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Modeling Porous PMDI-based Polyurethane Foam Decomposition in Pressurizing Systems

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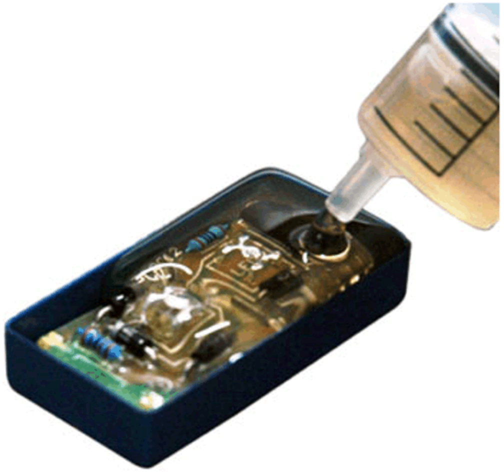
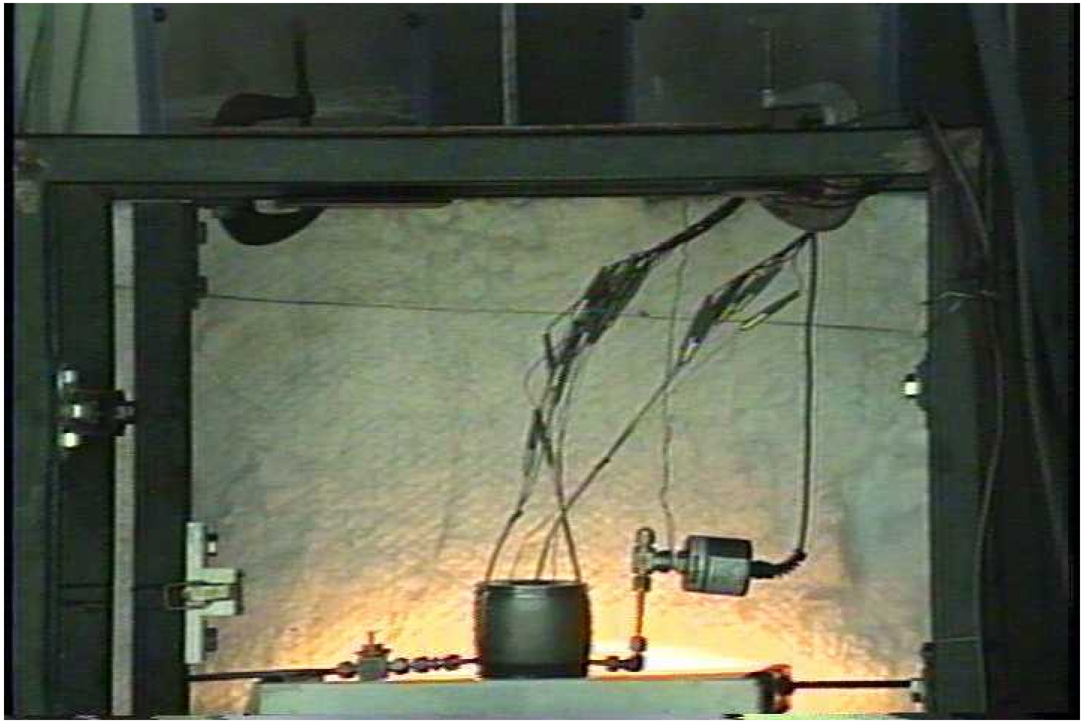
Motivation



- Electronic devices need protection from mechanical and thermal shocks under normal operating conditions
  - Foams can be used for this purpose
- Foams pyrolyze at relatively low temperatures (250C – 300C)
  - In a fire environment and in sealed systems, the foam pyrolysis can cause pressurization
- Need a model of heat transfer and pressurization
- Medium scale experiments for validation

Foam in a Can



Encapsulating 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

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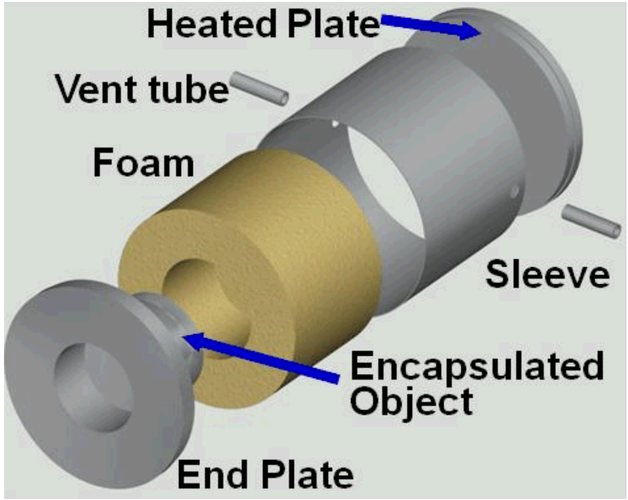
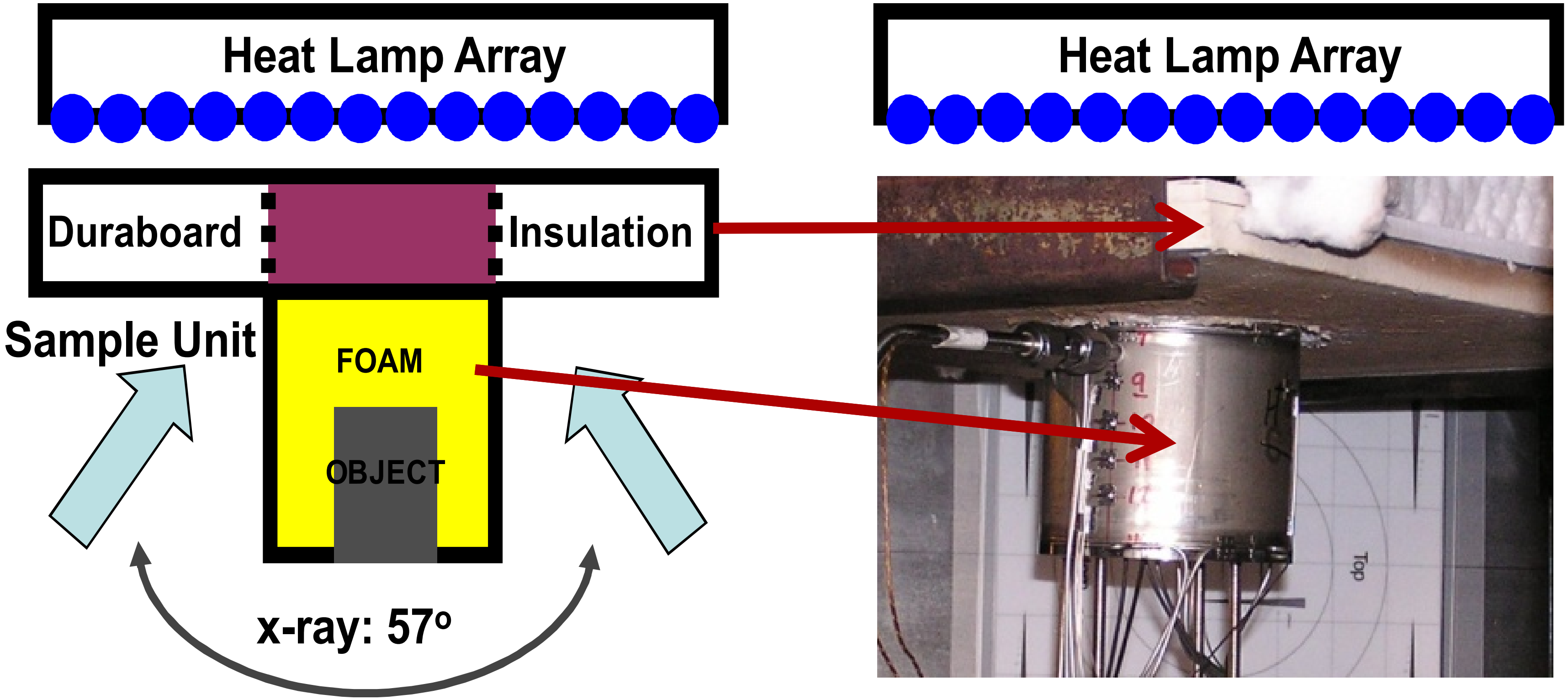


- Data Sets:
  - 320 kg/m^3 PMDI polyurethane foam (rigid, closed cell)
  - Heated to 800 C at a rate of 150 C/min and 50 C/min.
- Can dimensions are approximately
  - Diameters: 9 cm
  - Length: 6.5 cm
  - Side Wall Thickness: 0.5 mm

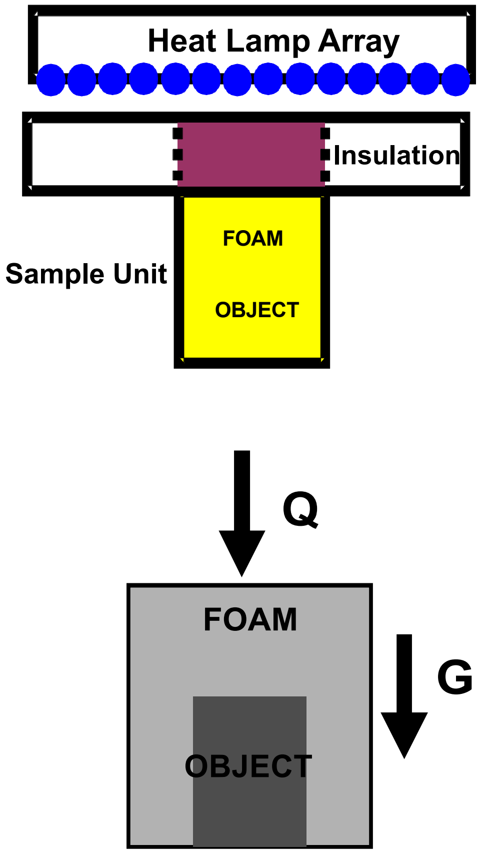
Foam in a Can Experiment



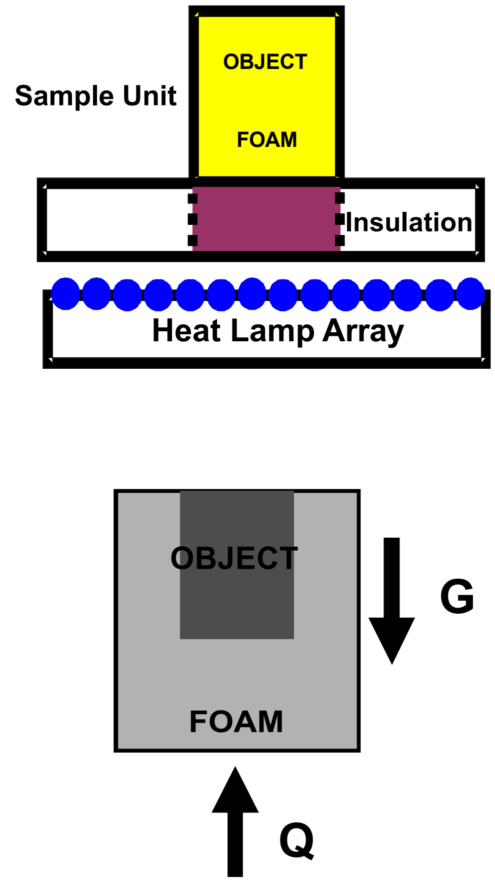
- Monitor pressure and temperature
- X-Rays to view can interior
- Experiments run to breach

Foam in a Can Experiment

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

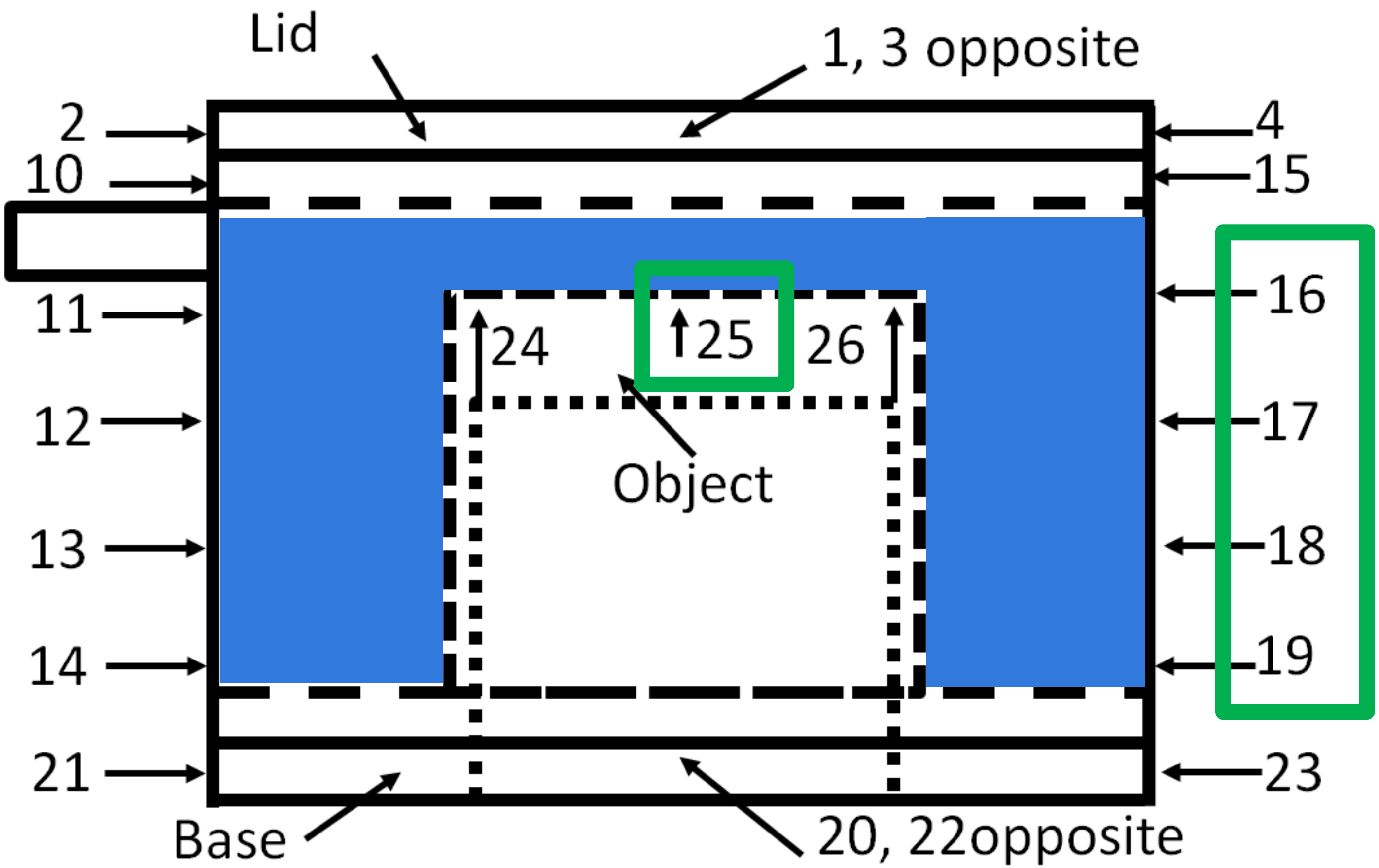


Upright – 0°



Inverted – 180°

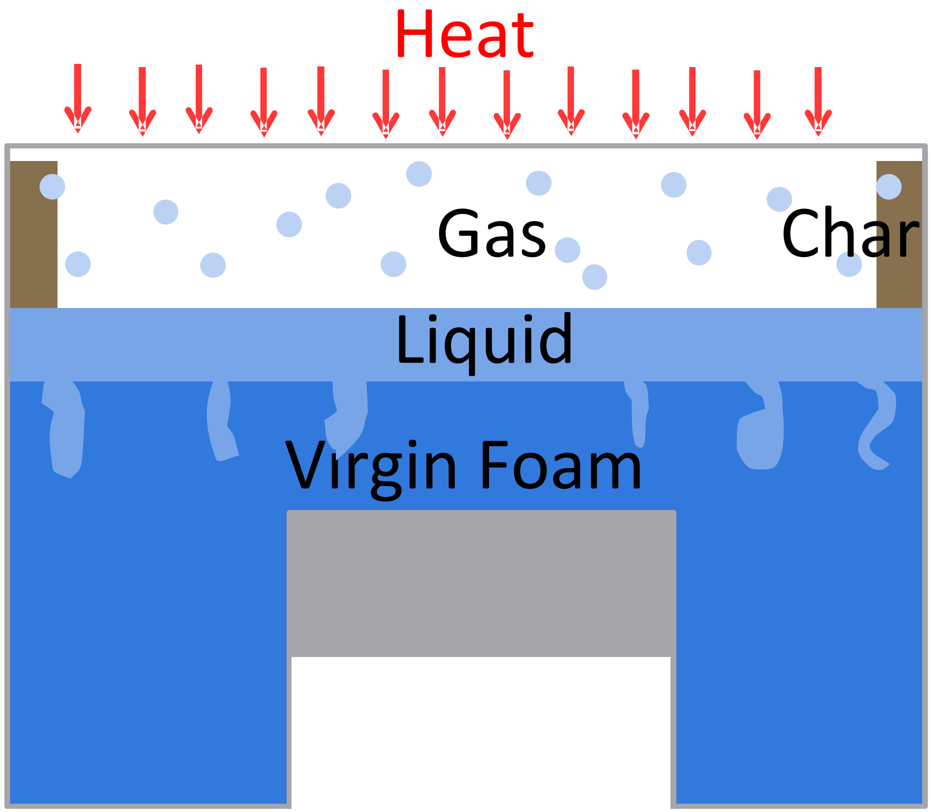
Foam in a Can Experiment



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

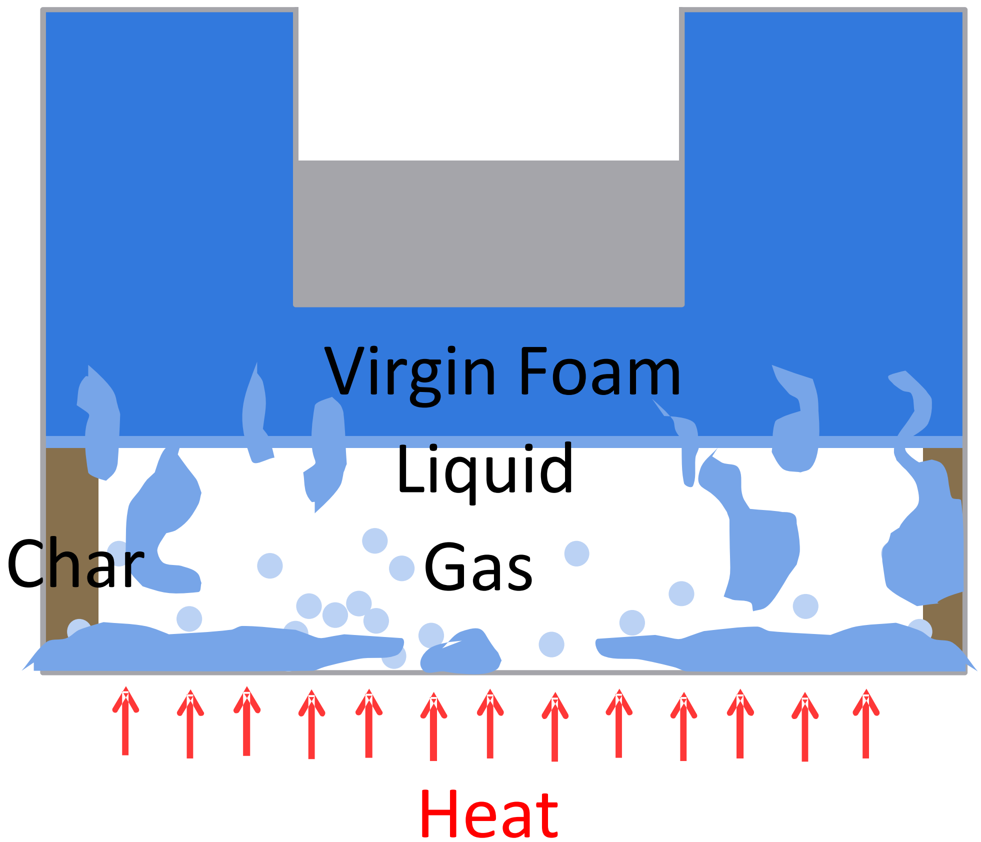
Decomposing Foam

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

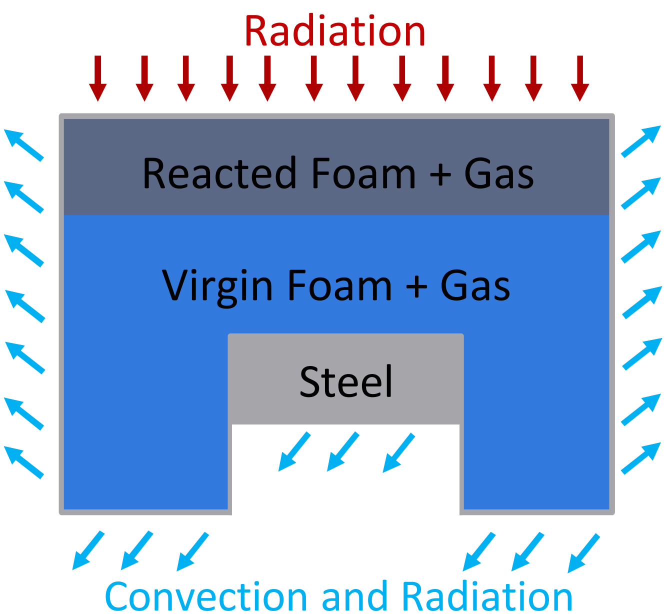


Decomposing Foam

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



Porous Flow Model Description



- 3D Model in Aria
- Three step reaction mechanism
  - PMDI Polyurethane -> CO_2, light and heavy organics (gas phase), char
- Continuity, species, and enthalpy equations
  - Solved for in condensed and gas phases
  - Gas velocity solved using Darcy's approximation for flow through a porous material
  - Ideal gas law used to relate density to pressure
  - Radiative and Convective boundary conditions
- Material Properties
  - Foam Effective Conductivity, Foam Porosity, Foam Permeability
    - Function of reaction
  - Other material properties
    - Constant or function of temperature

Parameter Calibration/Optimization

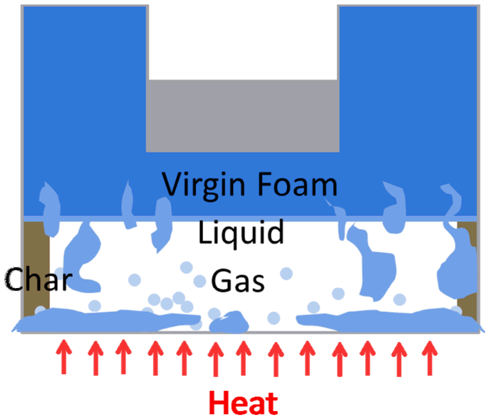
- Porous media equations introduce variables into that are unknown
  - Virgin foam permeability
    - The foam is closed cell, therefore a permeability can't be tested.
    - Virgin Foam Range: 10^{-14} to 10^{-7}
  - Char foam permeability
    - Can't be measured in-situ
    - Char Foam Range: 10^{-8} to $10^{-6.5}$
  - Organic gas fraction
    - Unclear what fraction of the decomposition products are in the gas vs condensed phase
    - Range: 0 to 0.44
  - Rosseland-mean extinction coefficient (β_R) to calculate the radiation contribution to the effective conductivity in the char
    - Absorption and scatter can't be measured in-situ
    - Range: 200 to 1990

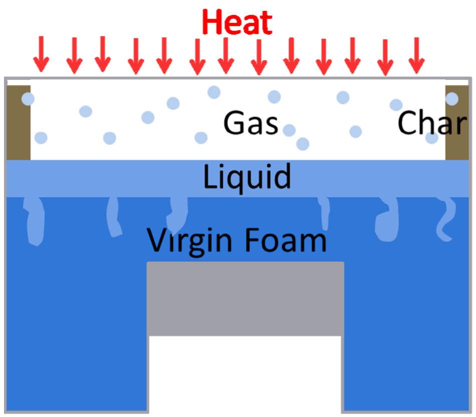
Organic Gas Fraction

$$PMDI\ RPU \ = 0.45\ FOAMA + 0.15\ FOAMB + 0.4\ FOAMC$$

$$FOAMA \rightarrow [0.56\ ]CO_2 + [\ 0.44 - gasorg]LMWO + [gasorg]char$$
$$FOAMB \rightarrow [1 - 2 * gasorg]HMWO + [2 * gasorg]char$$
$$FOAMC \rightarrow [0.5 - gasorg]\ HMWO + [0.5 + gasorg]\ char$$

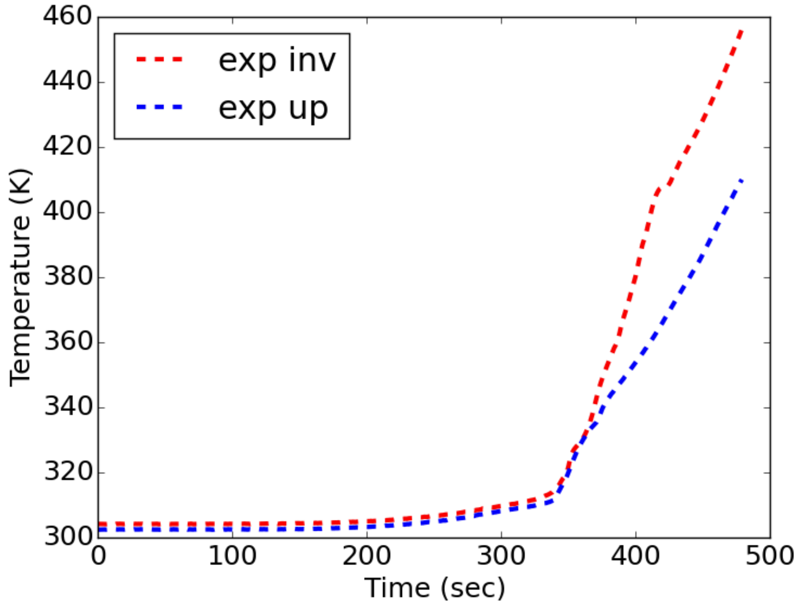
- Varied from 0 to 0.44
- Separate values for inverted and upright to approximate liquid dripping

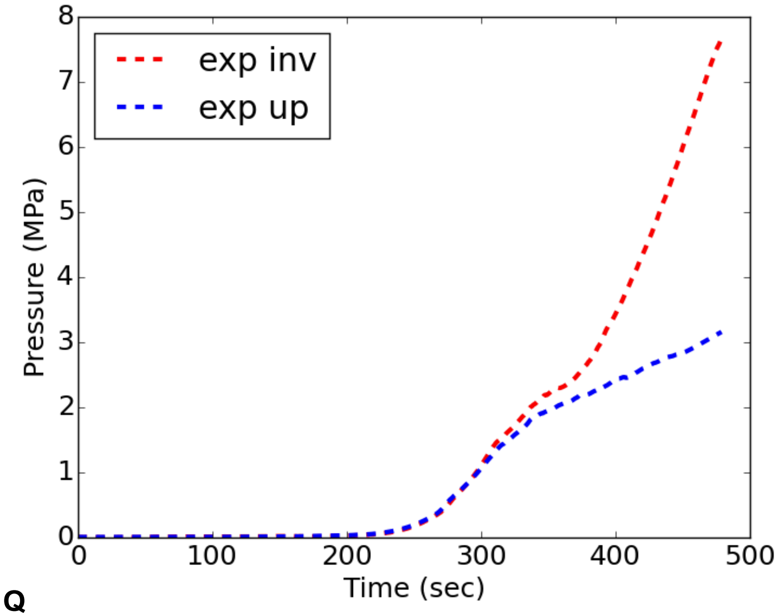


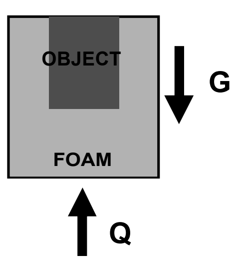


Parameter Calibration/Optimization

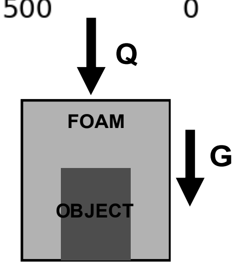
- Global method was used
- Pressure and temperature of the slug are the optimized response quantities (from 150 C/min data set)



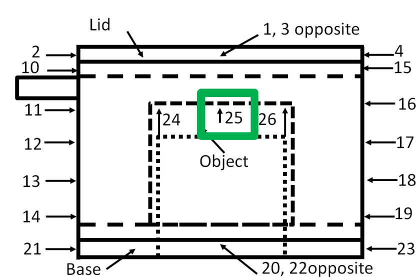




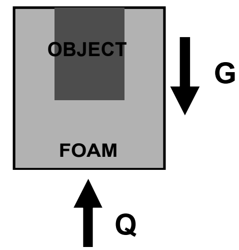
Inverted – 180°



Upright – 0°



150 C/min



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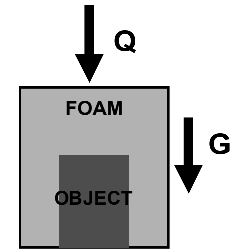

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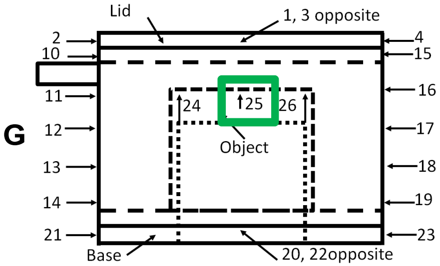
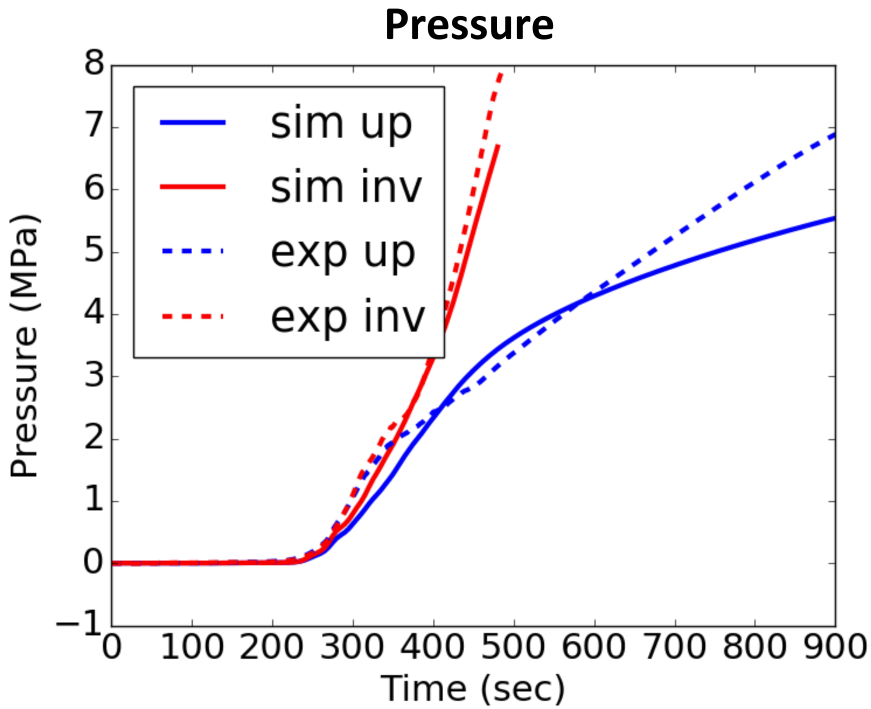
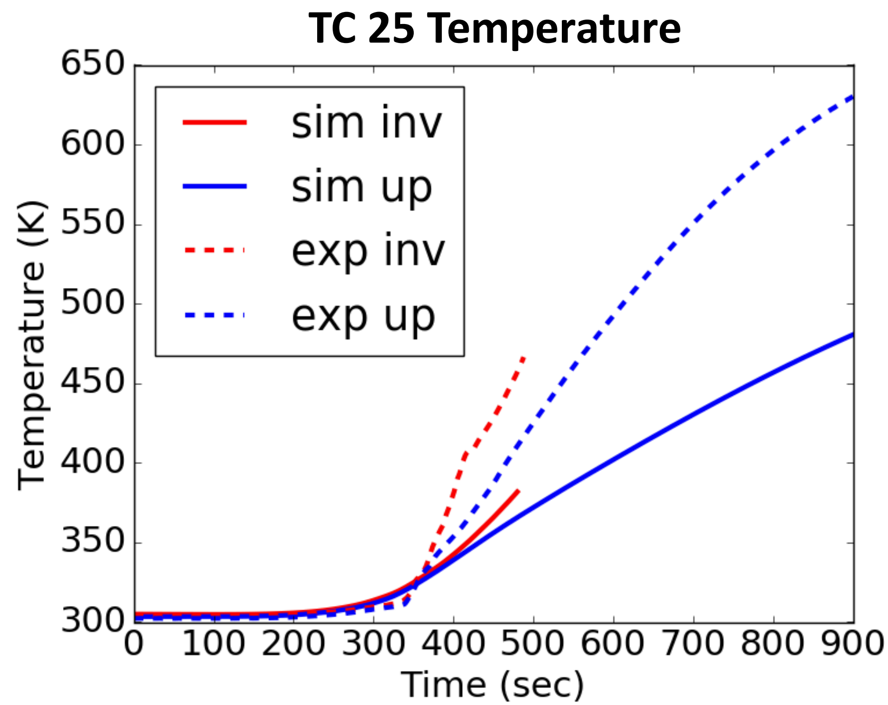
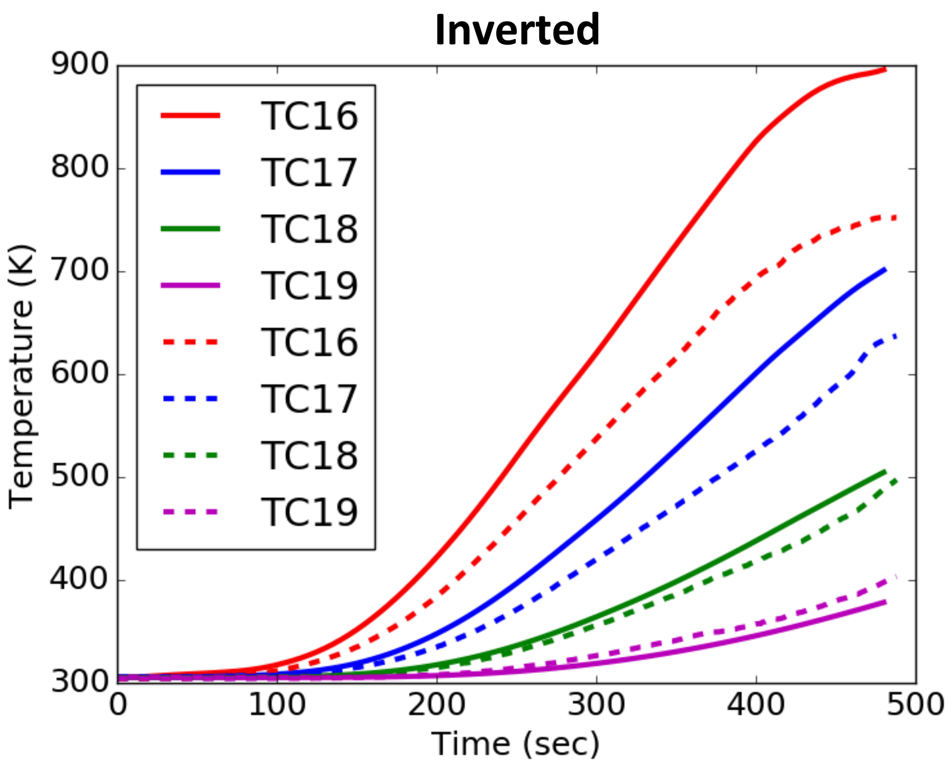


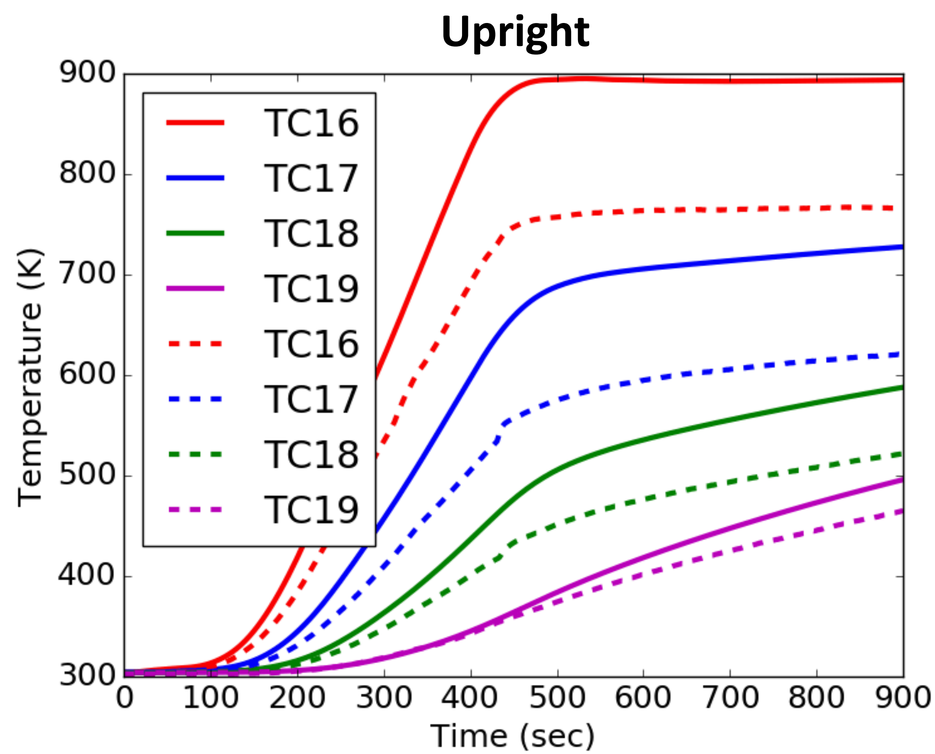


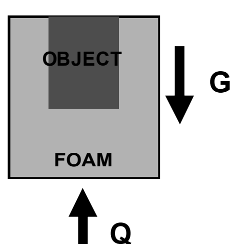


	Low Bound	High Bound	Optimized Value
Virgin Foam Permeability [m^2]	$1x10^{-14}$	$1x10^{-8}$	$7.76x10^{-13}$
Char Foam Permeability [m^2]	$1x10^{-8}$	$1x10^{-6.5}$	$1.48x10^{-8}$
Upright Organic Gas Fraction	0	0.44	0.37
Inverted Organic Gas Fraction	0	0.44	0.22
Char β_R [mK]	200	1990	579

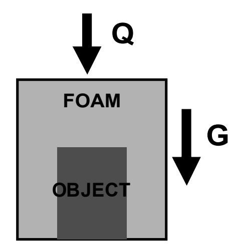
150 C/min



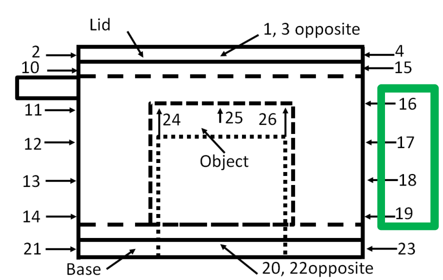




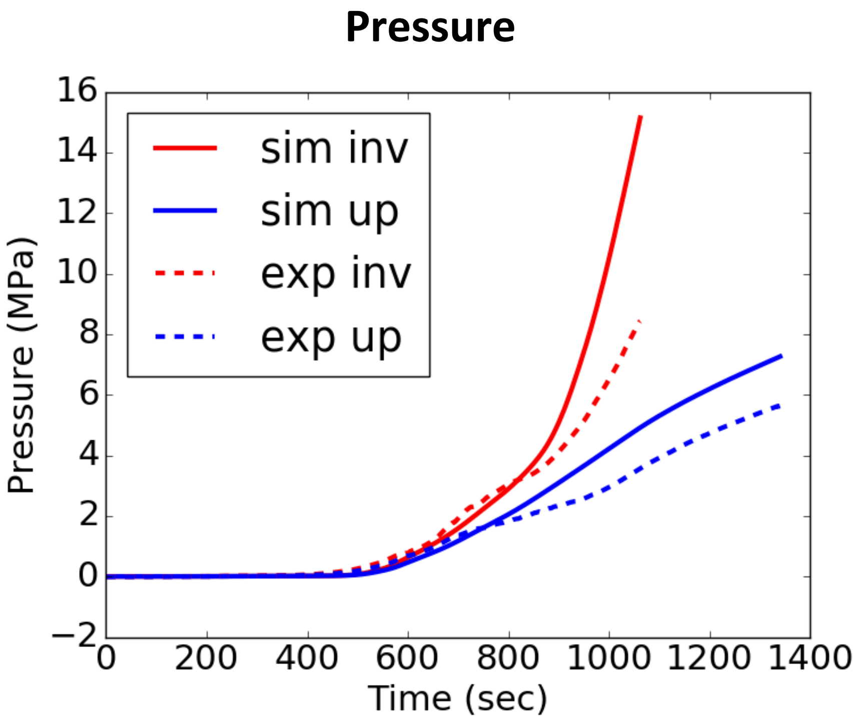
Inverted – 180º

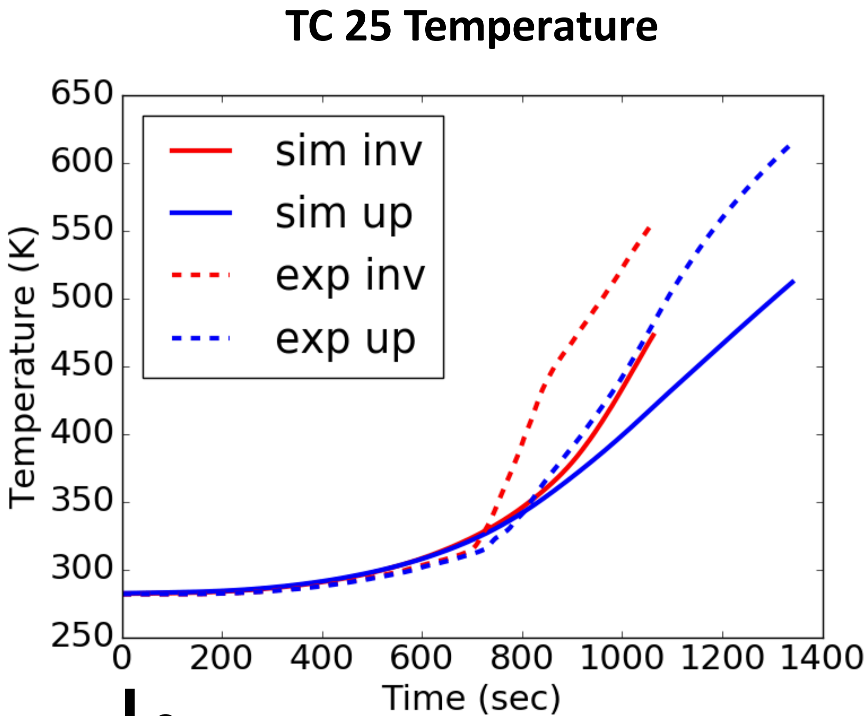


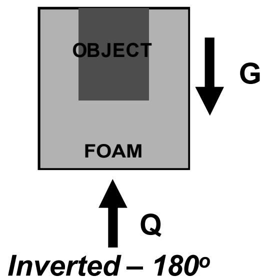
Upright – 0º

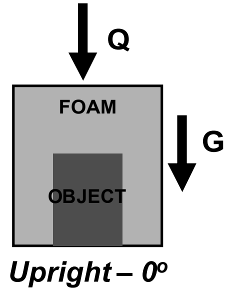


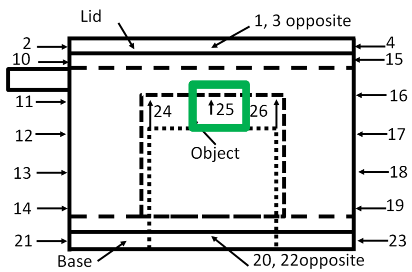
50 C/min


Pressure
sim inv
sim up
exp inv
exp up
Pressure (MPa)
Time (sec)


TC 25 Temperature
sim inv
sim up
exp inv
exp up
Temperature (K)
Time (sec)

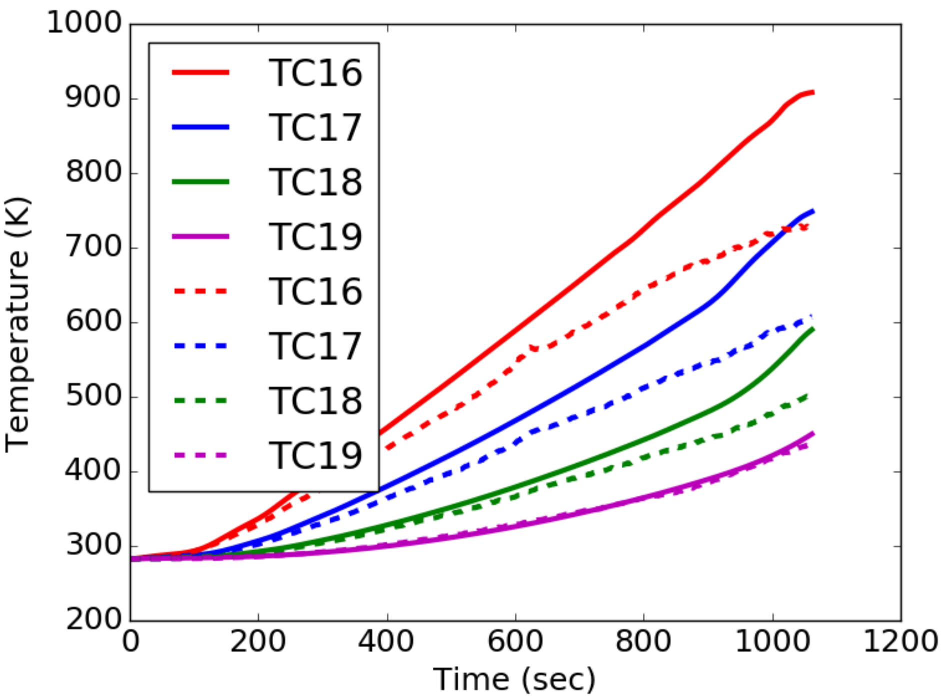

OBJECT
FOAM
G
Q
Inverted – 180°


Q
FOAM
OBJECT
G
Upright – 0°

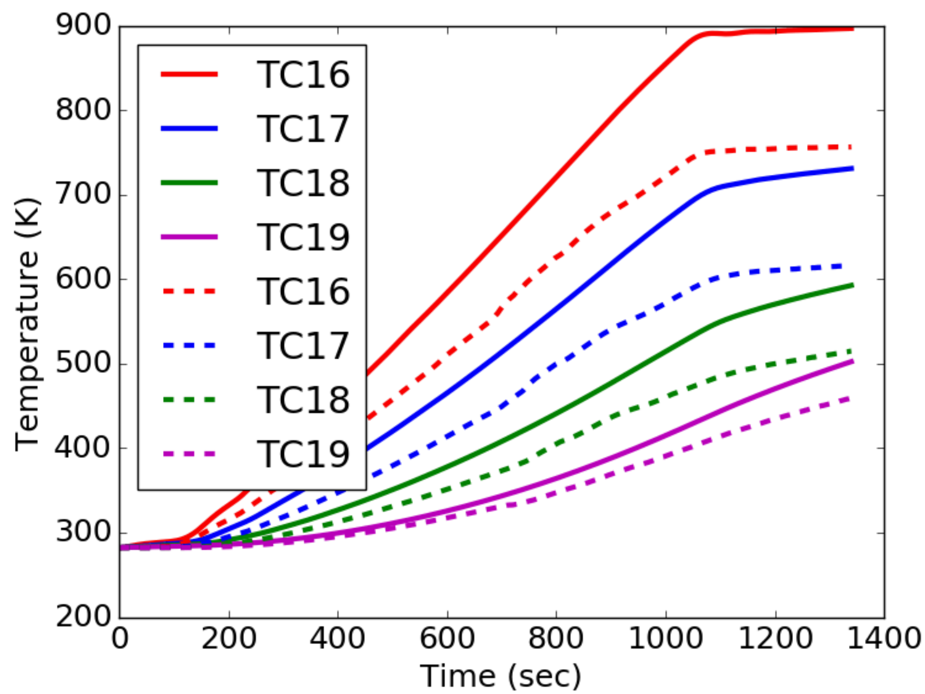

Lid
1, 3 opposite
Object
Base
20, 22opposite

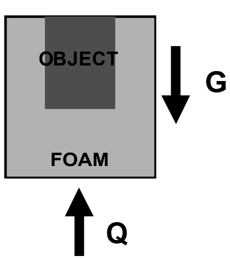
50 C/min

Inverted

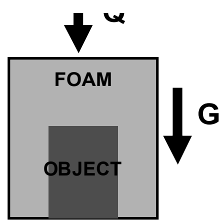


Upright

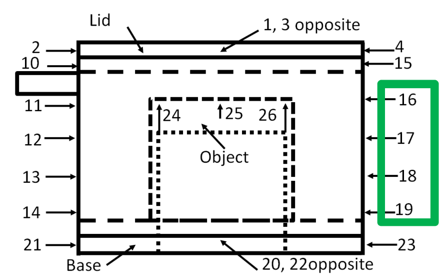




Inverted – 180°

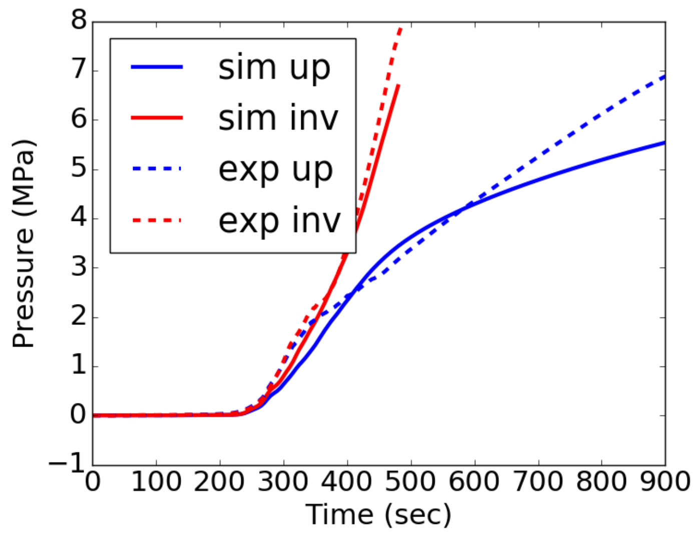


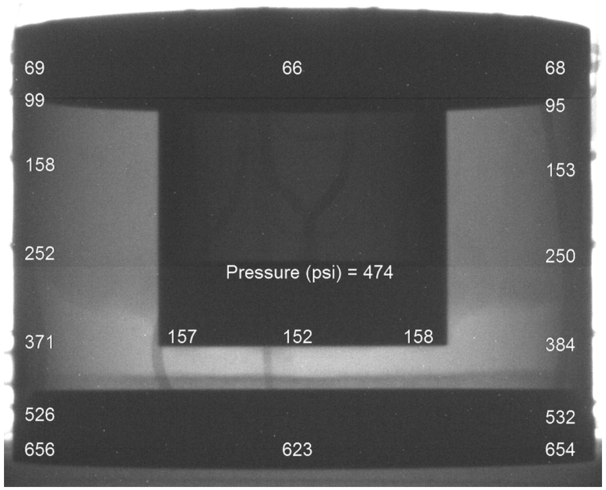
Upright – 0°

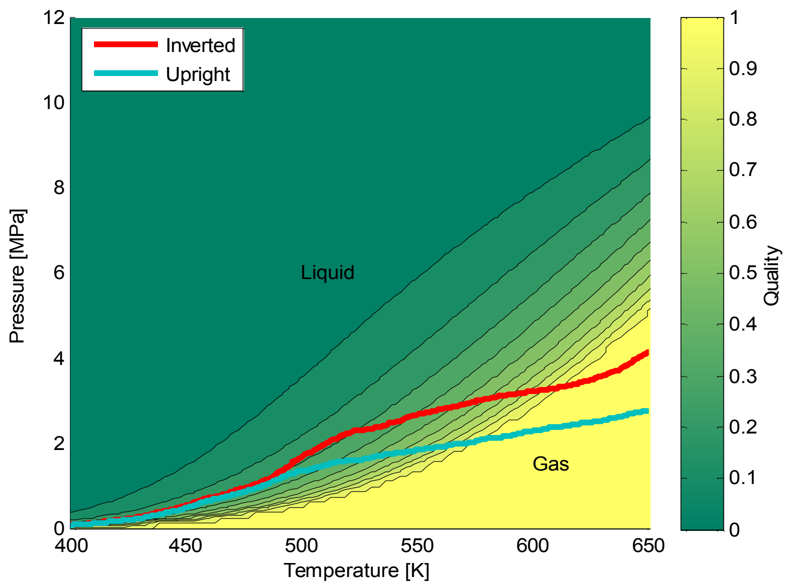


Future Work - Vapor Liquid Equilibrium

- This study more closely matched experimental data when separate values controlled the rate of gasification
- X-Rays of the experiments show what looks to be liquid decomposition products
- Early investigations show that major decomposition products can be liquids at pressures and temperatures seen in the experiments.







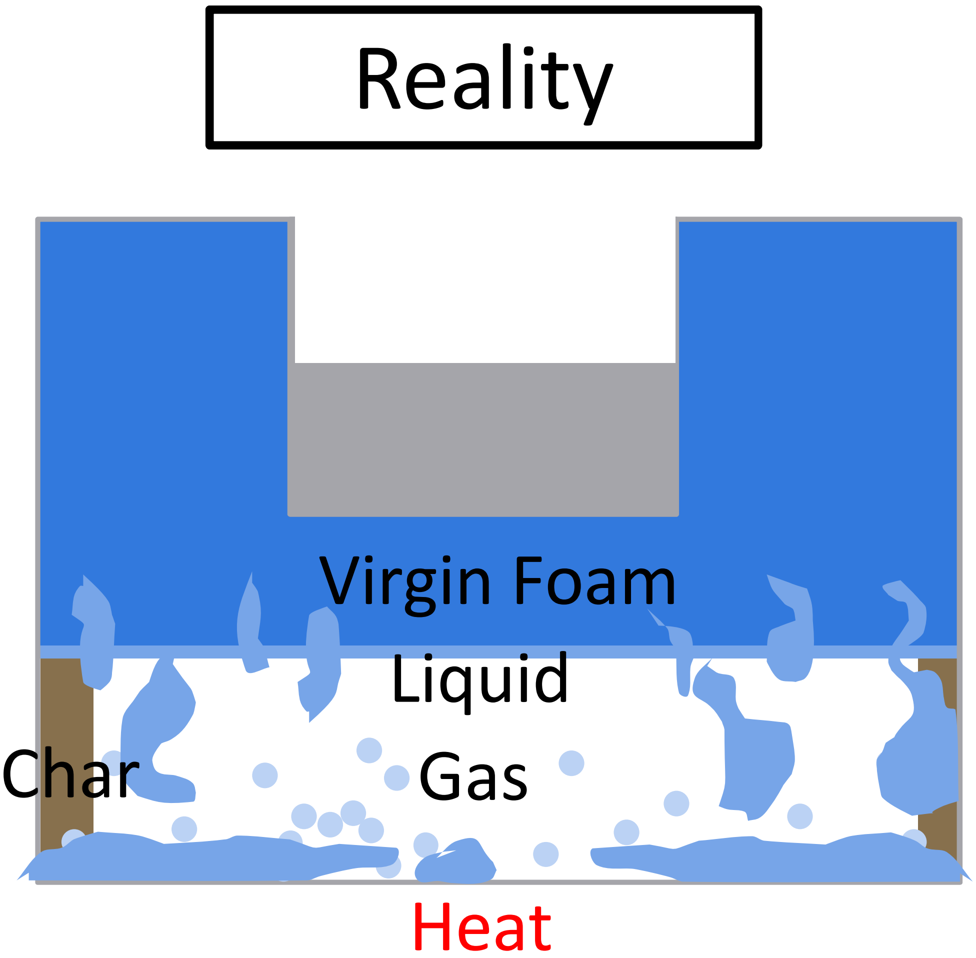
QUESTIONS?

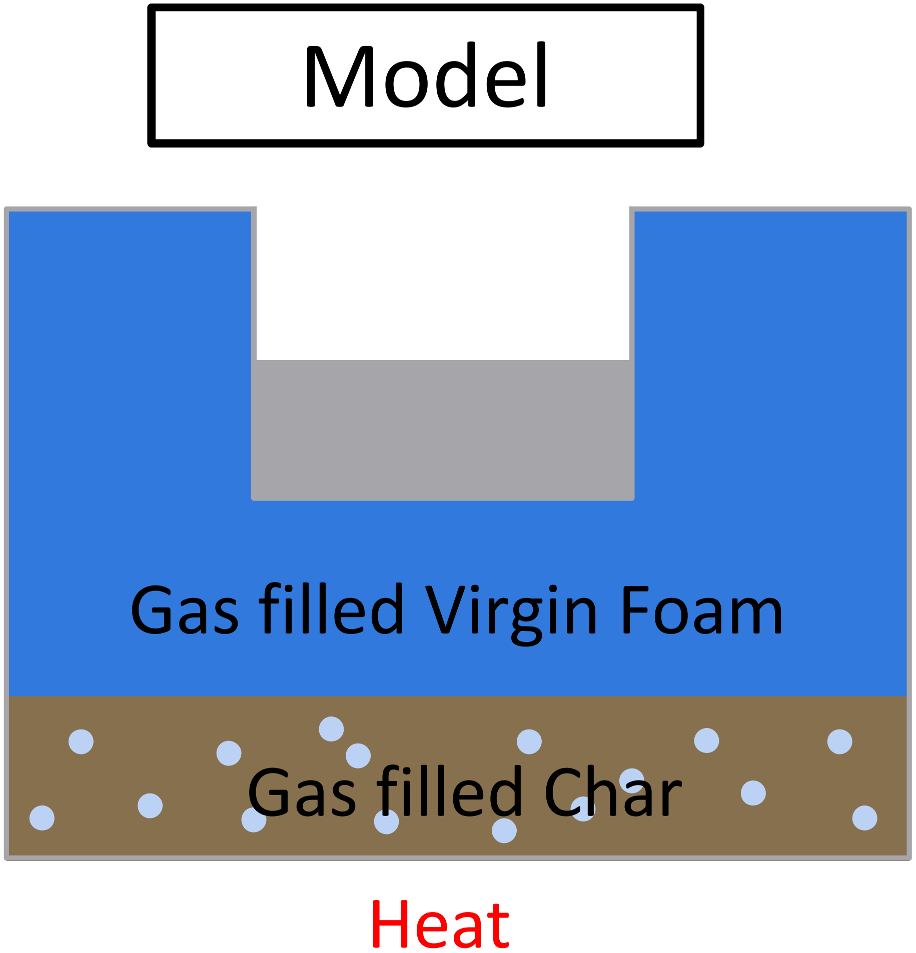
Previous Work

- Previous Model Development
  - No flow model
    - Model developed with foams that leave structured char
      - Good agreement in temperature and pressure with experiments
    - Erickson, K.L, *et al*. Proceedings of BCC 2010, Stamford, CT, May 2010
- Previous PMDI Polyurethane Development using Erickson (no flow) model
  - Scott, S.N., *et al*. Fire Technology Dec 2014
    - Validation of 150 C/min data set
    - Mean Value and Latin Hyper Cube were compared
  - Scott, S.N., *et al*. Mediterranean June 2015
    - Want understand the effect of heating rate

BACKUP SLIDES

Modeled Physics





Permeability

- Appears in the Darcy approximation

Permeability

Flow velocity → $$u_{j,g} = -\frac{\bar{K}}{\mu_g}\left(\frac{\partial P_g}{\partial x_j} + \rho_g g_j\right)$$ ← Body Force

Gas Viscosity

Pressure Gradient

- Virgin Foam Range: 10^{-18} to 10^{-7}
- Char Foam Range: 10^{-9} to 10^{-6}
- Exponent is varied
- Check to ensure Virgin Foam Permeability is lower than Char Foam Permeability

Rosseland-mean Extinction Coefficient

Radiation Effective Conductivity → $k_{rad} = \frac{16\sigma}{3\boldsymbol{\beta_R}} T^3$ ← Temperature

Stefan-Boltzmann (σ)

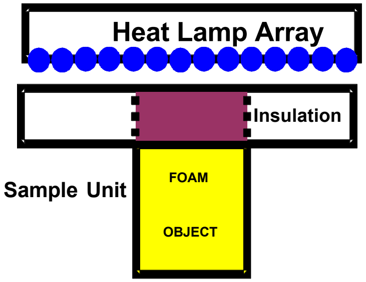
Rosseland-mean Extinction Coefficient (β_R)

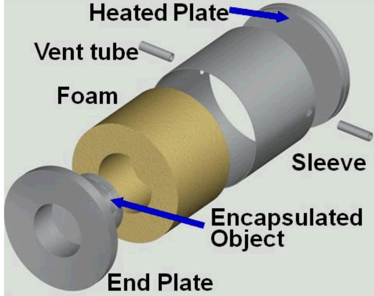
- Varied from 200 to 1900

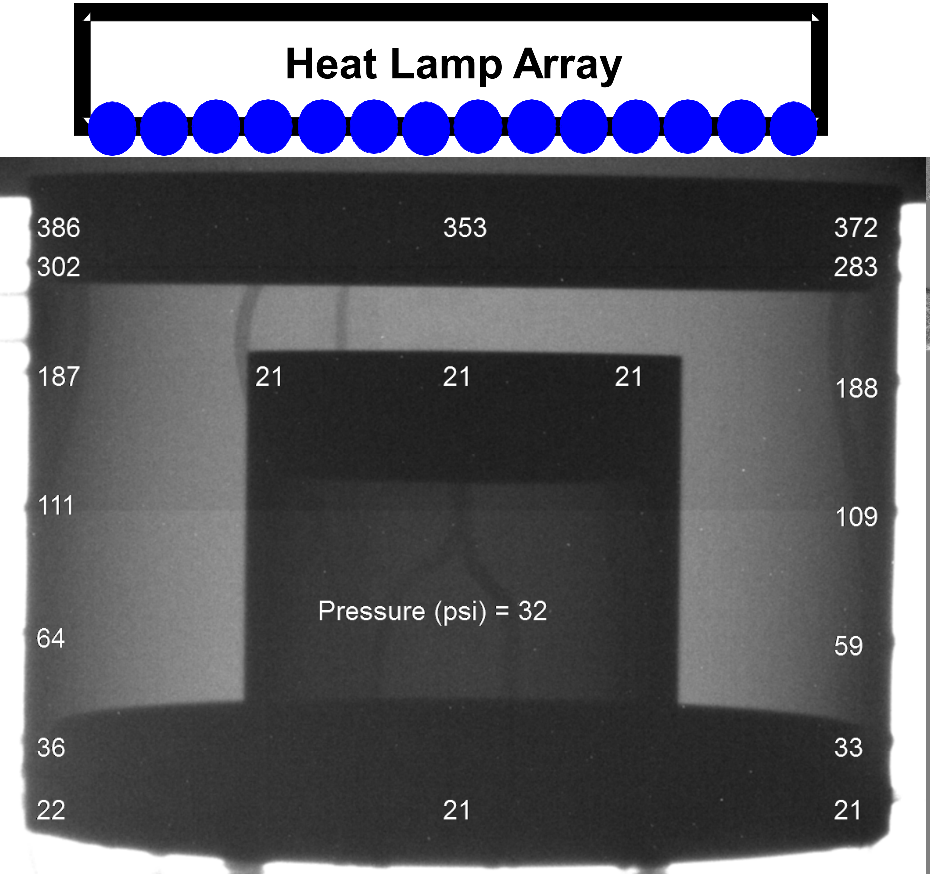
X-Ray Video

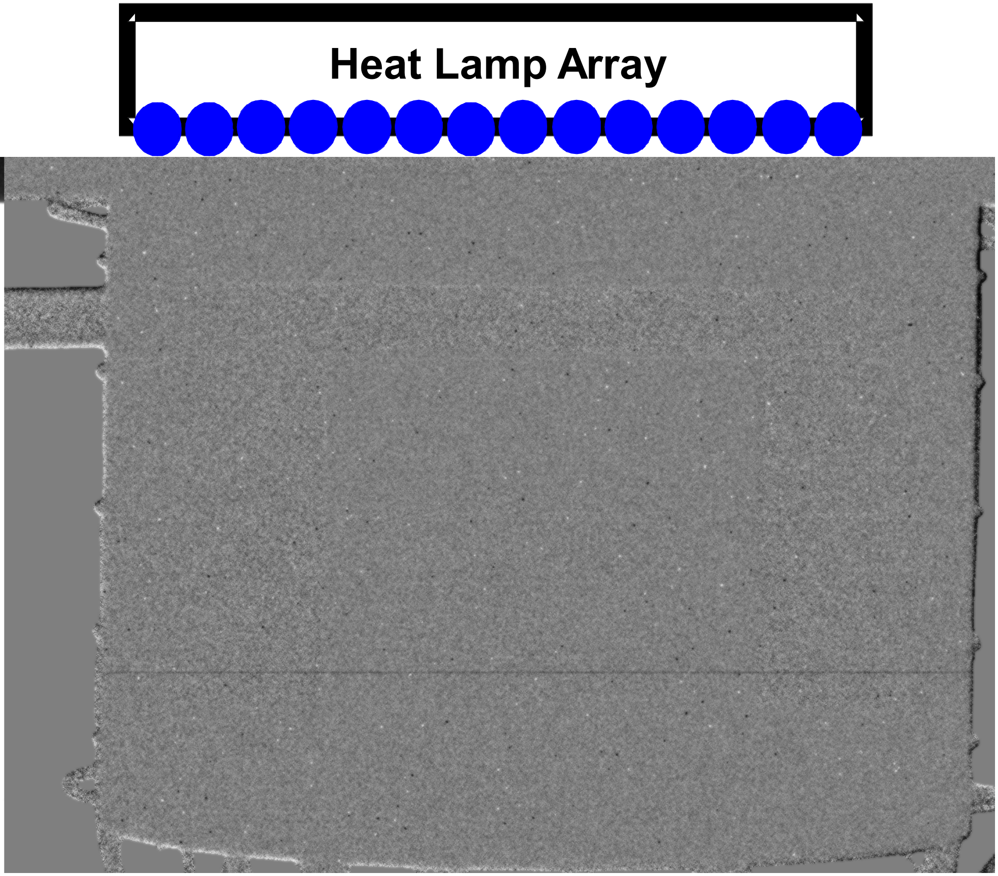
Upright Experiment

50 C/min









X-Ray Video

Inverted Experiment
50 C/min