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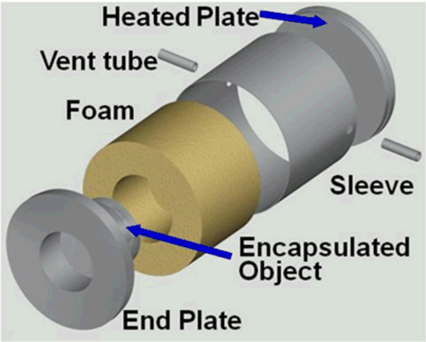

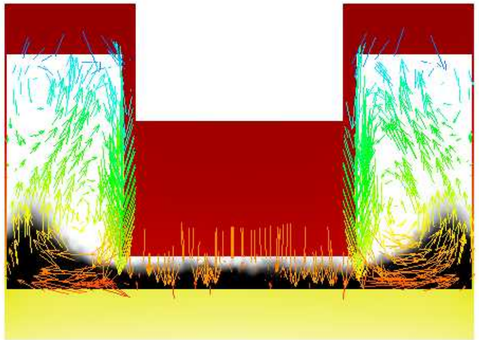

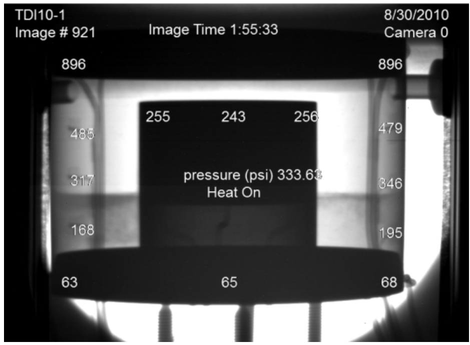

Uncertainty Quantification Assessment of Porous Media Modeling of Polyurethane Foam in a Sealed Container (VVS2015-8080)

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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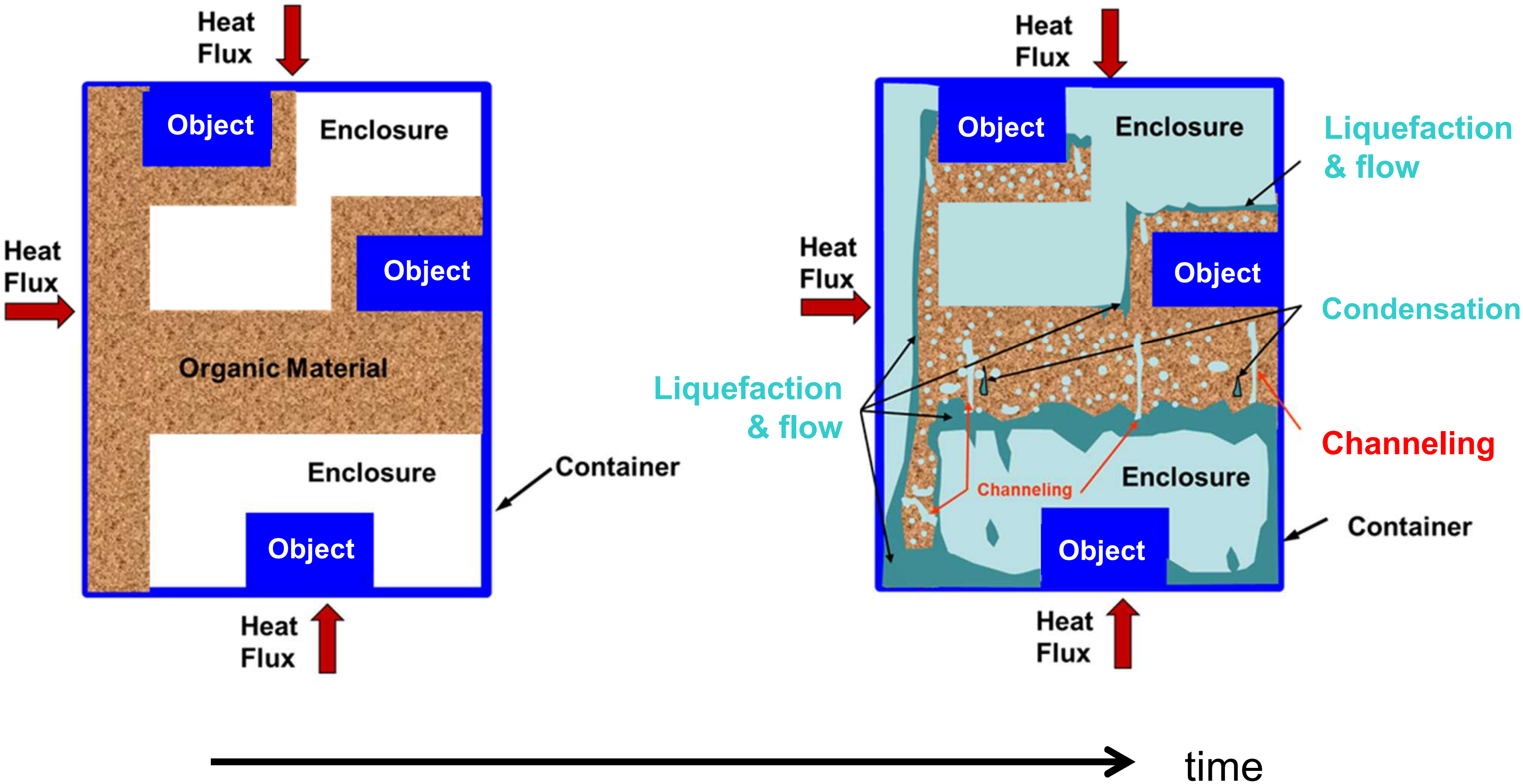
Presentation Outline

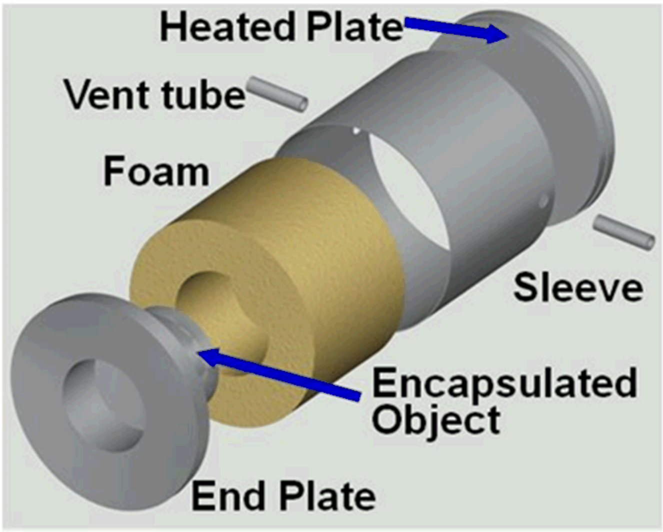
- Introduction to Organic Material Decomposition (OMD)
- Foam-in-Can Validation Experiments
- Simulation Capabilities
  - Porous media model
- Latin Hypercube Study (LHS)
  - Validation vs. Experiment
  - Parameter Sensitivities
- Future Work

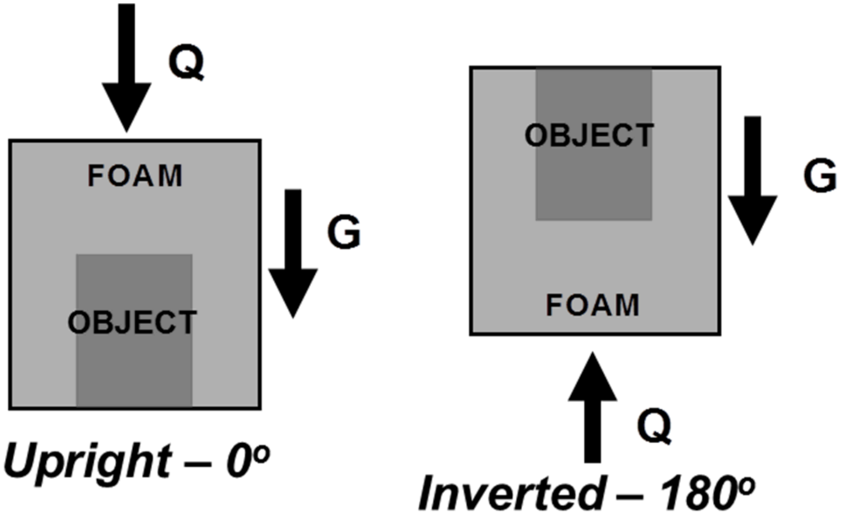
Organic Material Decomposition

Subject to heating (e.g. fire), porous foams open up and/or liquefy and decompose into char and products (gas+liquid)

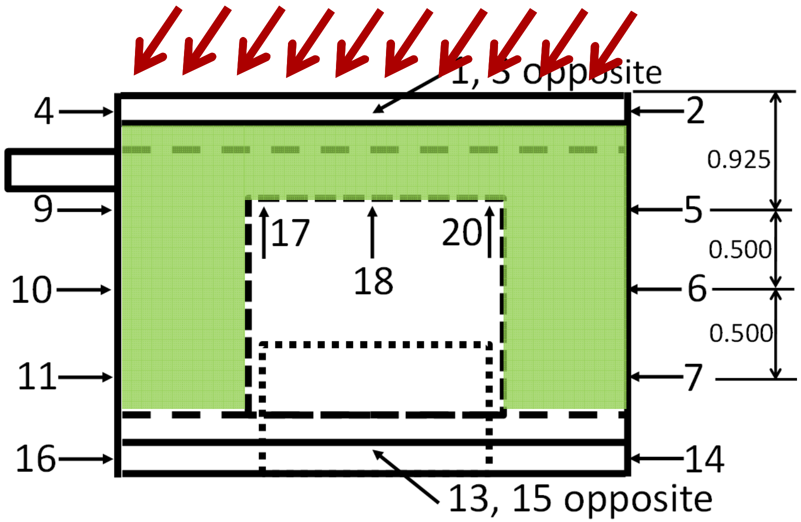


Validation Experiments



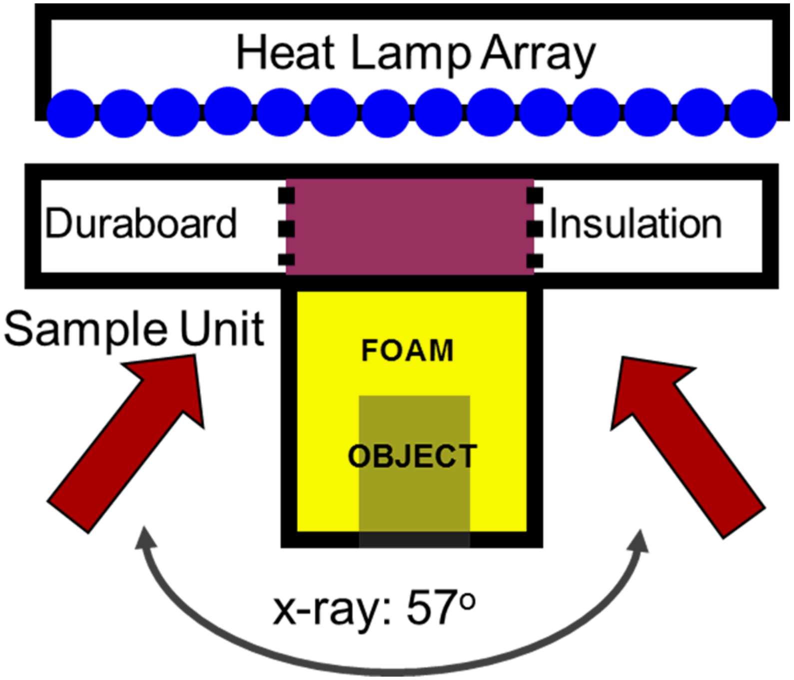


Heat applied such that can surface increases at 200 °C/min up to 900 °C



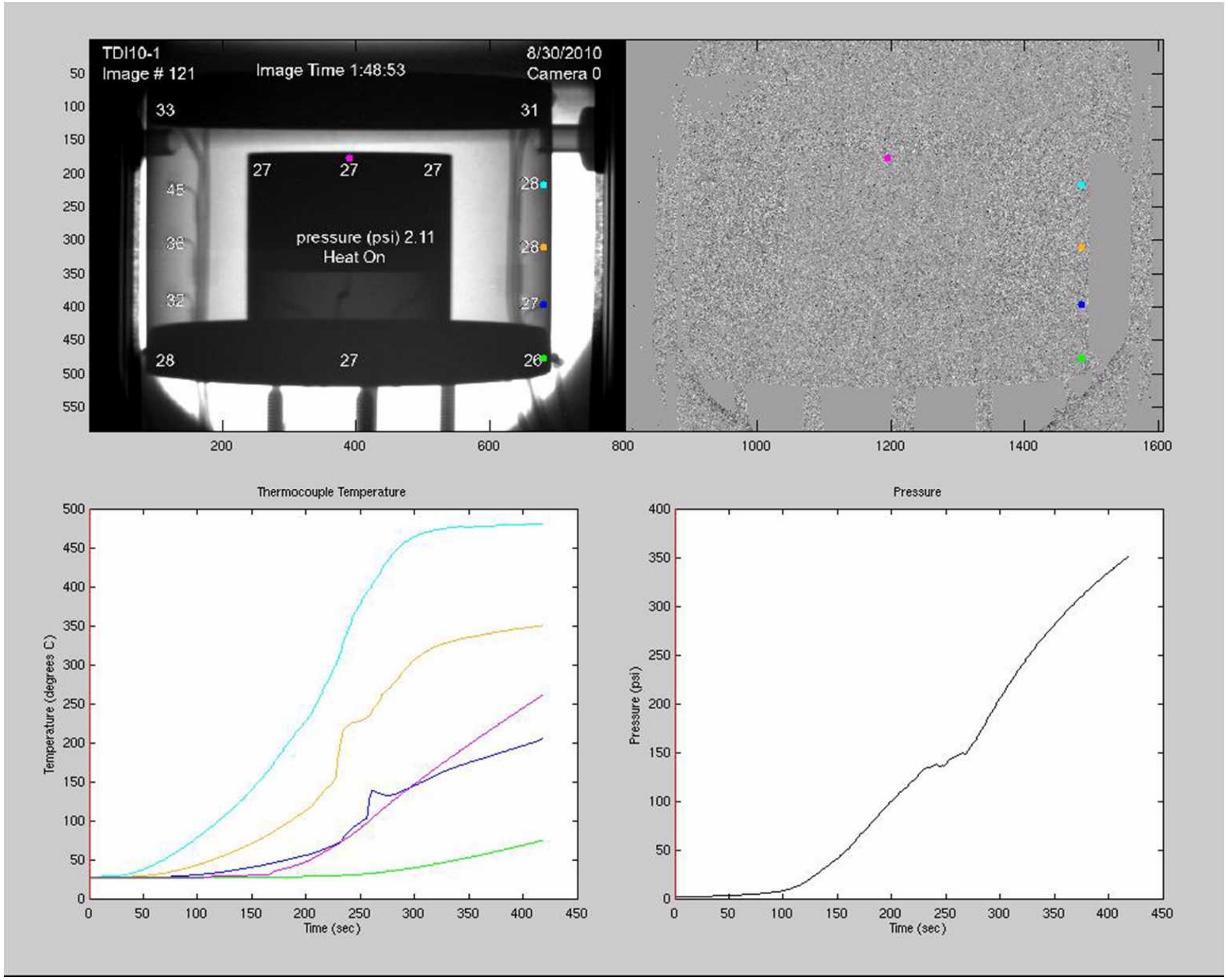
Polyurethane foam (TDI)
10 lb/ft³ (160 kg/m³)

Additional Experimental Figures



- Sample container
  - Sleeve 321 SS tubing
    - 8.89-cm OD, 5.40 cm long
    - 1.651-mm wall thickness
  - End plates: 0.602-cm thick 304 SS
    - Laser welded to Sleeve

Video of Experiment (Upright)

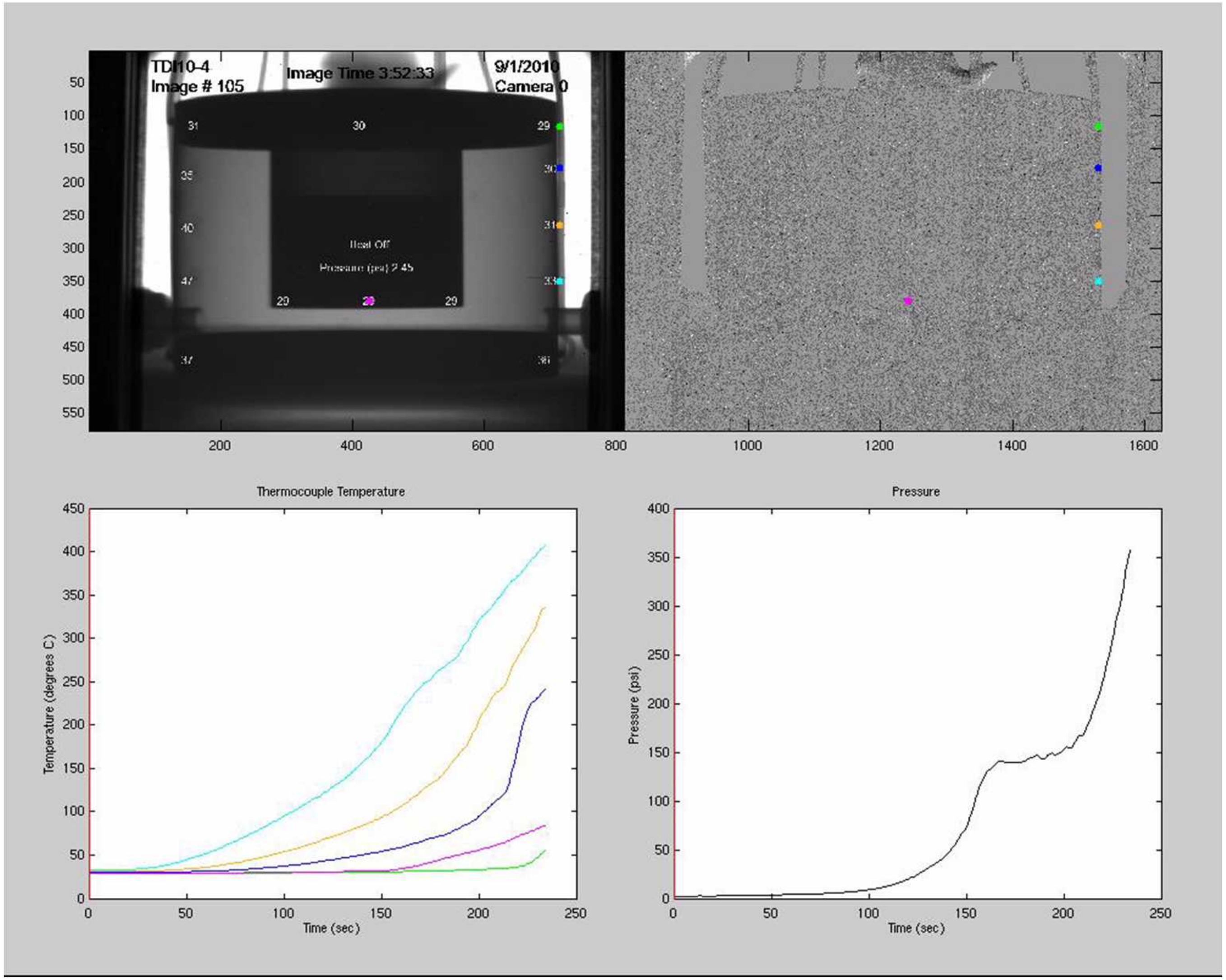


Temperature

Pressure

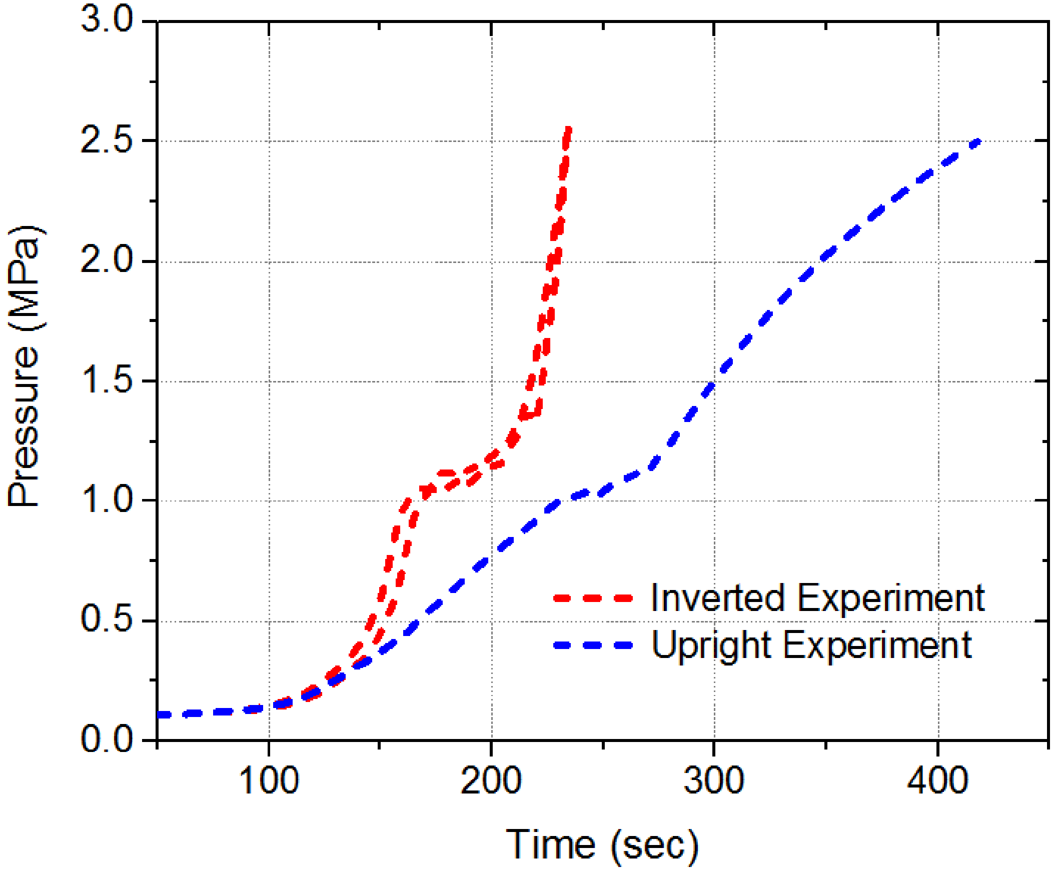
Video of Experiment (Inverted)

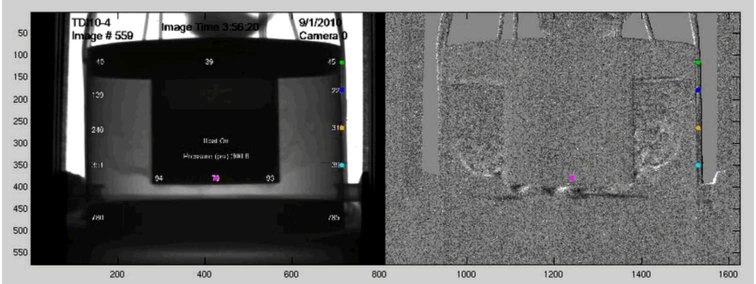
Temperature

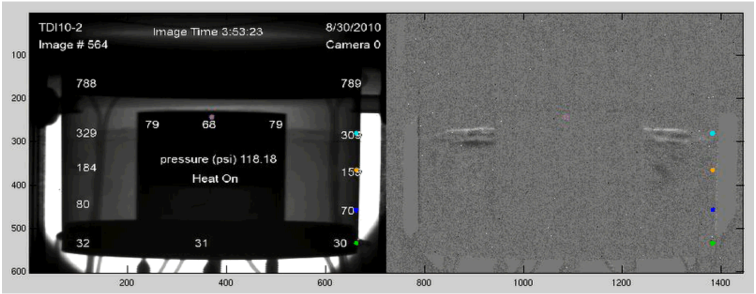


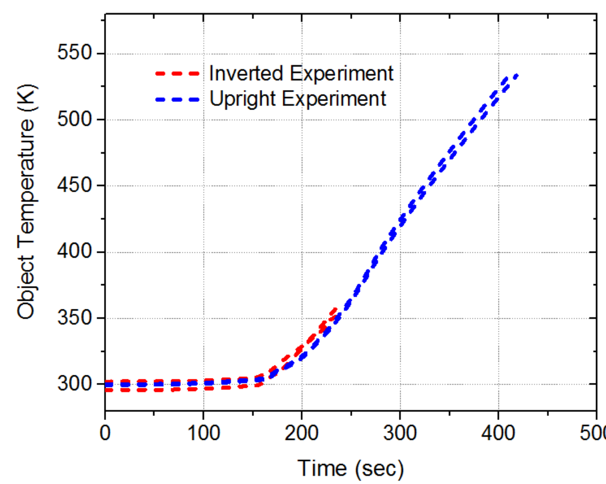
Pressure

Orientation Strongly Affects Pressurization









Simulation Approaches

Simulations were conducted with Aria – a multi-physics code that is part of the Sierra code suite

Previous

One-Temperature Effective Conductivity Model

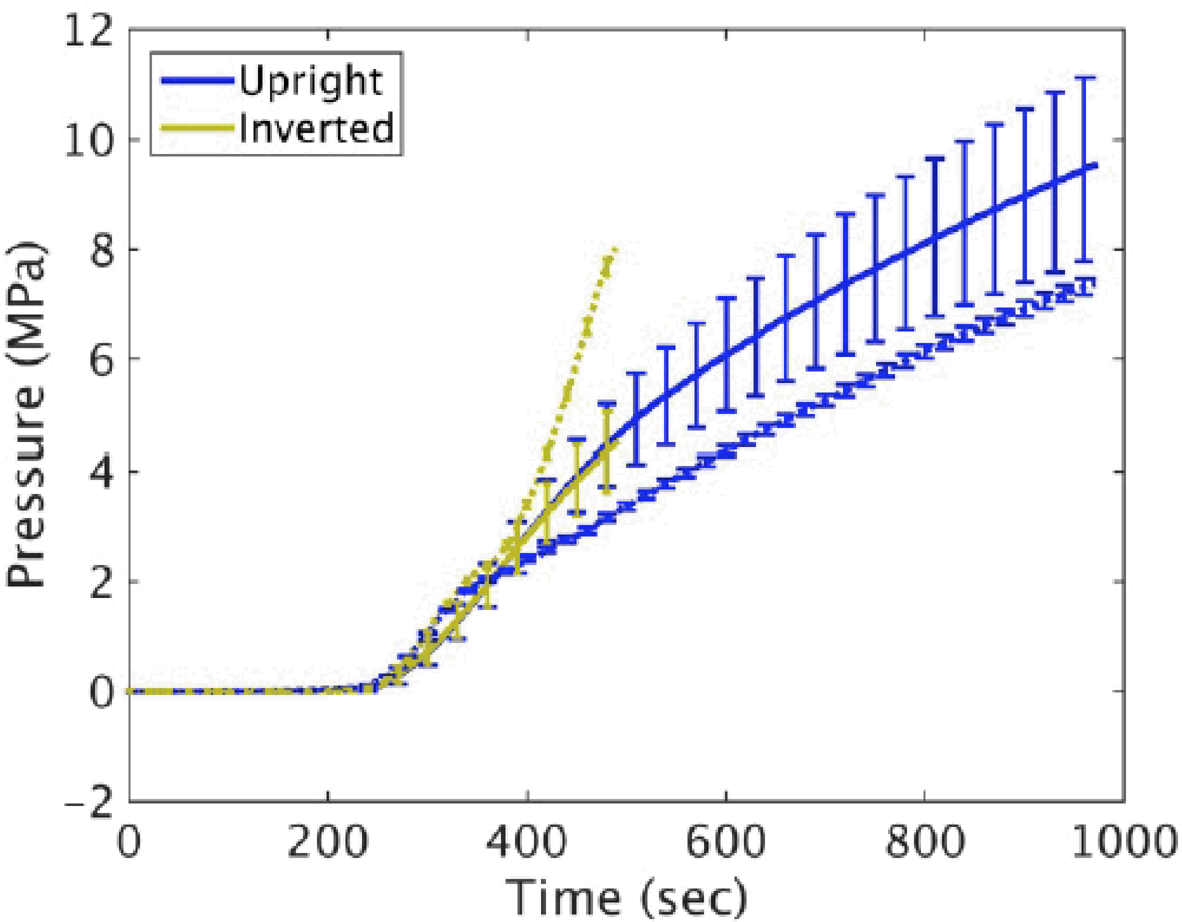
- *Energy conservation for metal and foam materials*
- *Chemical decomposition kinetics predict foam decomposition rate as a function of temperature*
- **Bulk pressure calculation**

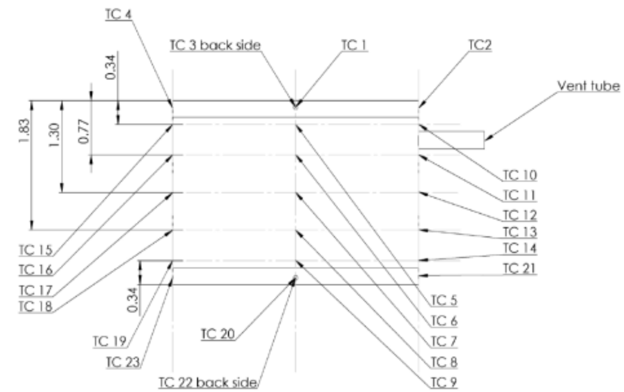
New

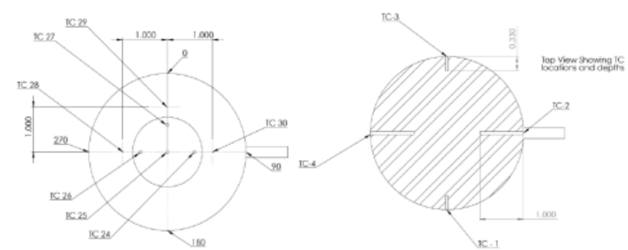
Porous Media Model

- *Energy conservation for metal and **both gas and solid phases of foam materials***
- *Chemical decomposition kinetics predict foam decomposition rate as a function of temperature*
- **Porous flow transport equations (spatially varying pressure)**
- **Species conservation**

Previous Validation Summary

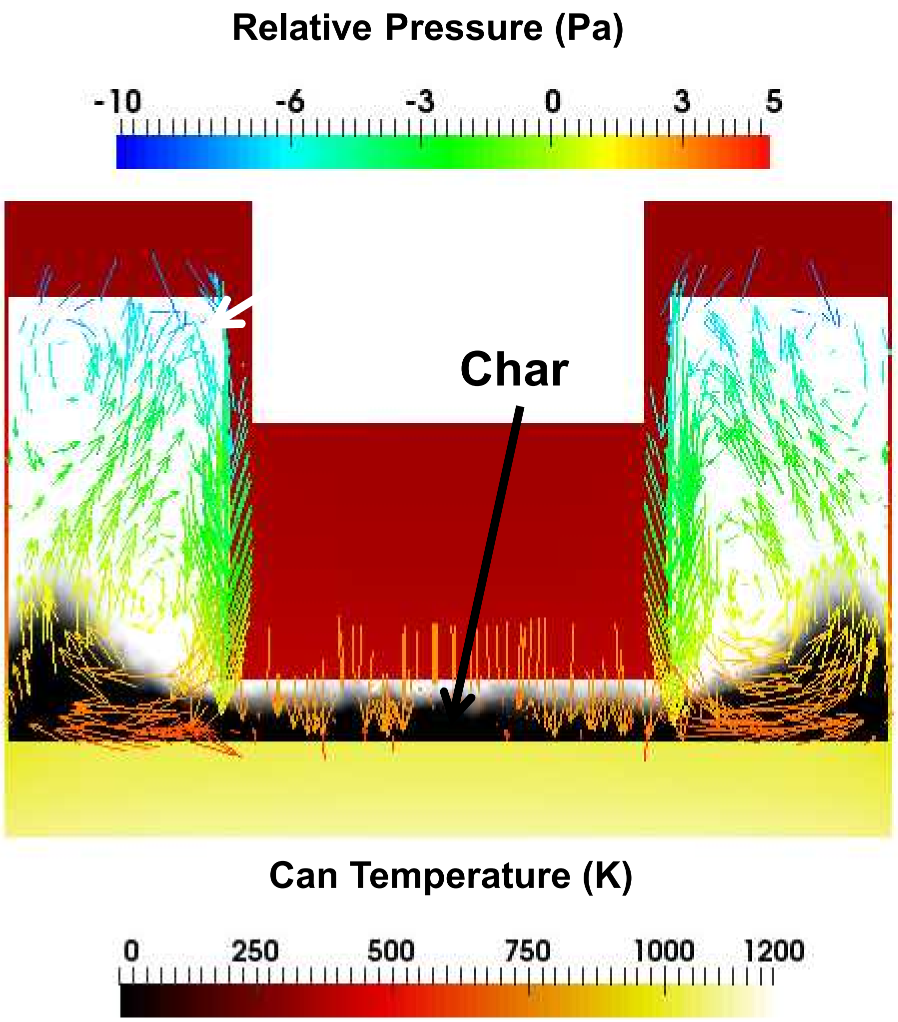






Porous Media Simulation

- Porous flow circulates gaseous products throughout the domain
- Heat transfer can be significantly impacted
- Gravity-induced convection may result in differentiation between upright and inverted pressurization



LHS Study Parameters of Interest

- 200 total simulations
  - 100 upright, 100 inverted orientations
- 19 parameters were selected
  - 12 properties were defined by normal distributions
  - 7 unknown quantities (next slide)
- Dakota management

Parameter	Mean Value	Uncertainty (Standard Deviation)
Foam		
Bulk Density	161.3 kg/m^3	5%
Solid Density	1500 kg/m^3	25%
Radiative Conductivity (β_r)	1073.1	15%
Heat of Reaction	25e4 J/kg	15%
Activation Energy	3.33e15 J/kg	2%
Bulk Conductivity	0.035691 W/m/K	10%
Specific Heat Capacity	~1800 J/kg/K	10%
Char		
Bulk Density	16.1 kg/m^3	25%
Gas Products		
Molecular Weight	100 g/mol	15%
Specific Heat Capacity	1000 J/kg/K	20%
Mass Diffusivity	2e-5 m^2/sec	30%
Miscellaneous		
Convection coefficient	10	30%

LHS Study Parameters of Interest

- Seven quantities are quite poorly characterized
- Currently using uniform distribution of parameter values

Parameter	Low Value	High Value
Foam		
Permeability	1e-11 m^2	1e-8 m^2
Char		
Solid Density	150 kg/m^3	2000 kg/m^3
Permeability	1e-11 m^2	1e-8 m^2
Radiative Conductivity (β_r)	200	3000
Bulk Conductivity	0.01 W/m/K	0.06 W/m/K
Specific Heat Capacity	1000 J/kg/K	5000 J/kg/K
Gas Products		
% Organic Gases	0	0.787

Upright Temperature Comparison

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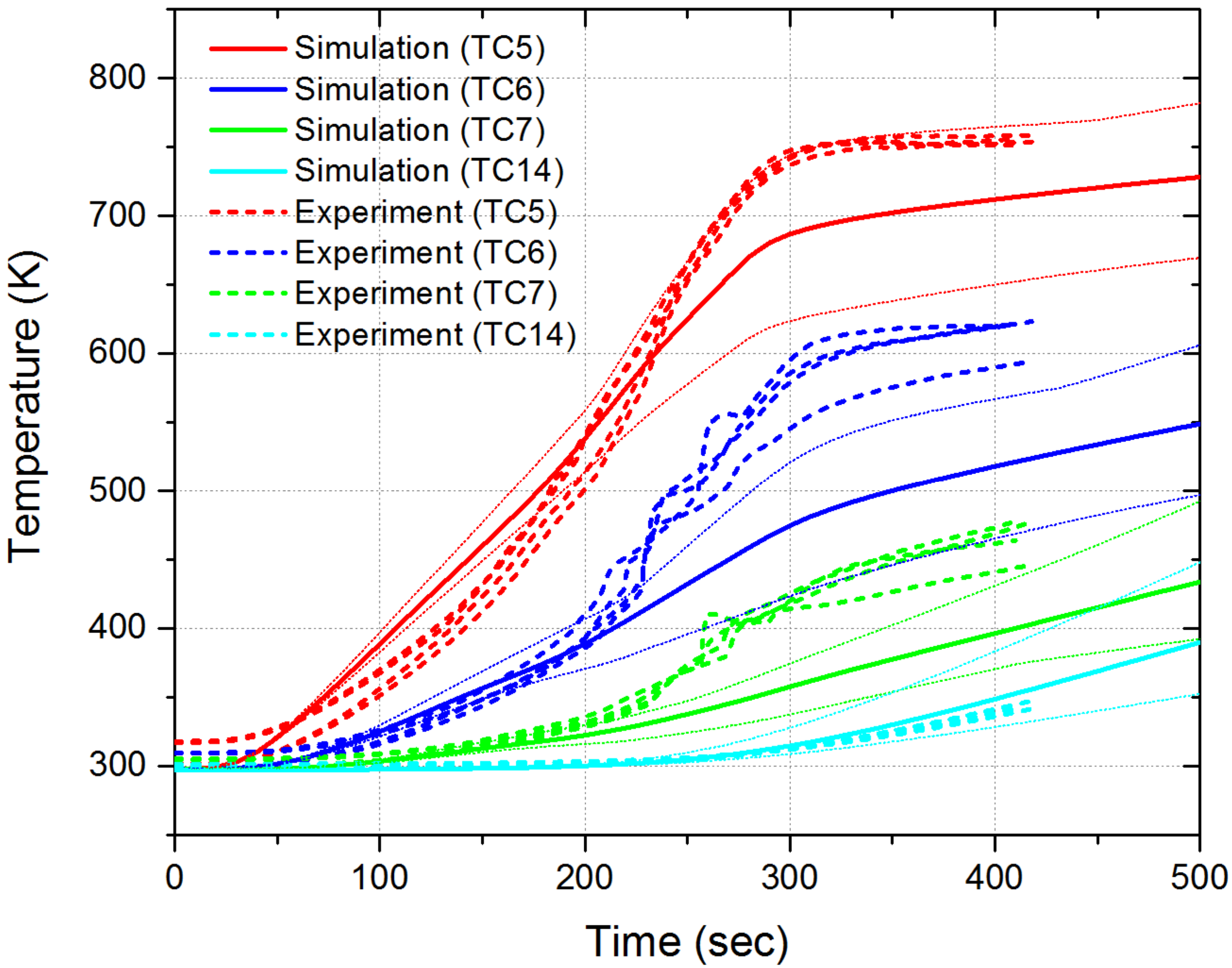
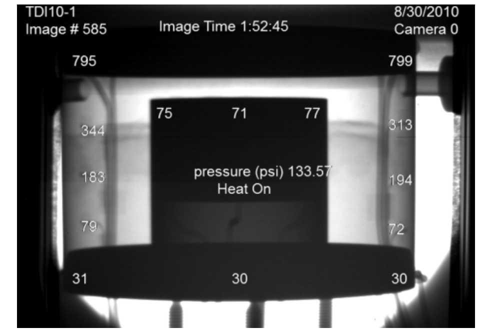
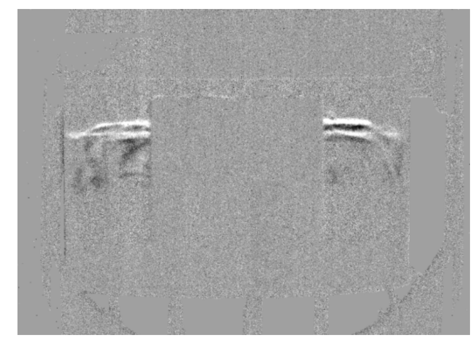
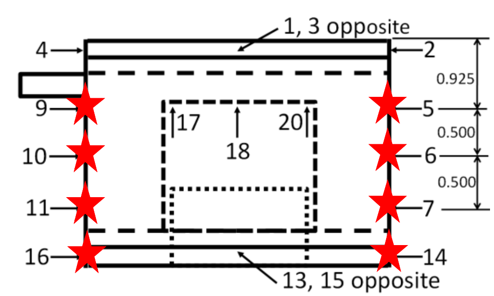
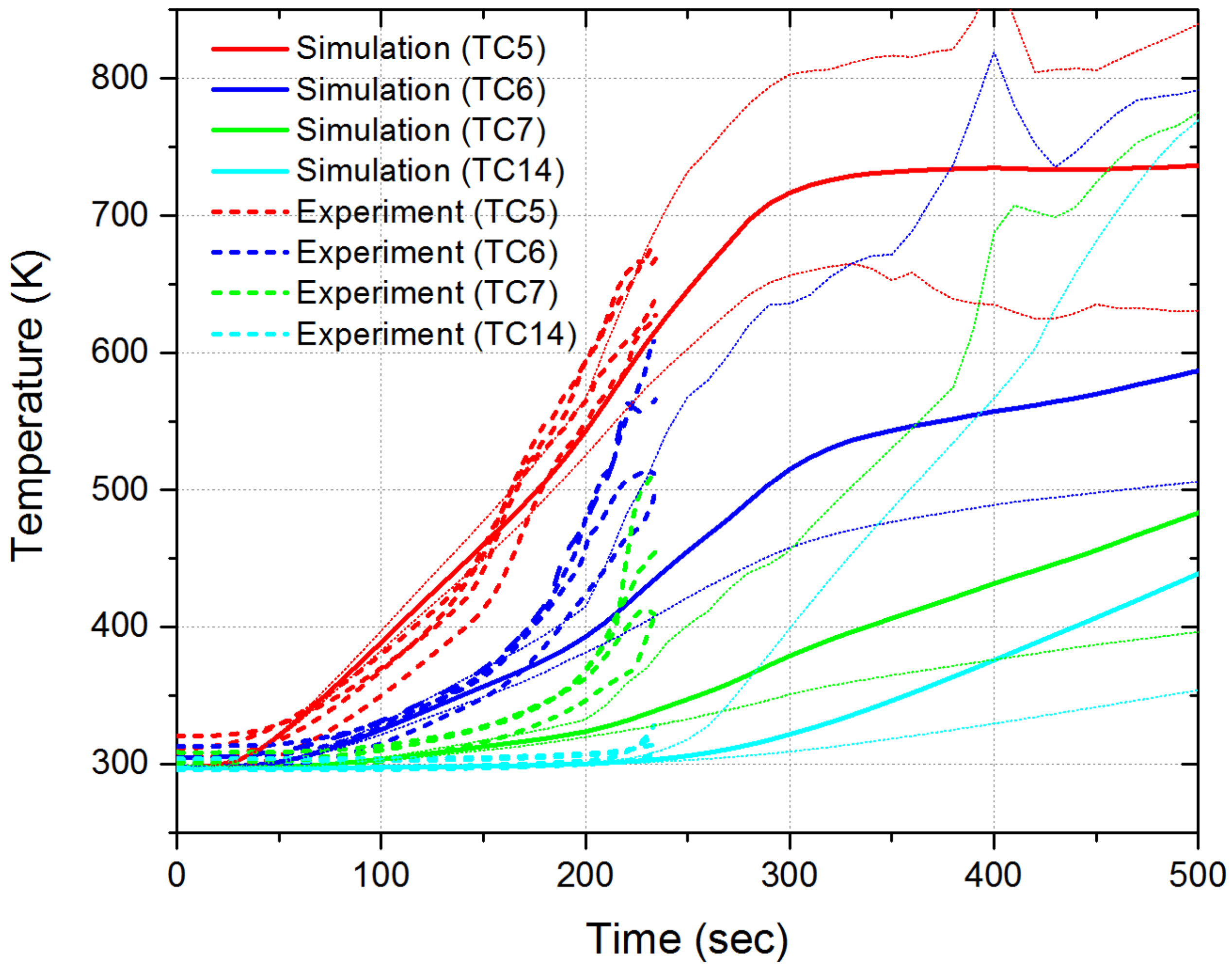


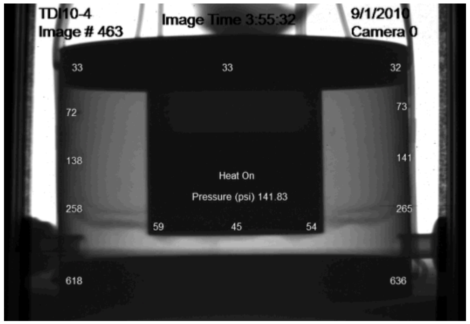


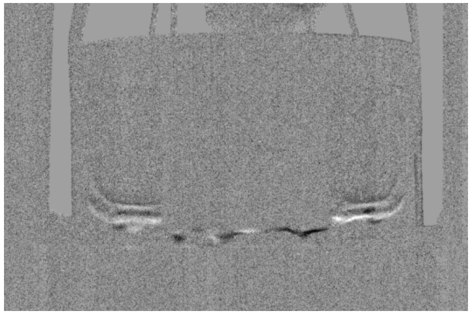


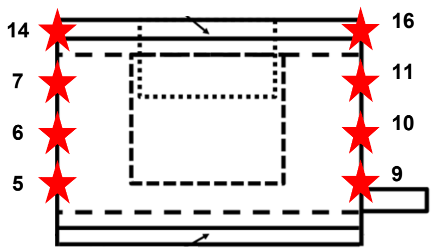


Inverted Temperature Validation

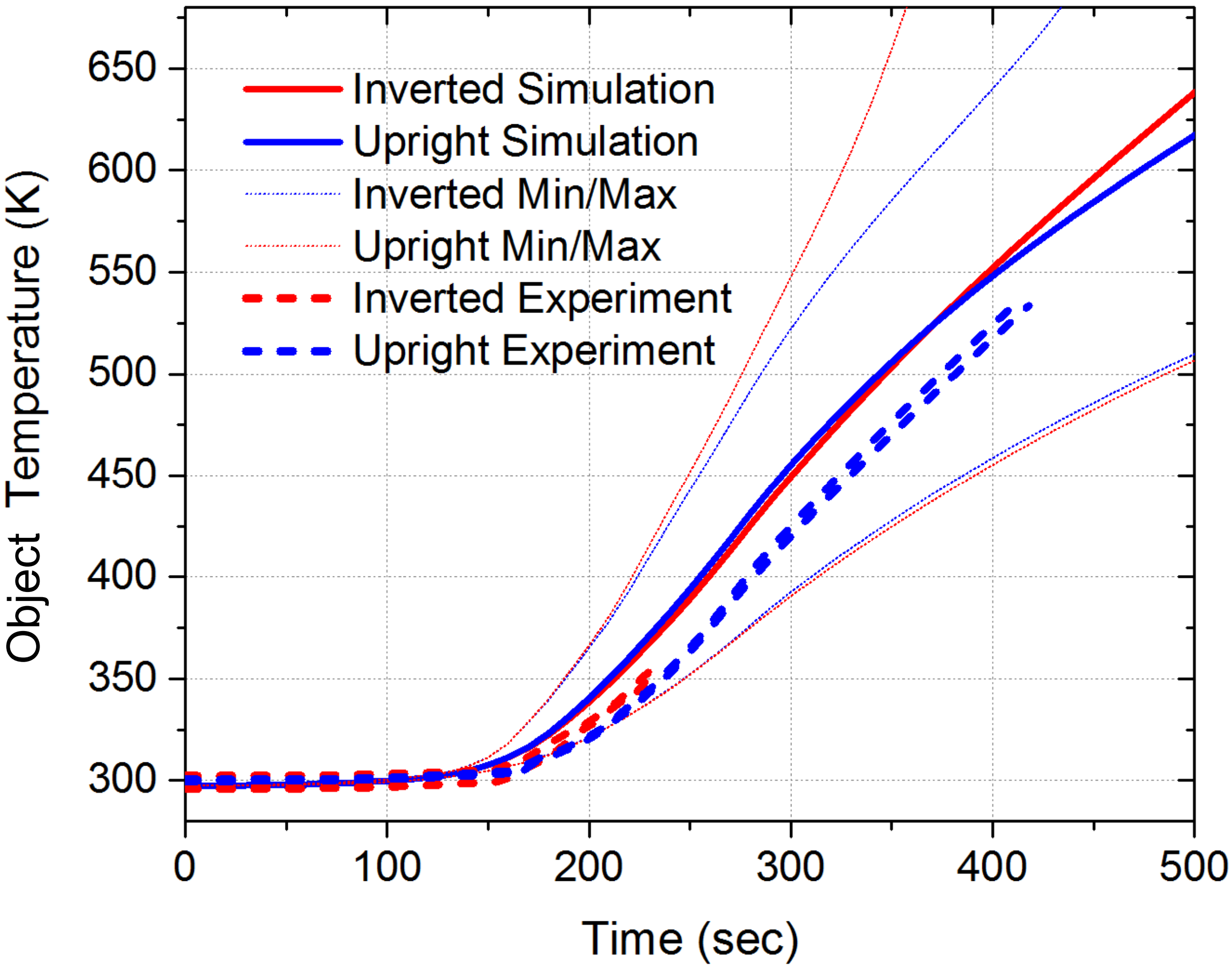


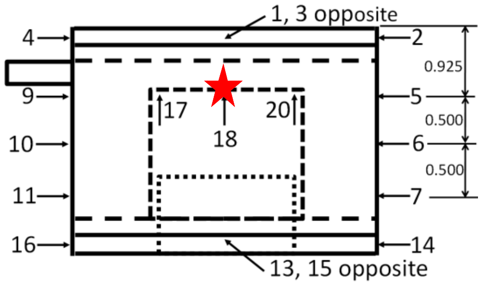




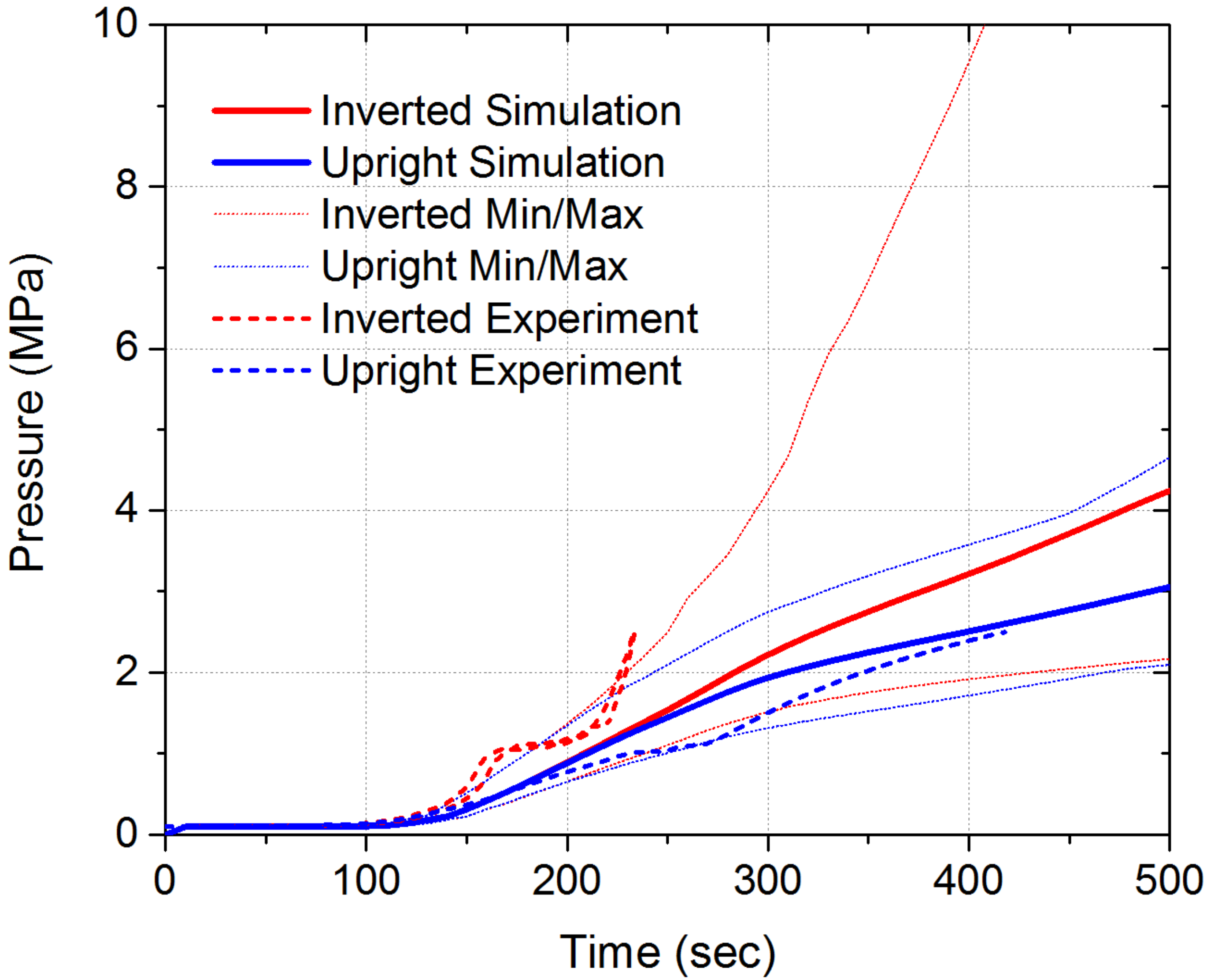


Object Temperature Results

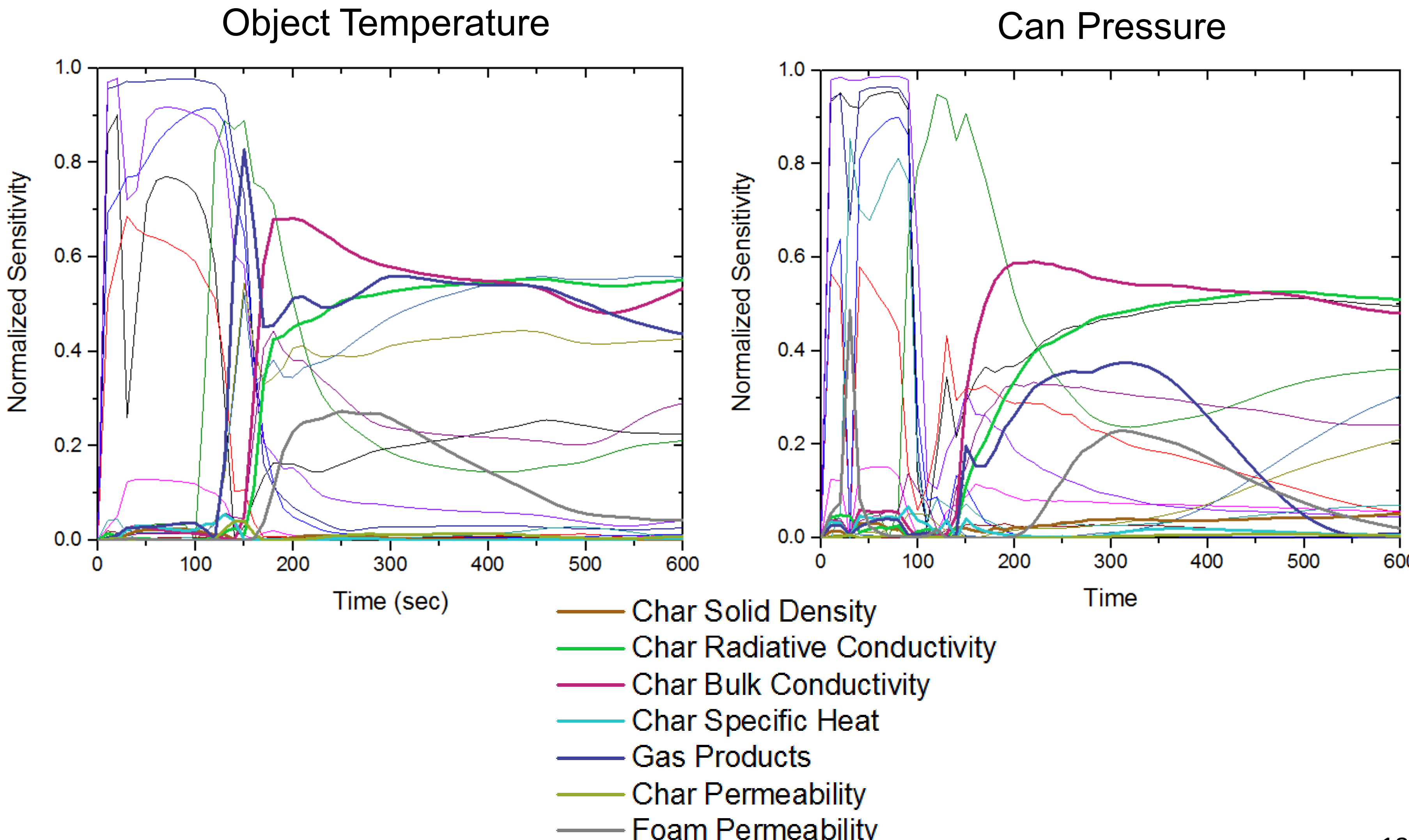




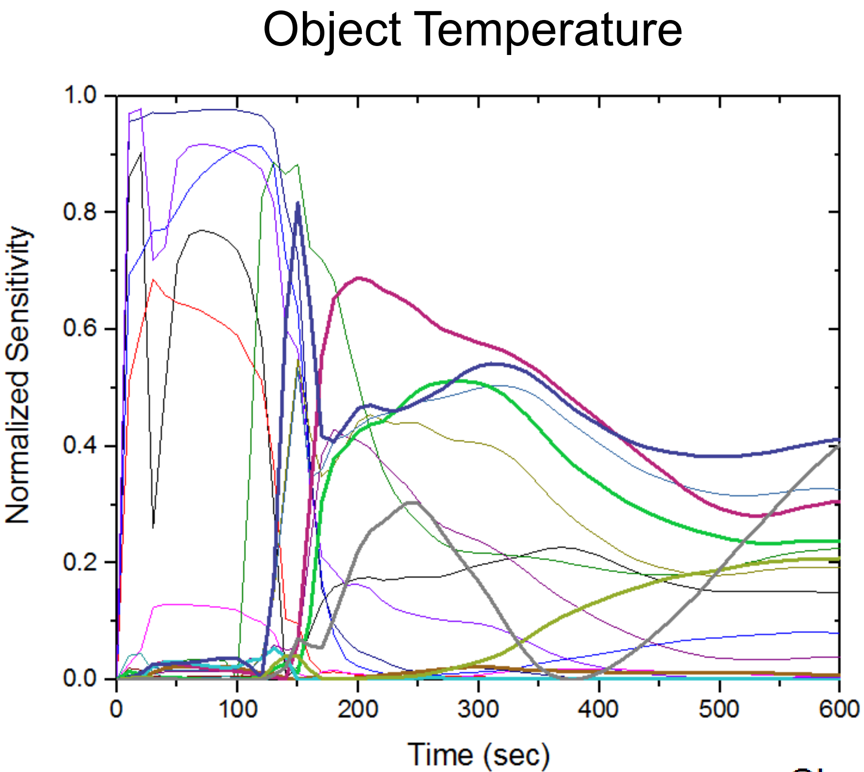
Pressurization Results

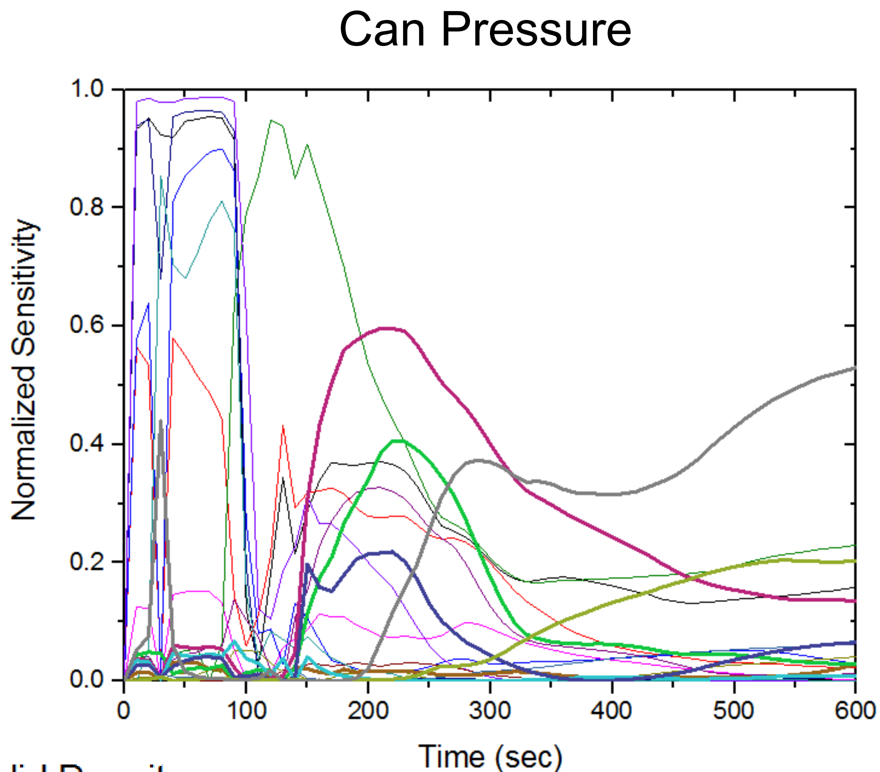


Upright Orientation



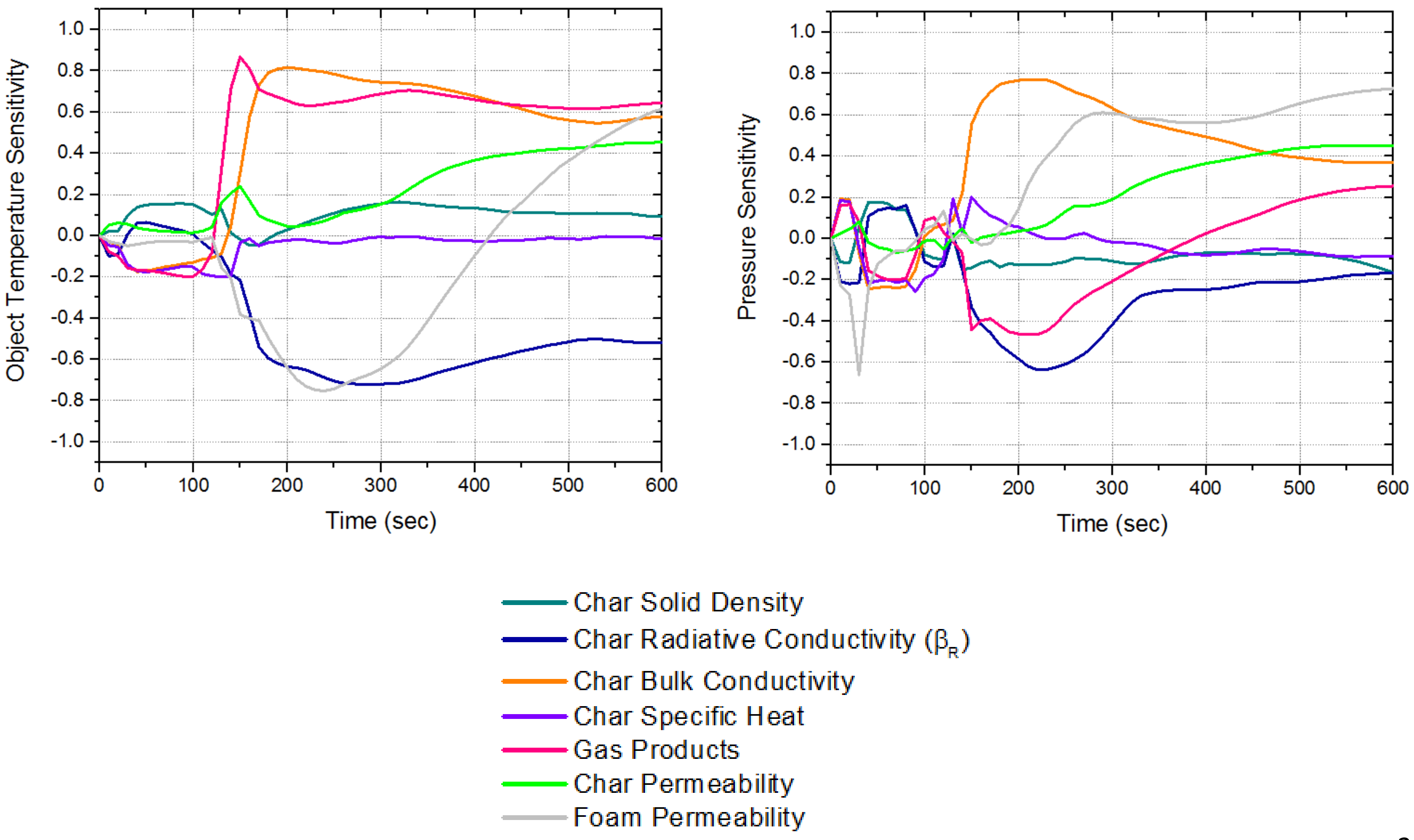
Inverted Orientation





- Char Solid Density
- Char Radiative Conductivity
- Char Bulk Conductivity
- Char Specific Heat
- Gas Products
- Char Permeability
- Foam Permeability

Inverted Orientation



Conclusions

- Porous media model improves predictive ability by differentiating between upright and inverted configurations
  - Within uncertainty, we see agreement for object temperature for both orientations; pressure for upright orientation
  - Strong evidence that additional model physics are necessary to have a fully-validated model
- Sensitivity study illuminates need for future work
  - Prioritization of parameter characterization
  - More refined selection of parameter ranges
  - Motivation for inclusion of additional physics

Future Work

- Additional LHS studies with more selective parameter ranges
- Increase Darcy flow stability to allow for higher permeability
- Incorporate additional fluid physics
  - Navier-Stokes description of gases
  - Model for liquefaction
- Explore other radiation modeling approaches
  - Enclosure radiation
  - Participating media radiation