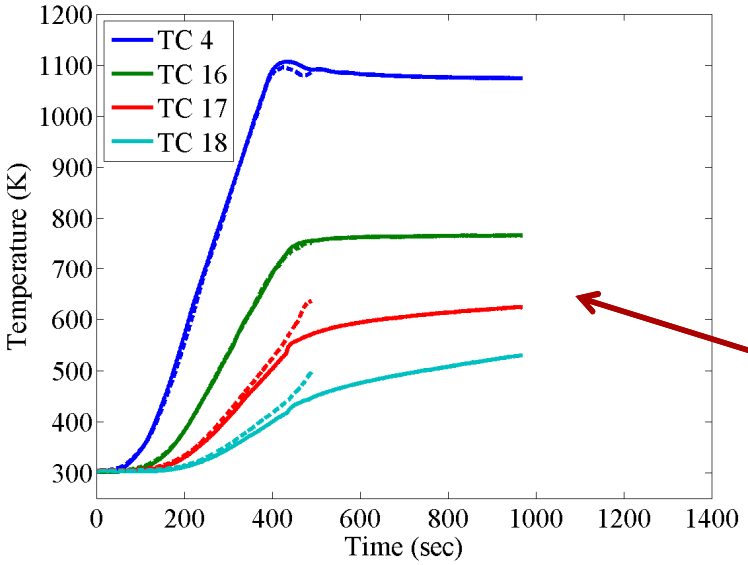
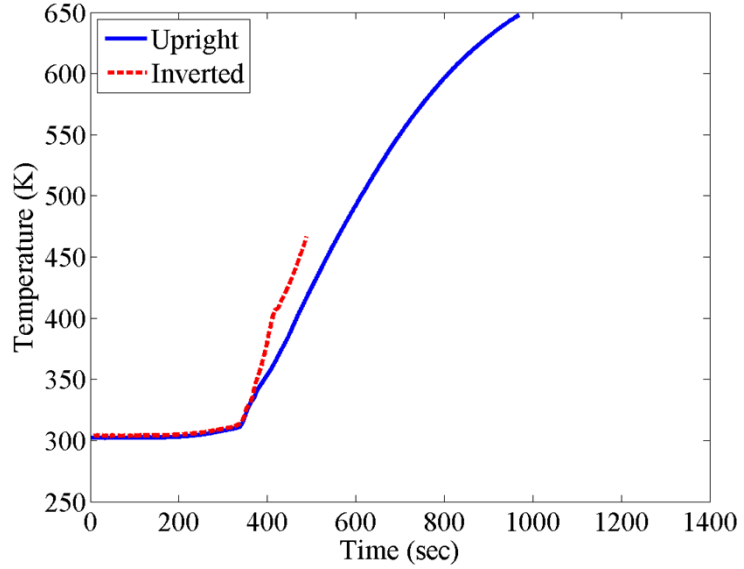
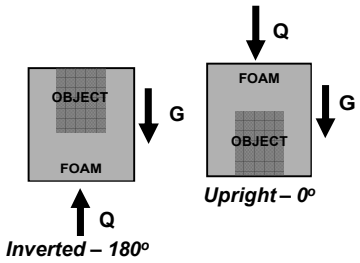
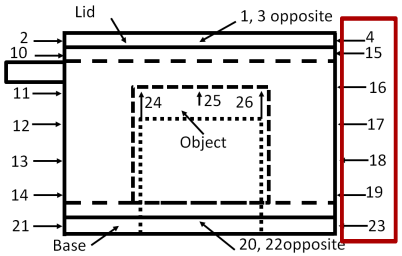
150 C/min



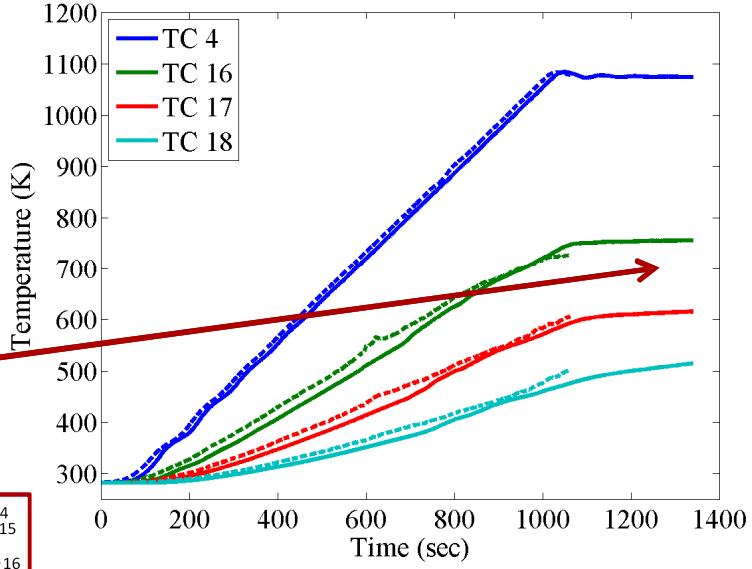


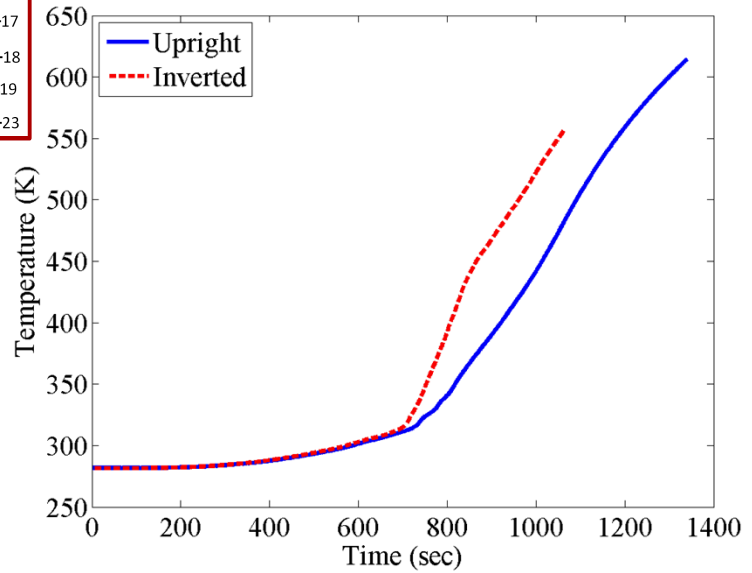


Final temperatures are the same



50 C/min

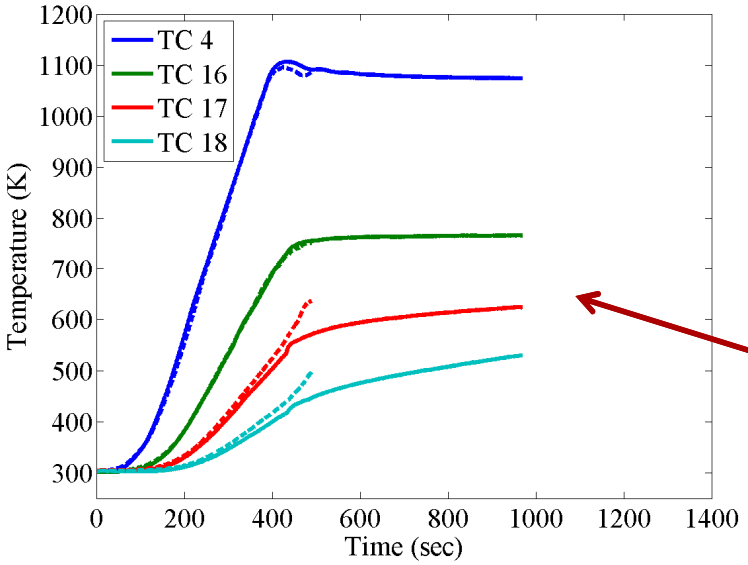


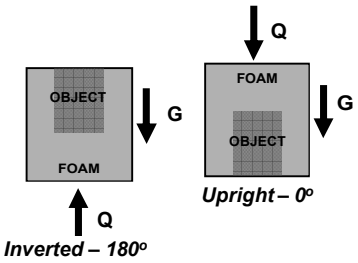


Experimental Results: Temperature

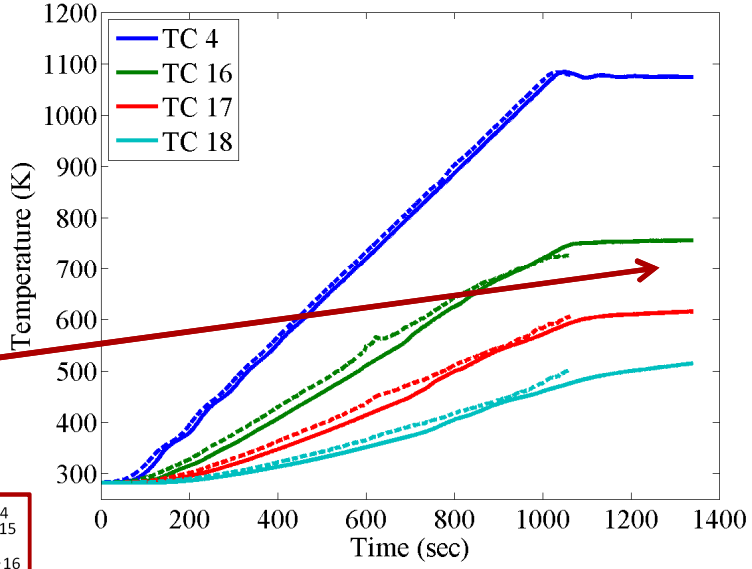
Sandia National Laboratories

150 C/min

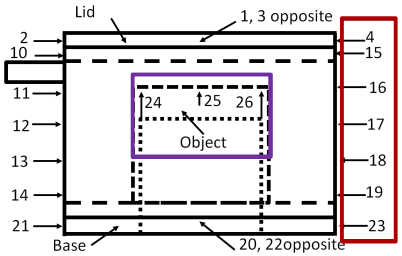


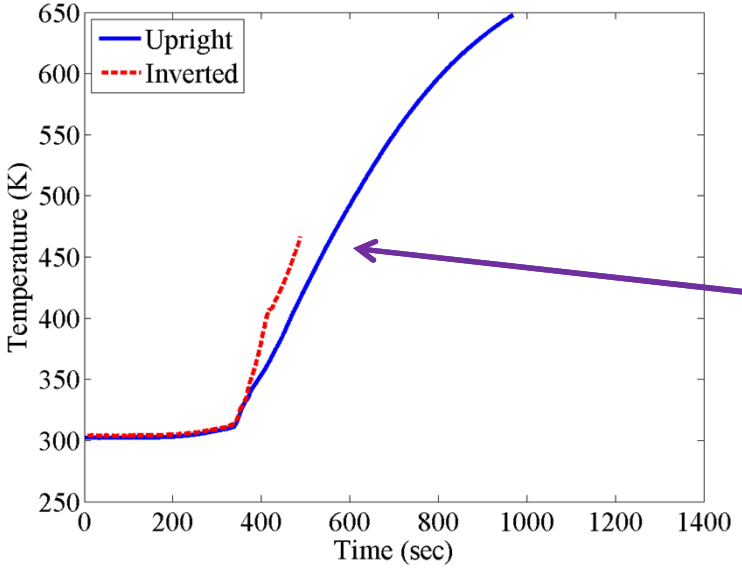


50 C/min

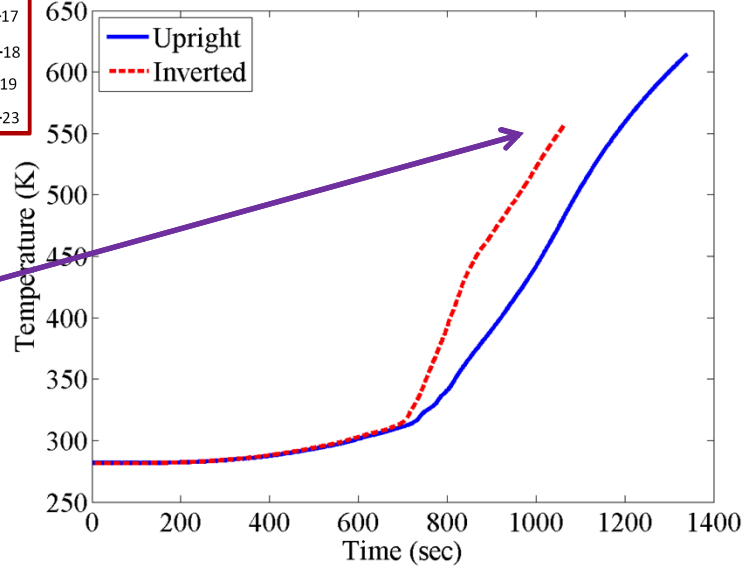


Final temperatures are the same





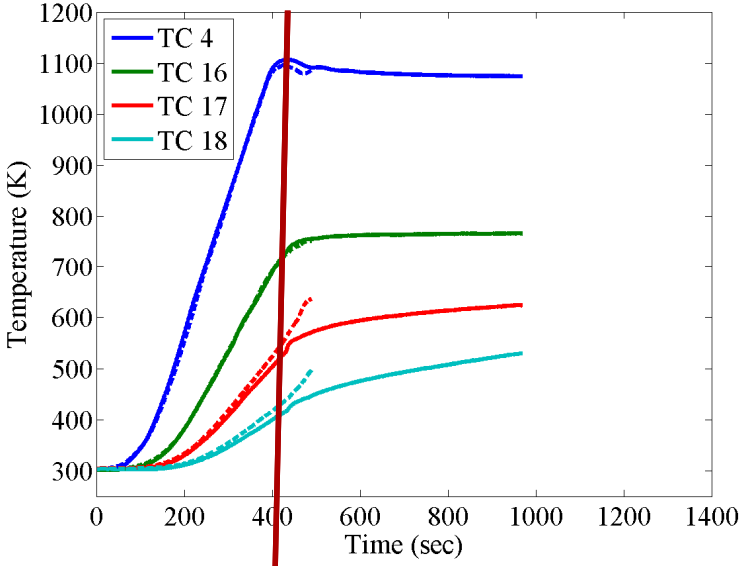
Final temperatures are different

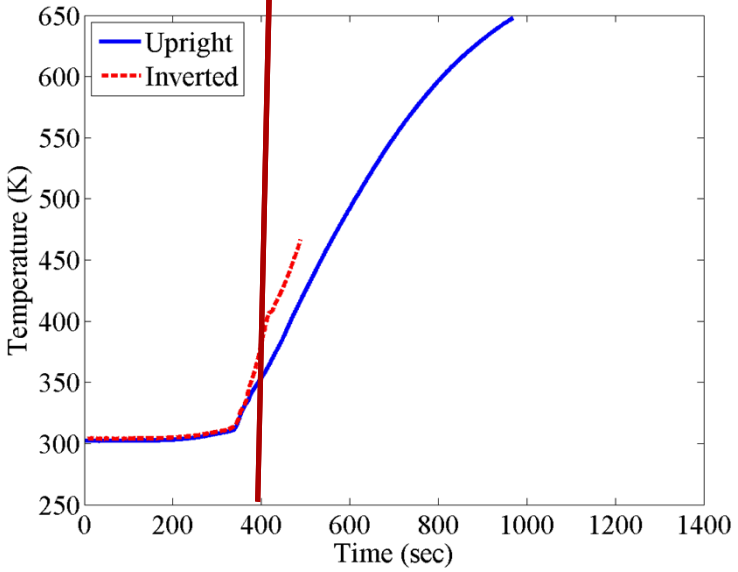


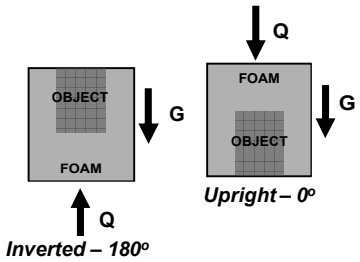
Experimental Results: Temperature

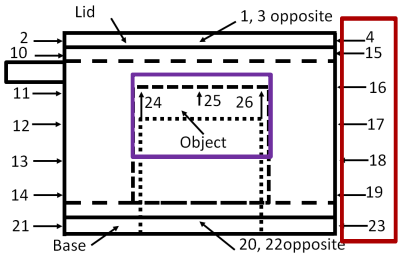
Sandia National Laboratories

150 C/min

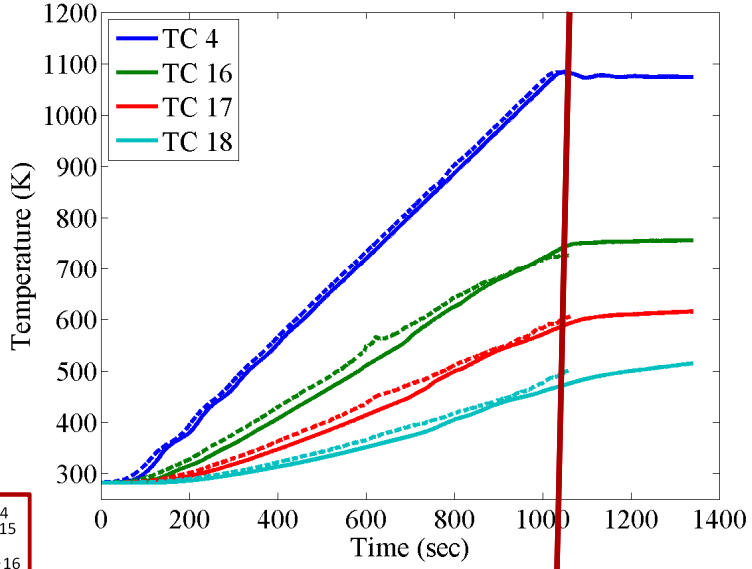


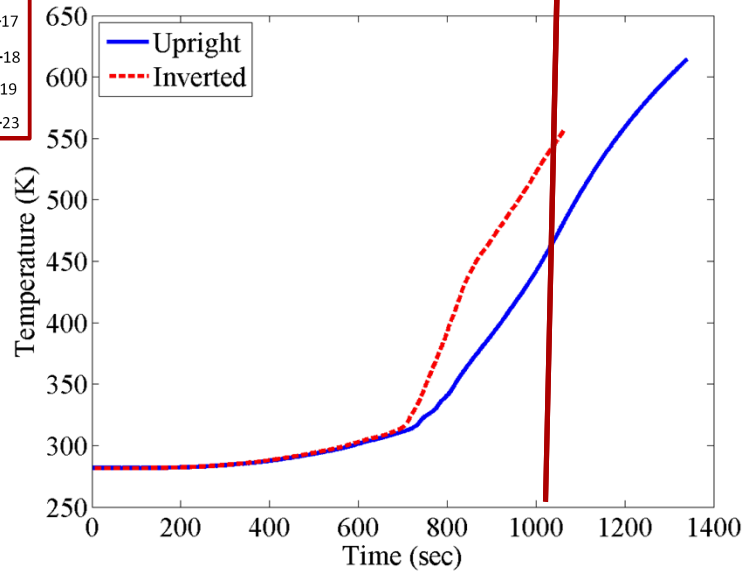






50 C/min





Experimental Results: Temperature

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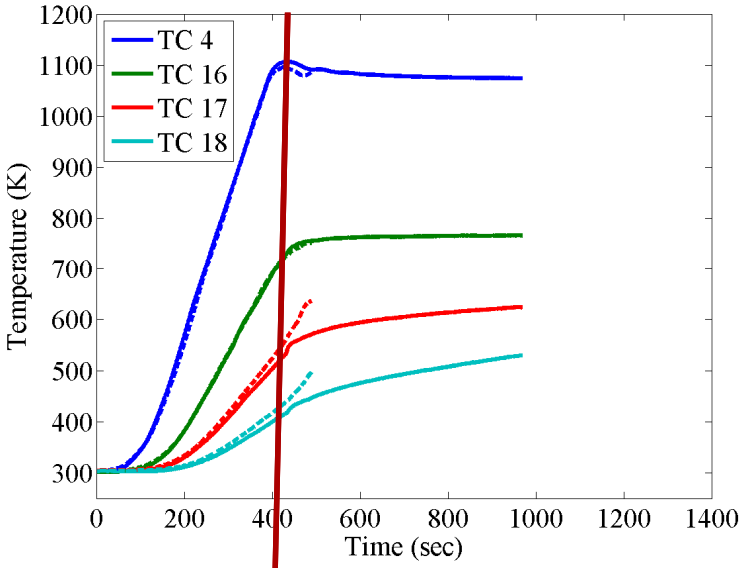
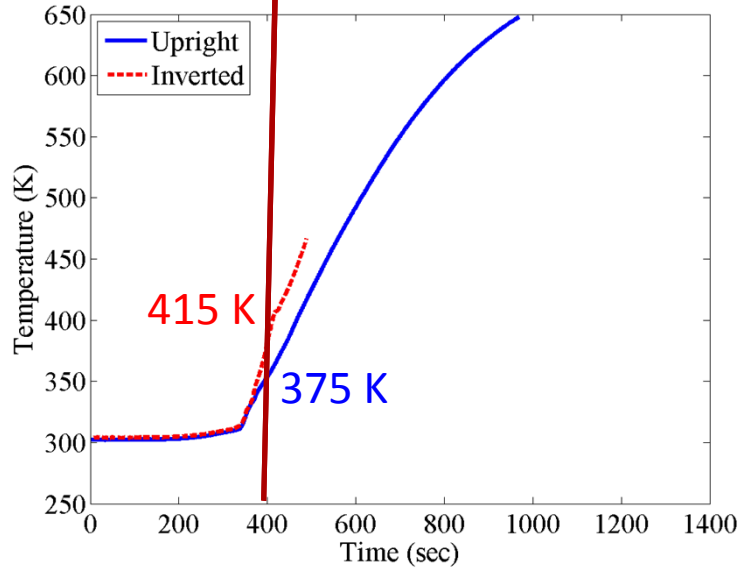
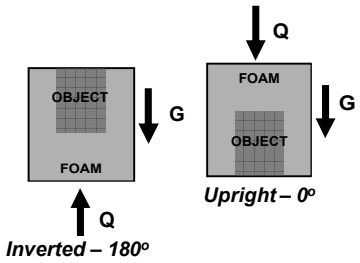
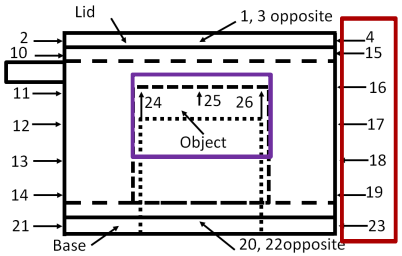
150 C/min

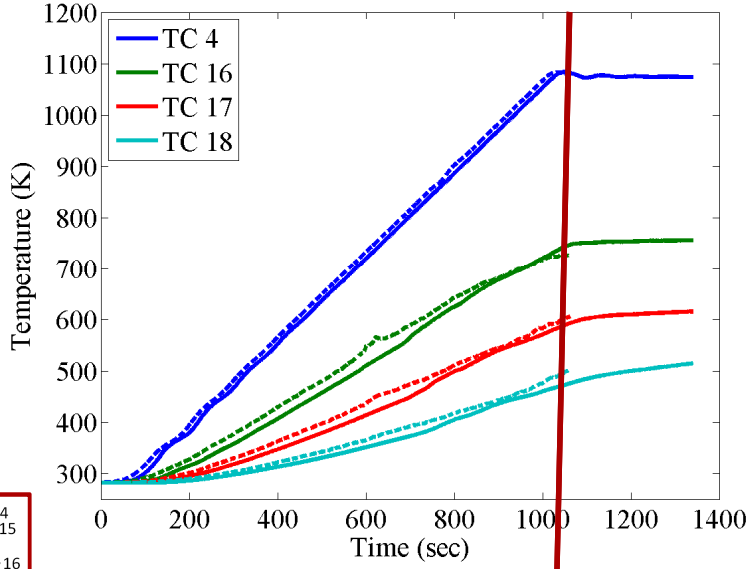


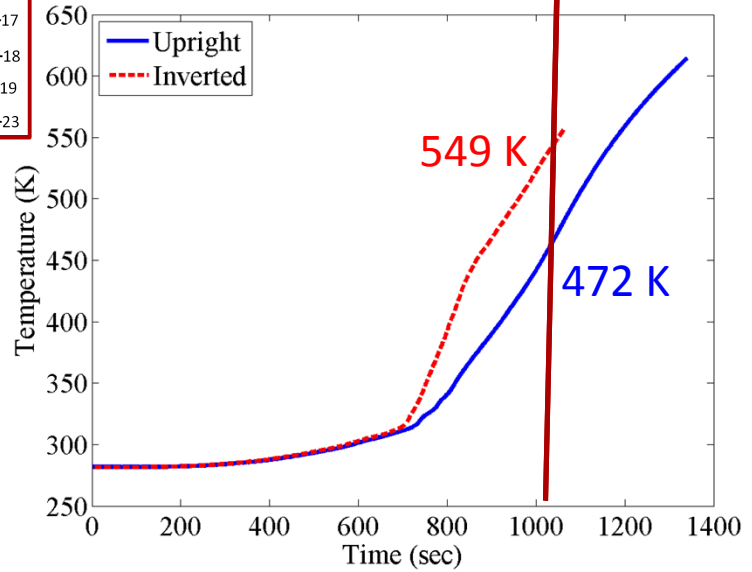






50 C/min





Experimental Results: Summary

- Inverted cans have a steeper pressure increase than upright
- Slower heating rate increases temperature of the embedded object at breach and decreases the pressure at which breach occurs.
- This result indicates that different modes of heat