SAND2018-7723C

Thermally Decomposing Polyurethane Foam in Sealed Containers

Sarah Scott[1,2], Matthew Kury[1], Ryan Keedy[1], Victor Brunini[1], Amanda Dodd[1], James Urban[2], Carlos Fernandez-Pello[2]

[1]Sandia National Laboratories, California

[2]University of California, Berkeley

37th International Symposium on Combustion

July 29 – August 3, 2018

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Outline

Motivation for Studying Foams in Fires

Validation Experiments

Porous Media with Vapor Liquid Equilibrium Model

Motivation for Studying Foams in Fires

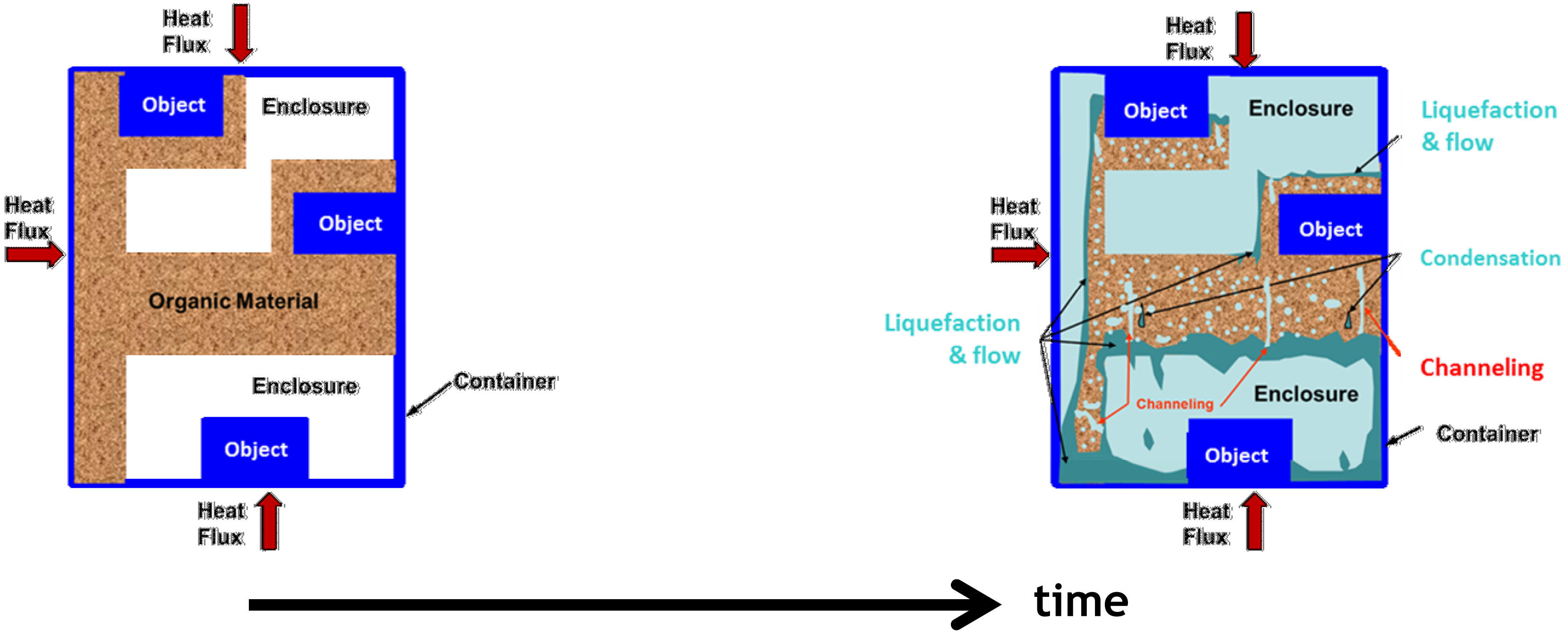
Motivation for Studying Foams in Fires

Foams (and other organics) are used to protect electronic devices from mechanical and thermal shocks under normal operating conditions.

In accident scenarios, these systems can be exposed to high heat fluxes, such a fire.

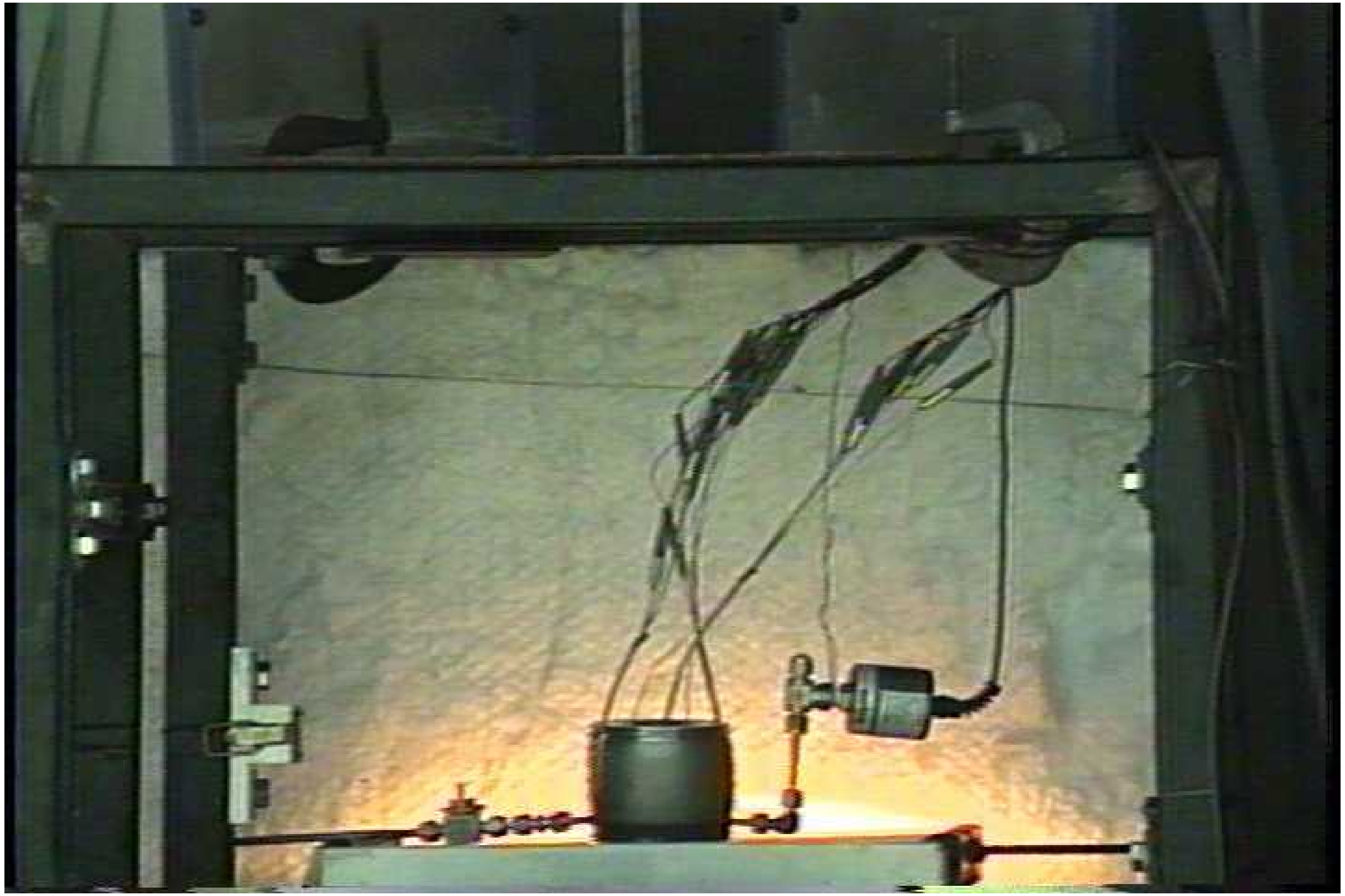
The Trouble with Organic Materials

- Organic materials decompose at low temperatures compared to other engineered materials, such as metals
- Organic material decomposition can impact heat transfer and pressurization



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

Foam in a Can Experiment




Validation Experiments

Experimental Motivation

Experiments showed that steel containers could breach from pressurization created by the gases of the thermally decomposing organics

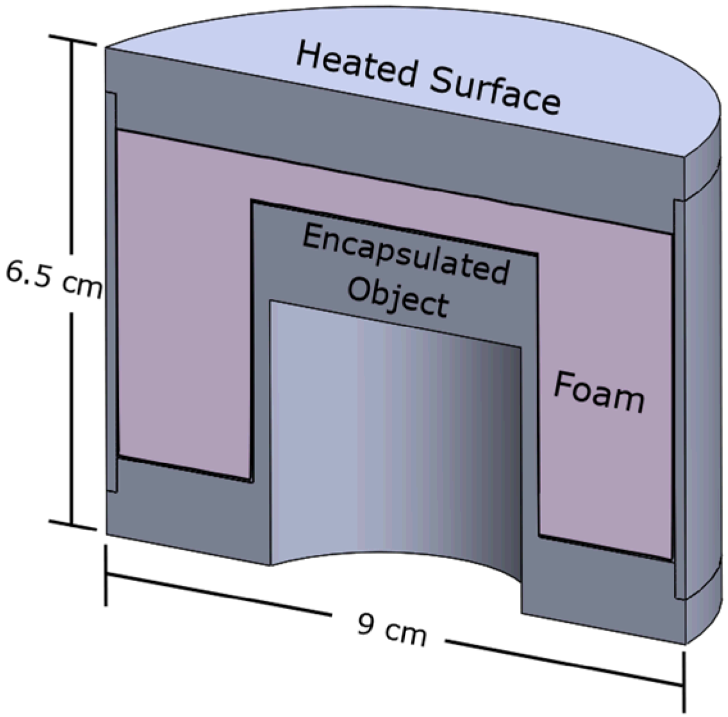
Existing thermal models could not predict this behavior

- When heated, organic materials undergo thermo-physical process that need to be better understood

A new series of experiments were conducted to better understand the problem in order to model it

- These experiments were used both to gain insight into the physics as well as to validate the model

Foam in a Can Experiment



Data Sets:

- 320 kg/m^3 PMDI polyurethane foam (rigid, closed cell)
- Heated to 800 C at a rate of 150 C/min.

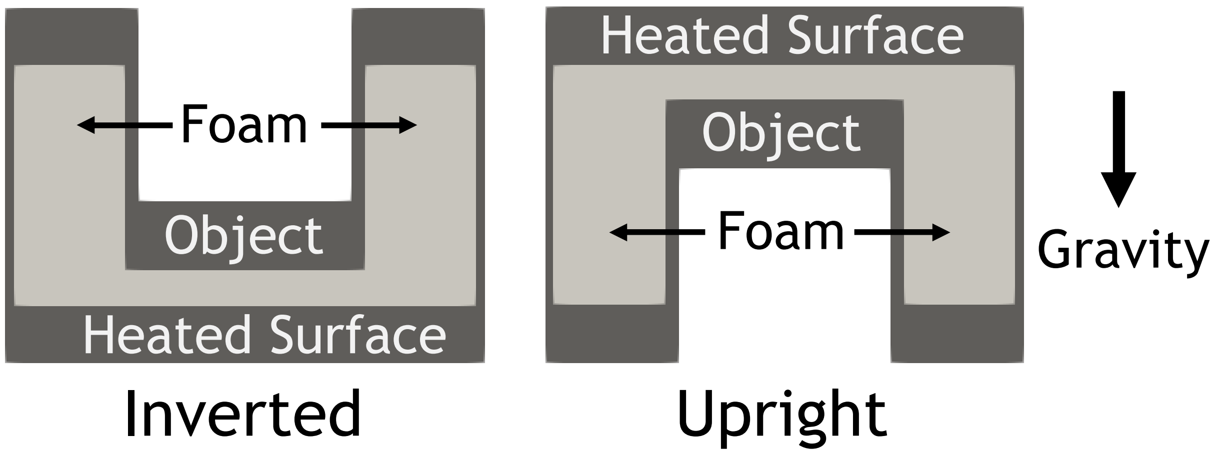
Can dimensions are approximately

- Diameter: 9 cm
- Length: 6.5 cm
- Side Wall Thickness: 0.5 mm

Monitor pressure and temperature

X-Rays to view can interior

Experiments run to breach



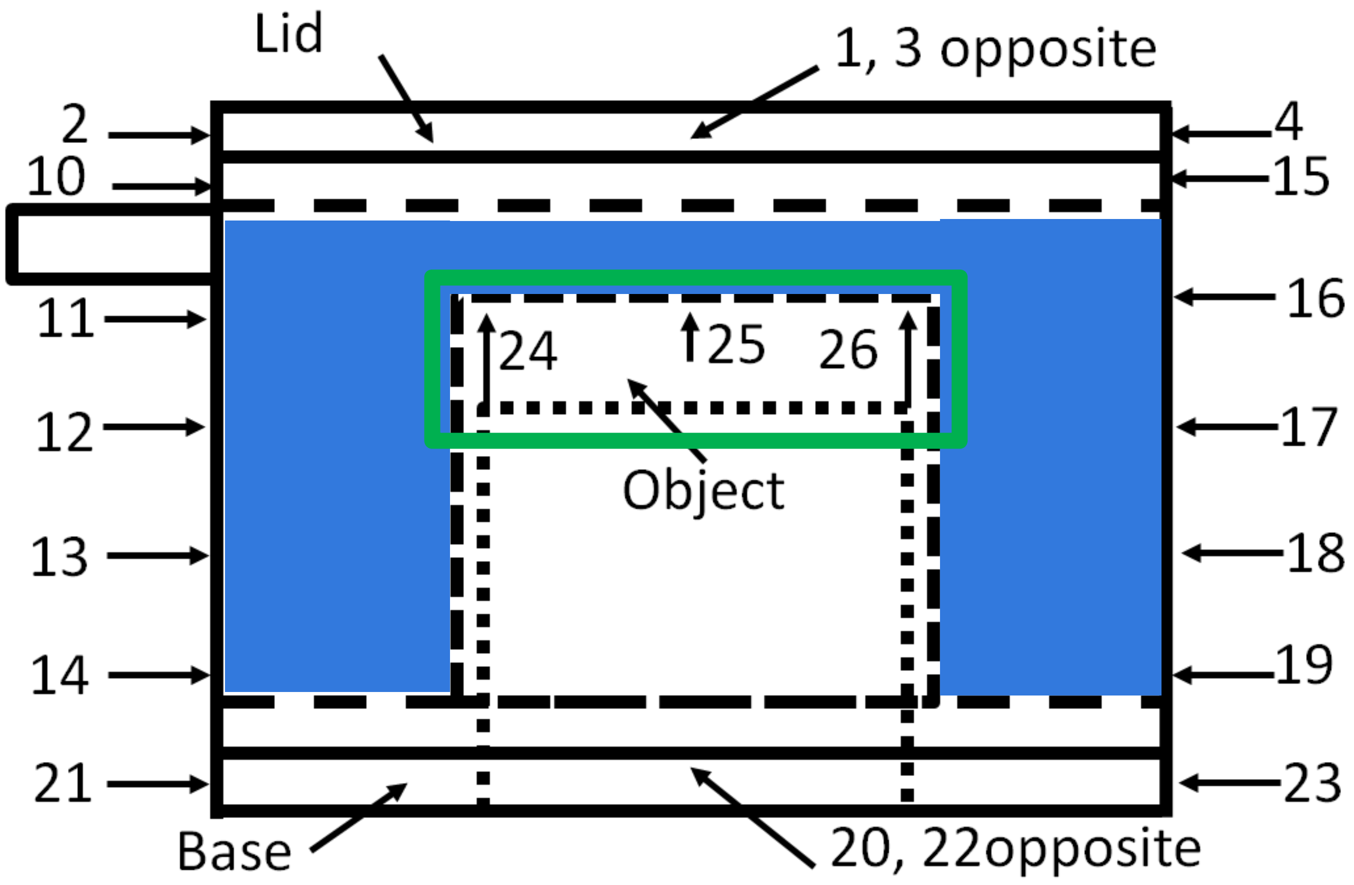
Experiment conducted in upright and inverted orientations

- Material bulk movement towards or away from heat source

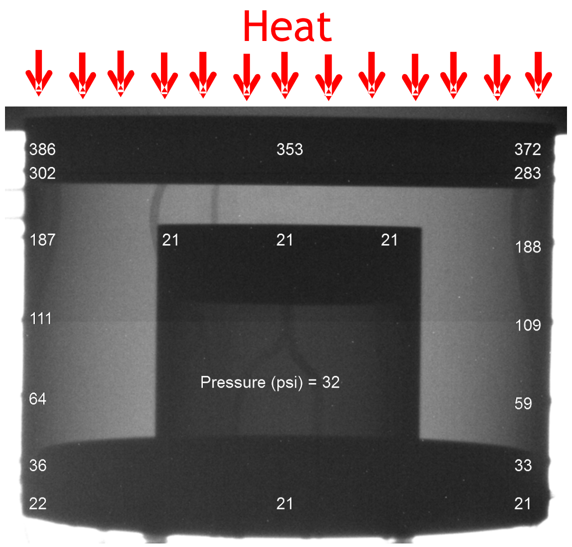
Acknowledgement: Jill Suo-Anttila

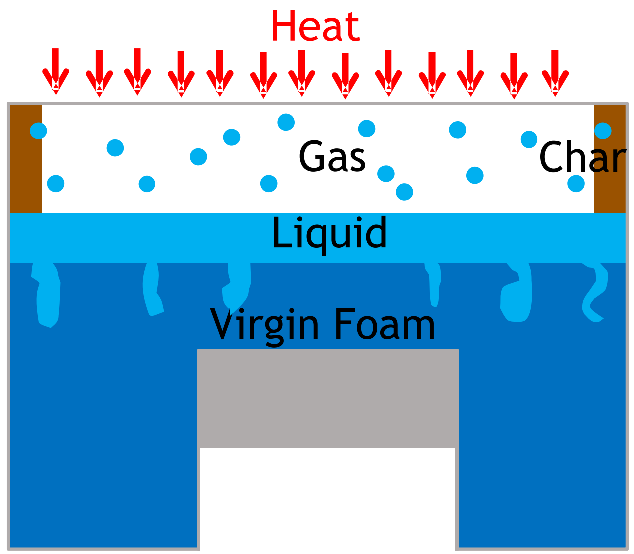
Foam in a Can Experiment: Thermocouples

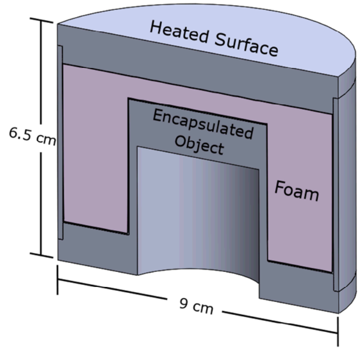
Temperature is monitored on the top, along the sides, and on the bottom of the can as well as on an embedded object.



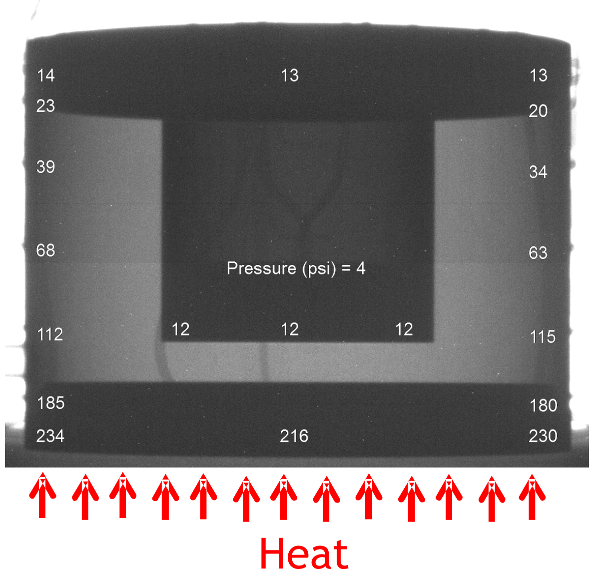
X-Ray Video of Experiments

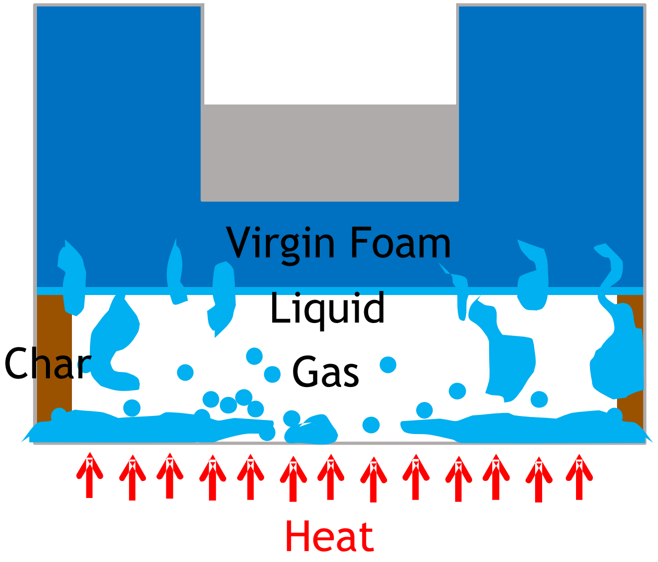






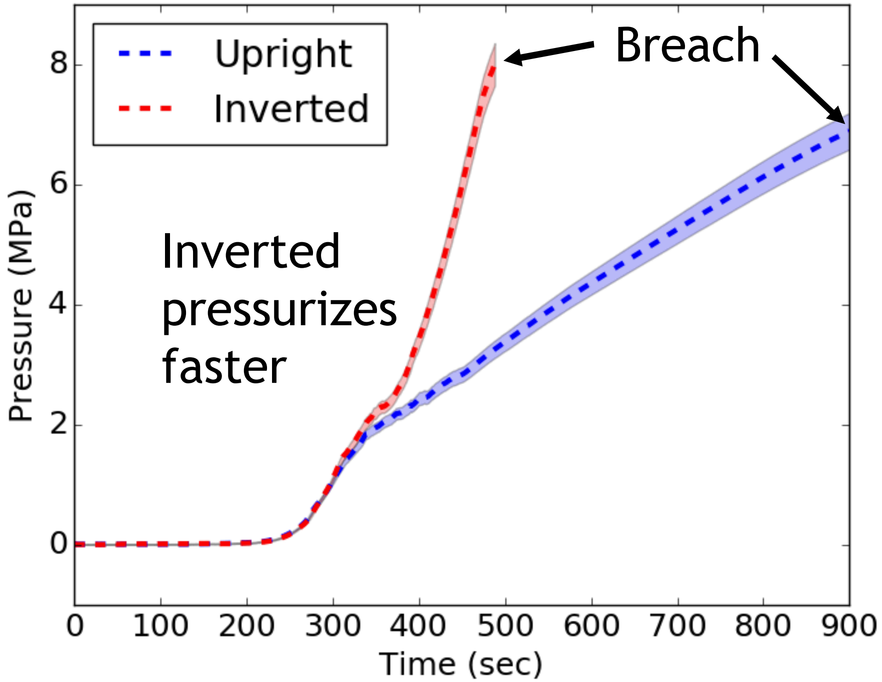
Upright

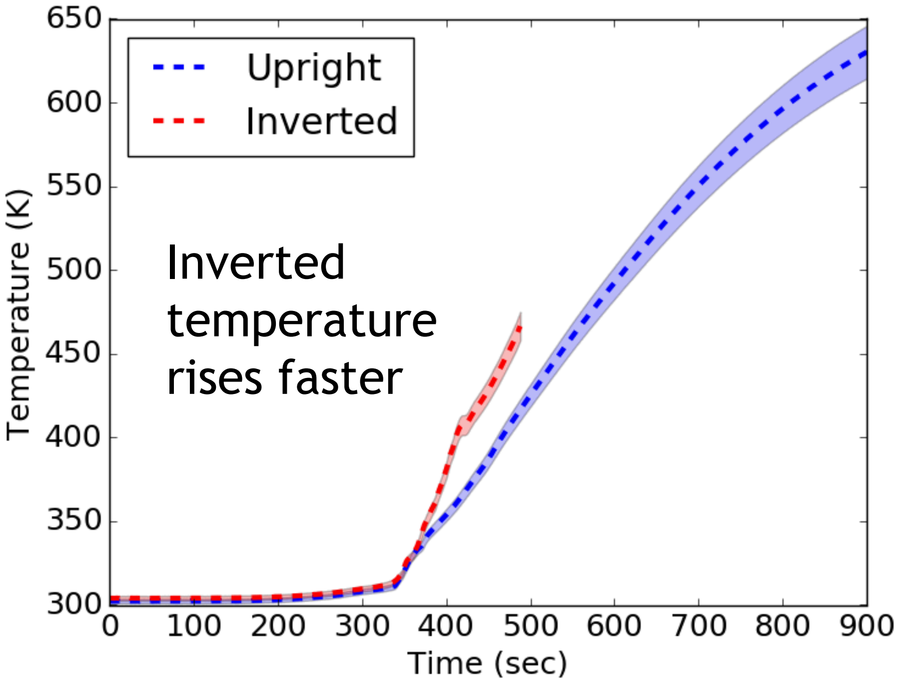


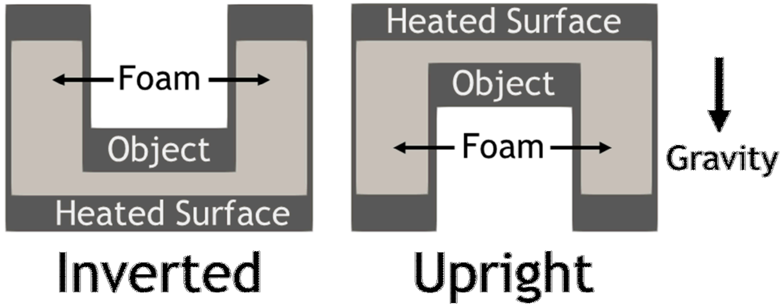


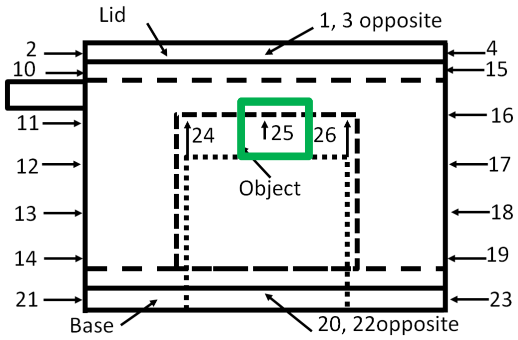
Inverted

Experimental Quantities of Interest



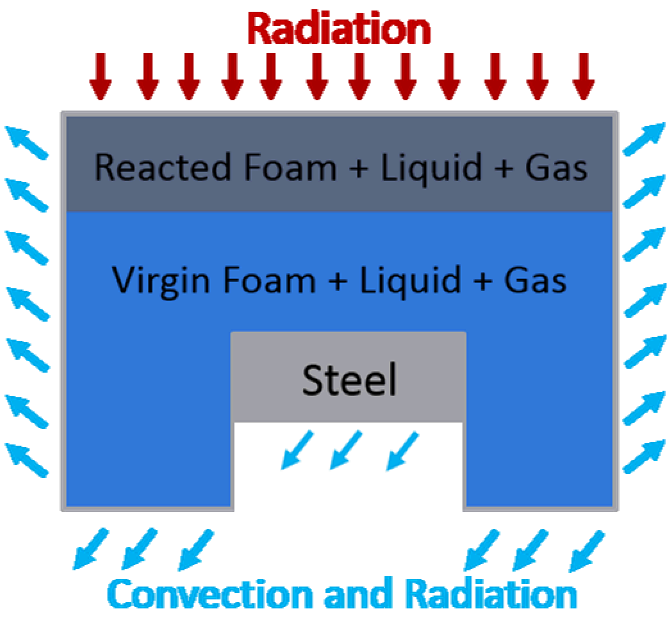






Porous Media with Vapor Liquid Equilibrium Model

Model Description



2D Axisymmetric Model in Sierra Thermal/Fluids

Three step reaction mechanism

- PMDI Polyurethane -> CO_2, light and heavy organics, char
- Phase of light and heavy organics determined by Henry's or Raoult's law
  - When liquid is formed, it is treated as part of the motionless matrix

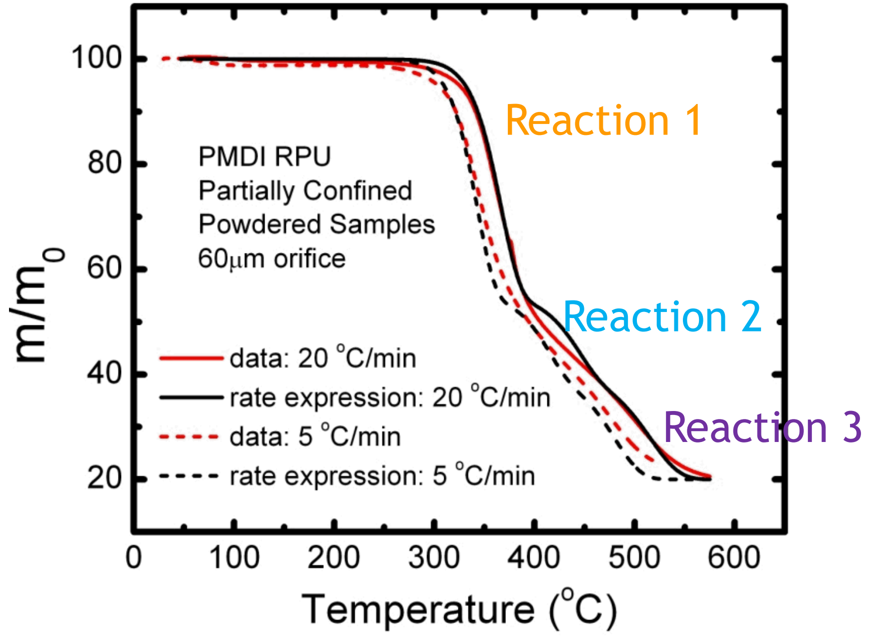
Continuity, species, and enthalpy equations

- 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

Decomposition Reactions and VLE



Three step reaction mechanism:
(Acknowledgment: Ken Ericson)

$$0.45\, \boldsymbol{foam} \xrightarrow[k_1]{} 0.20\, \boldsymbol{organics} + 0.25\, \boldsymbol{CO_2}$$

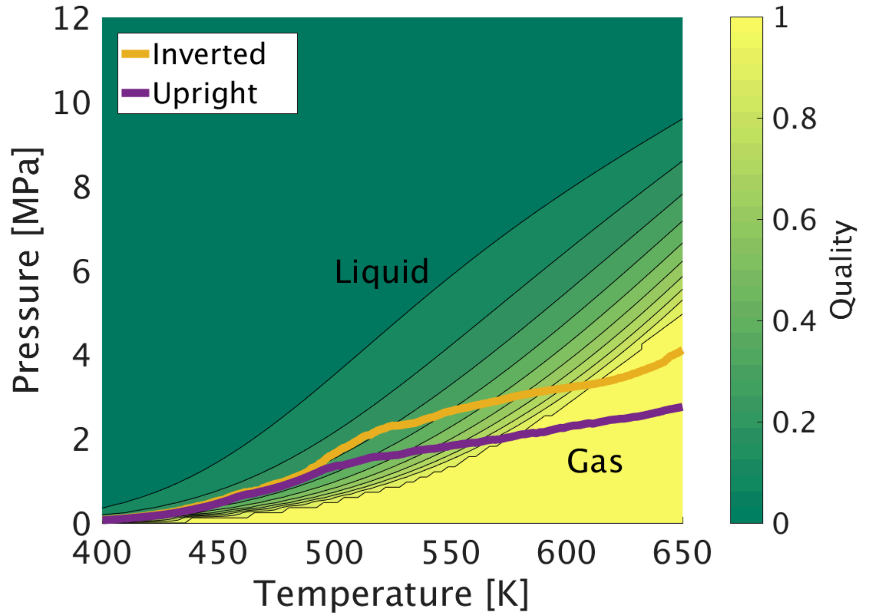
$$0.15\, \boldsymbol{foam} \xrightarrow[k_2]{} 0.15\, \boldsymbol{organics}$$

$$0.40\, \boldsymbol{foam} \xrightarrow[k_3]{} 0.20\, \boldsymbol{organics} + 0.20\, \boldsymbol{char}$$

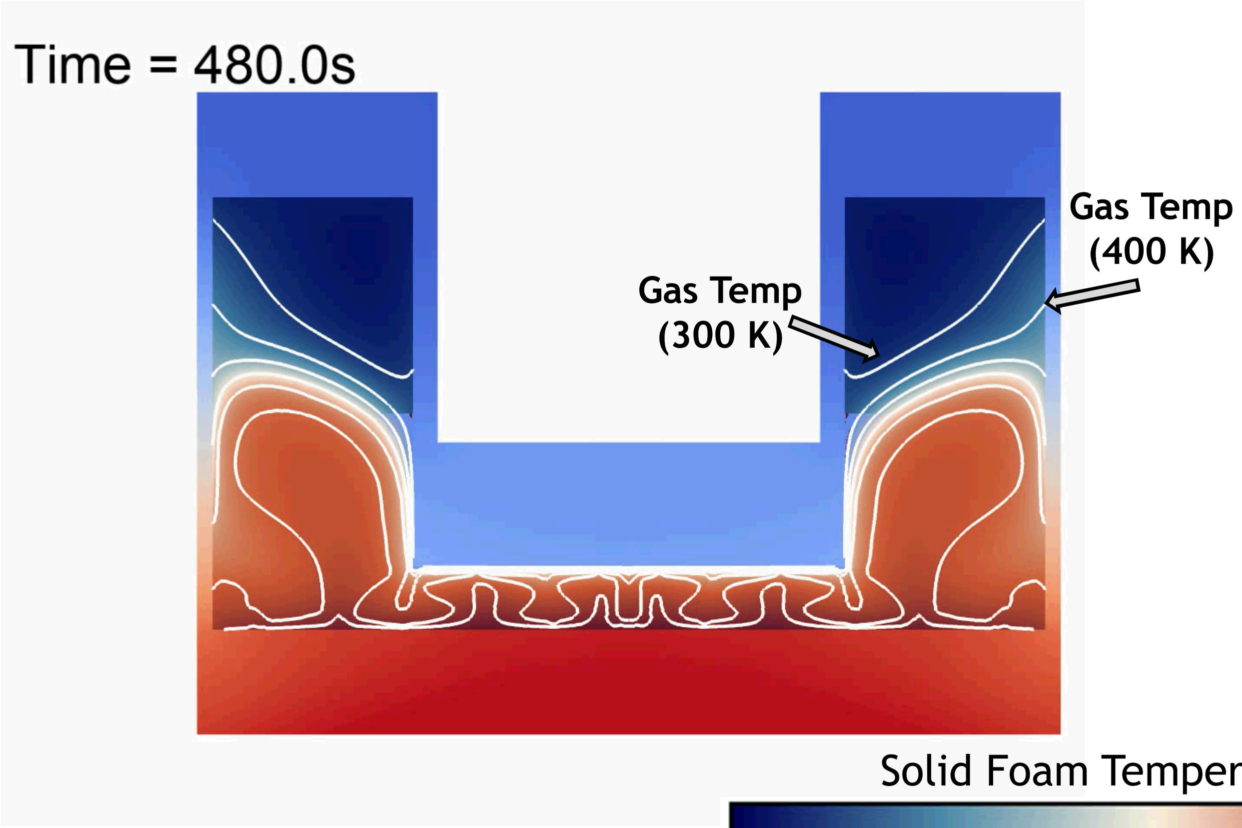
The major organic decomposition products of the reaction:

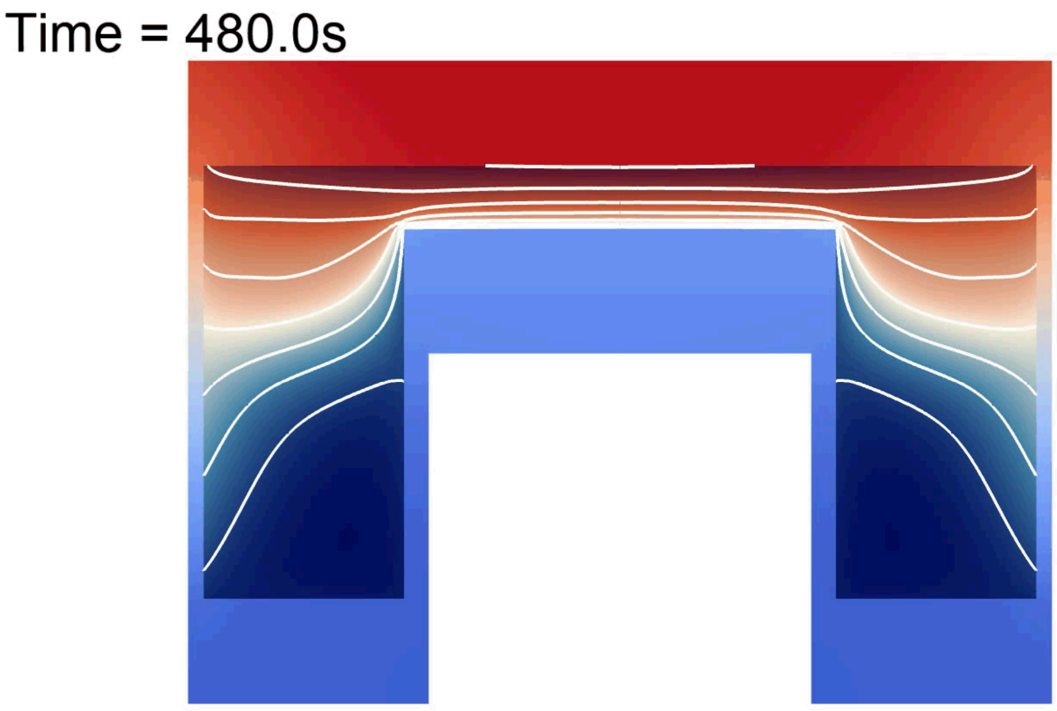
- Propylene glycol
- Aniline
- 4-methylaniline
- Phenyl isocyanate

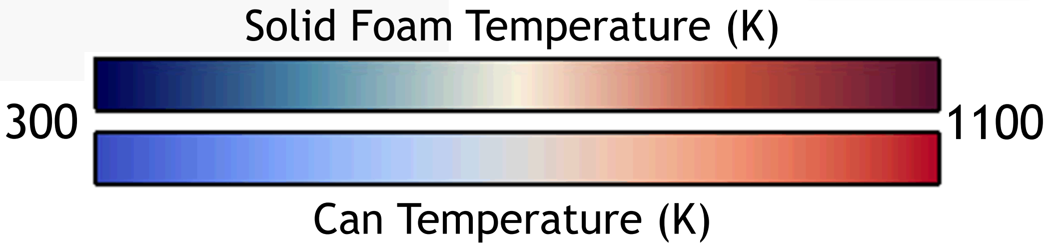
These products can exists in either the liquid or gas phase at the temperatures and pressures seen in the can



Gas and Solid Temperatures

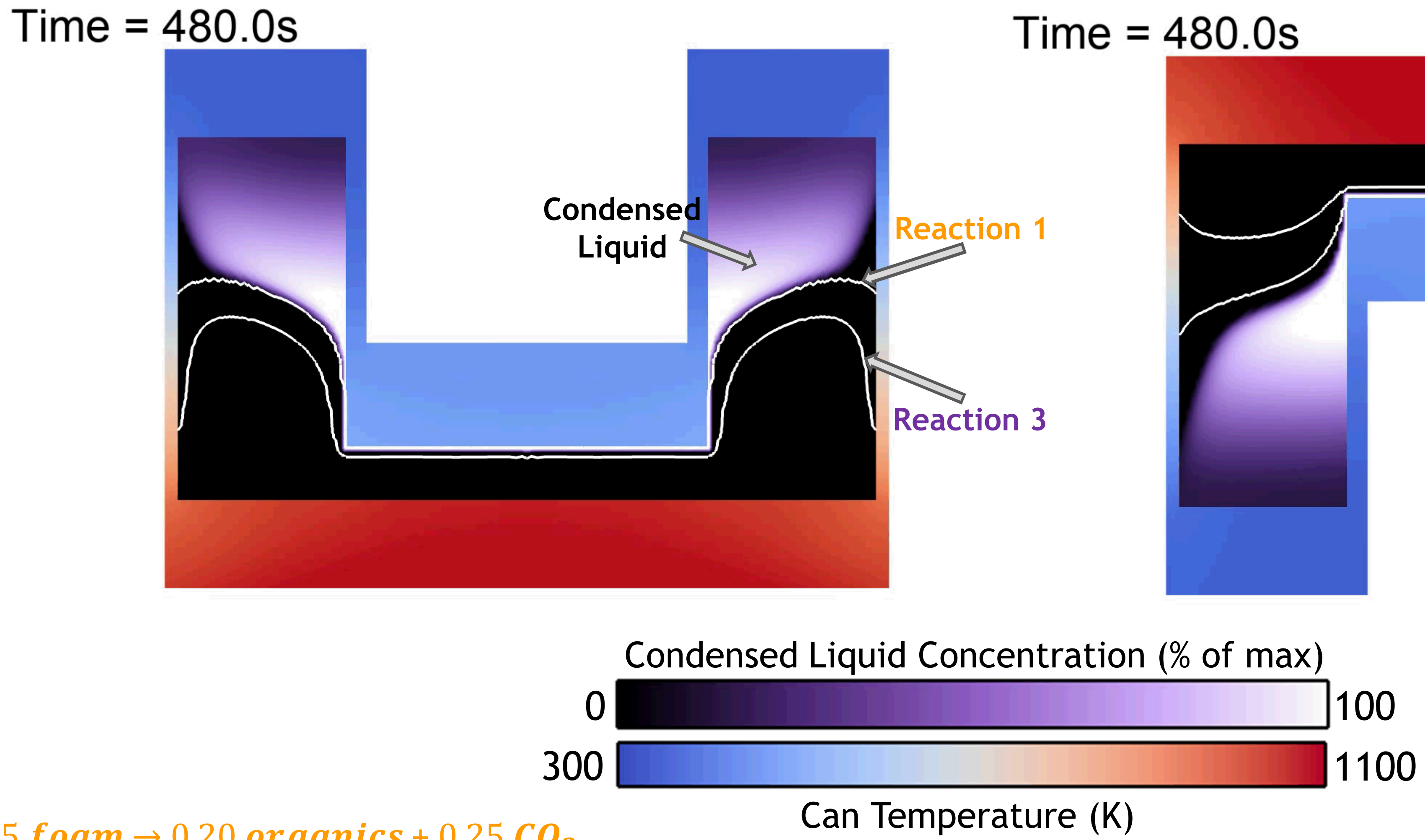






Gas Temperatures in increments of 100K

Condensed Liquid and Reactions

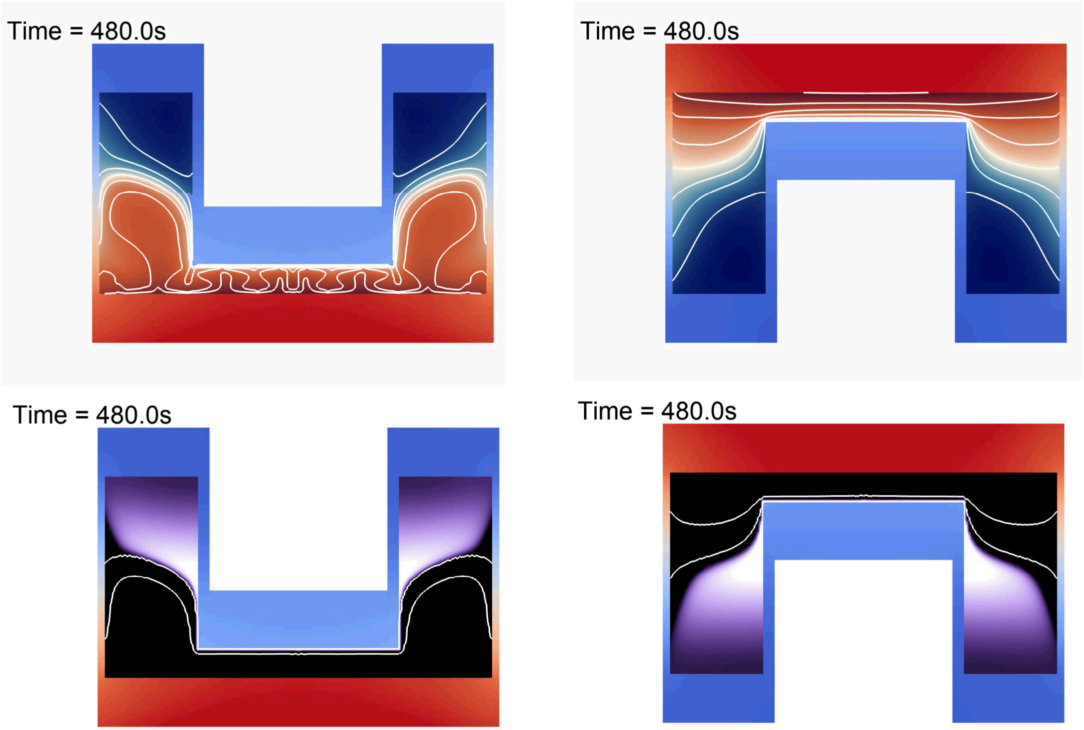


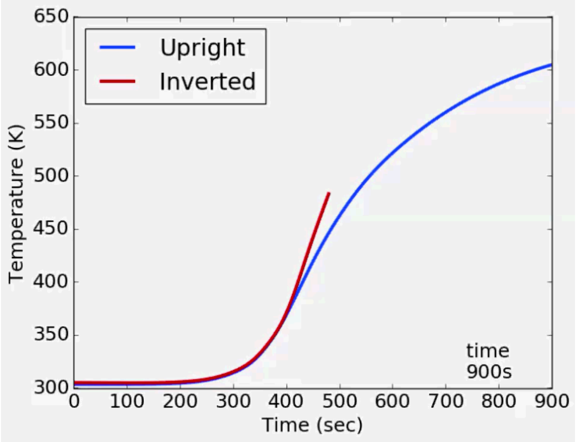
$0.45\ \boldsymbol{foam} \xrightarrow[k_1]{} 0.20\ \boldsymbol{organics} + 0.25\ \boldsymbol{CO_2}$

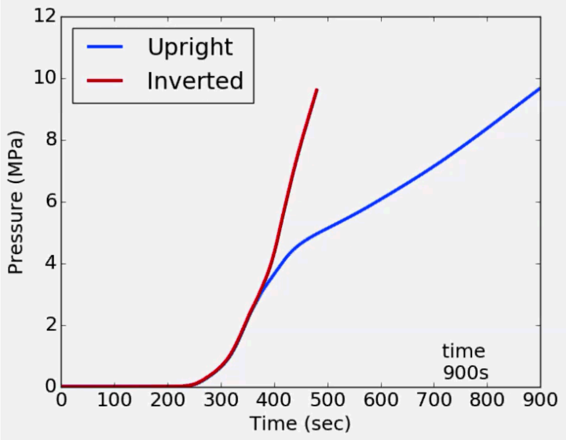
$0.15\ \boldsymbol{foam} \xrightarrow[k_2]{} 0.15\ \boldsymbol{organics}$

$0.40\ \boldsymbol{foam} \xrightarrow[k_3]{} 0.20\ \boldsymbol{organics} + 0.20\ \boldsymbol{char}$

Effects of Heat Transfer and Flow







Buoyant flow accelerates heat transfer in the inverted orientation, leading to a higher temperature gradient.

Gasses produced by the reaction flow to cooler areas of the can where they can condense. They can gasify again when heated.

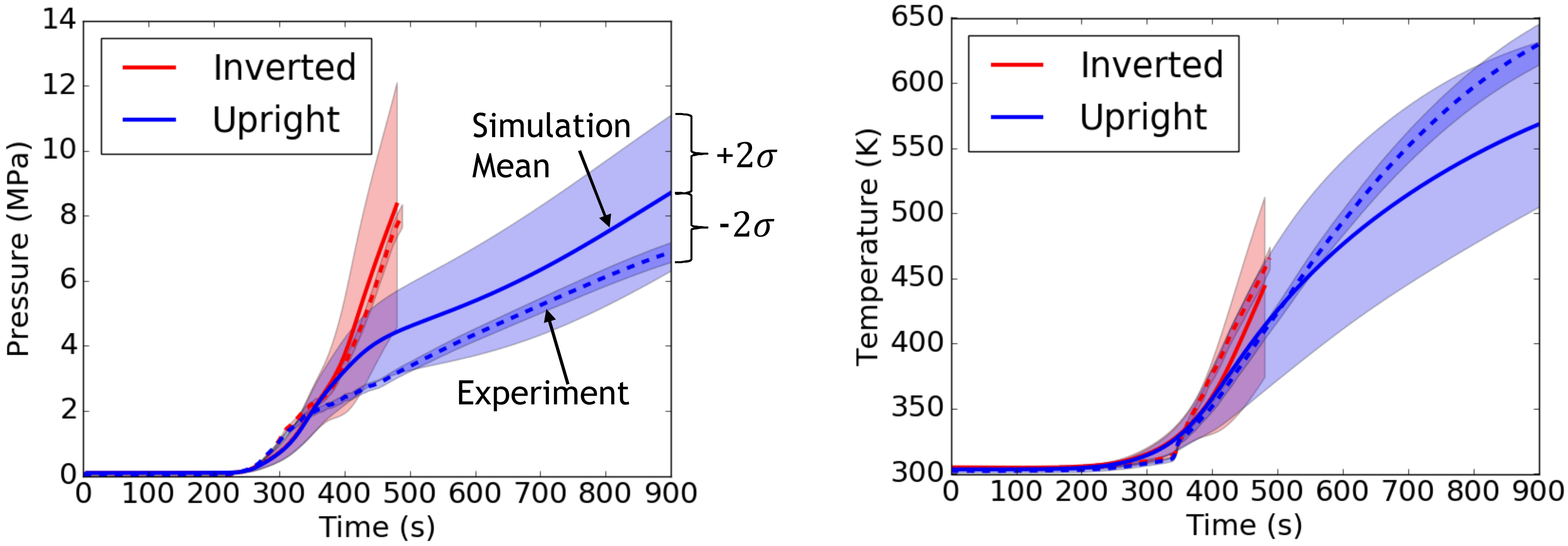
Accelerated heat transfer progress reaction faster and narrows reaction band.

Uncertainty Quantification (UQ)

The input parameters were varied using a Latin Hypercube Study (LHS) in Dakota

- 31 parameters were included
- 310 simulations in both the upright and inverted orientation were preformed (total 620 simulations)

The mean and standard deviation of the ensemble were calculated



Summary and Future Work

Summary

A model was created to predict pressure and temperature of a decomposing foam.

- The model incorporated porous media flow with vapor liquid equilibrium equations to better predict orientation dependence

An uncertainty quantification study was performed to understand the influence of parameter uncertainty on responses

- 100-125 K spread in temperature and 4-8 MPa in pressure

Future Work

Porous Media VLE model

- Investigate additional heating rates and densities of foam
- Using 2D models to handle computationally expensive activities for 3D models
- Implement additional statistical and UQ techniques

Condensed Phase Advection

- Include physics that would allow the matrix phase to flow

Questions?

Effective Conductivity and β_R

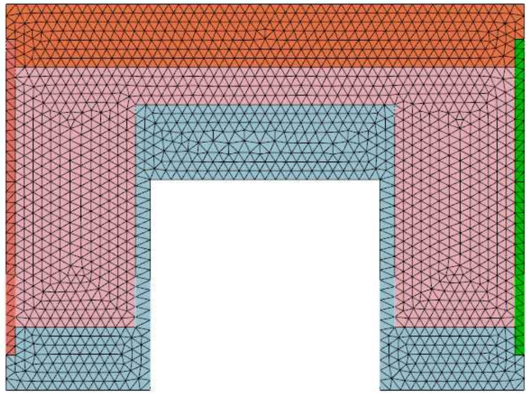
Radiative heat transfer is accounted for by an effective conductivity calculated by the diffusion method for an optically thick media

$$k_{rad} = \frac{16\ \sigma}{3\ \boldsymbol{\beta}}\ T^3$$

β is the absorption plus scattering, which is the properties that is measured. It varies as the inverse of k_{rad}.

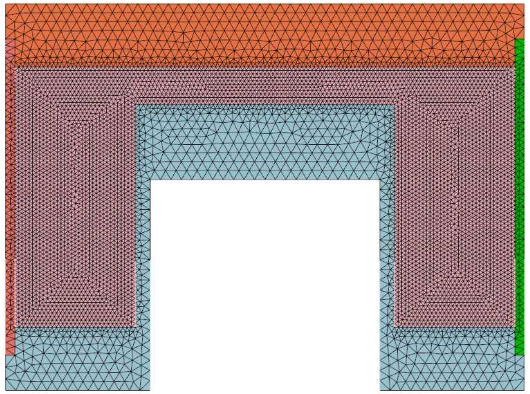
Mesh Resolution

Coarse



1.77mm
1,914 nodes

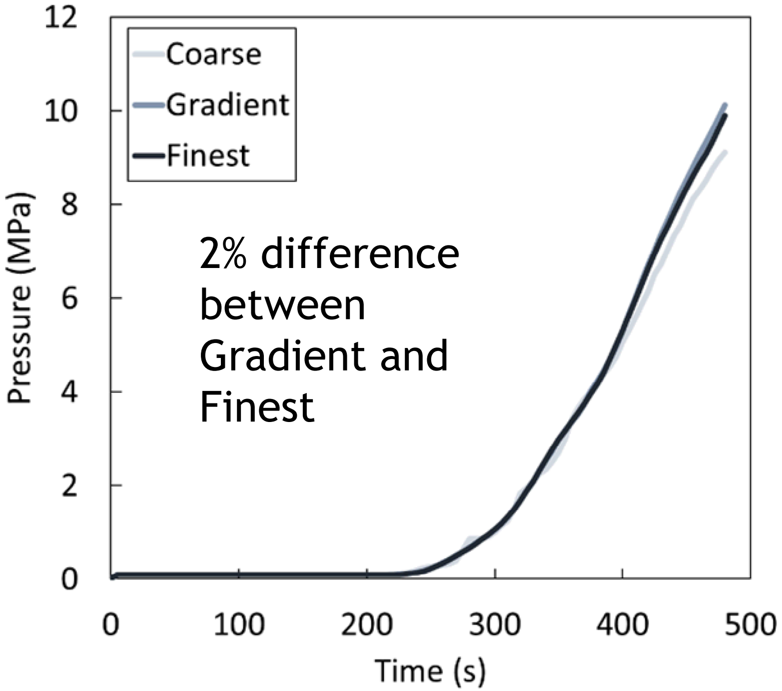
Gradient

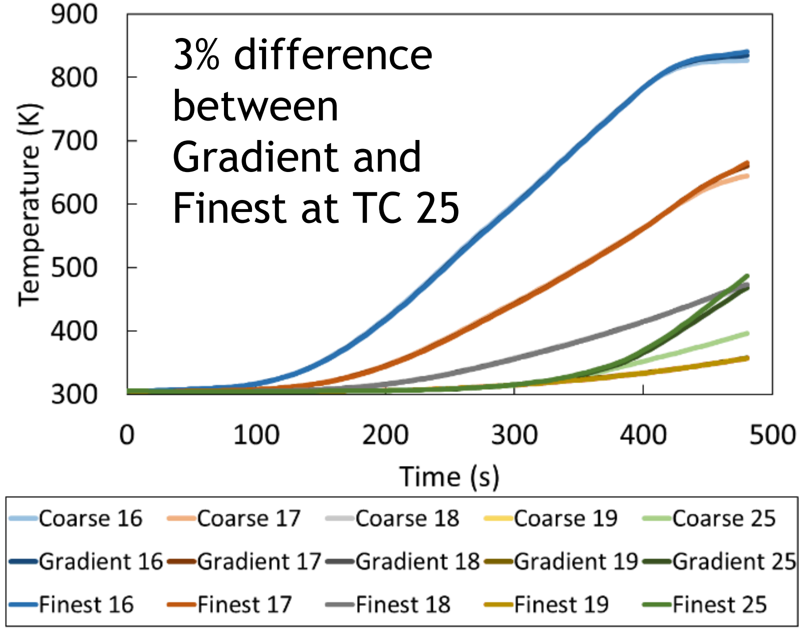


0.77mm
7,067 nodes

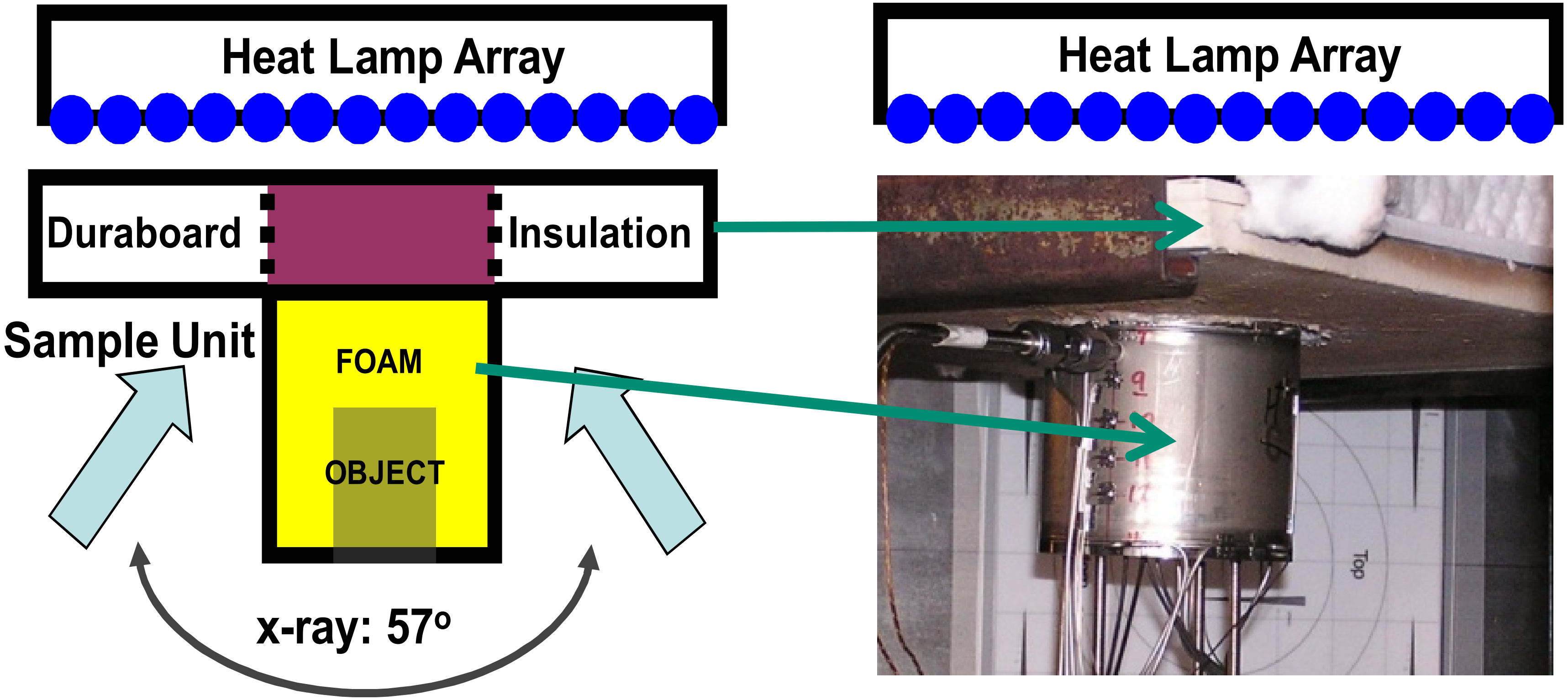
Finest

0.35mm
43,055 nodes





Foam in a Can Experiment



Monitor pressure and temperature

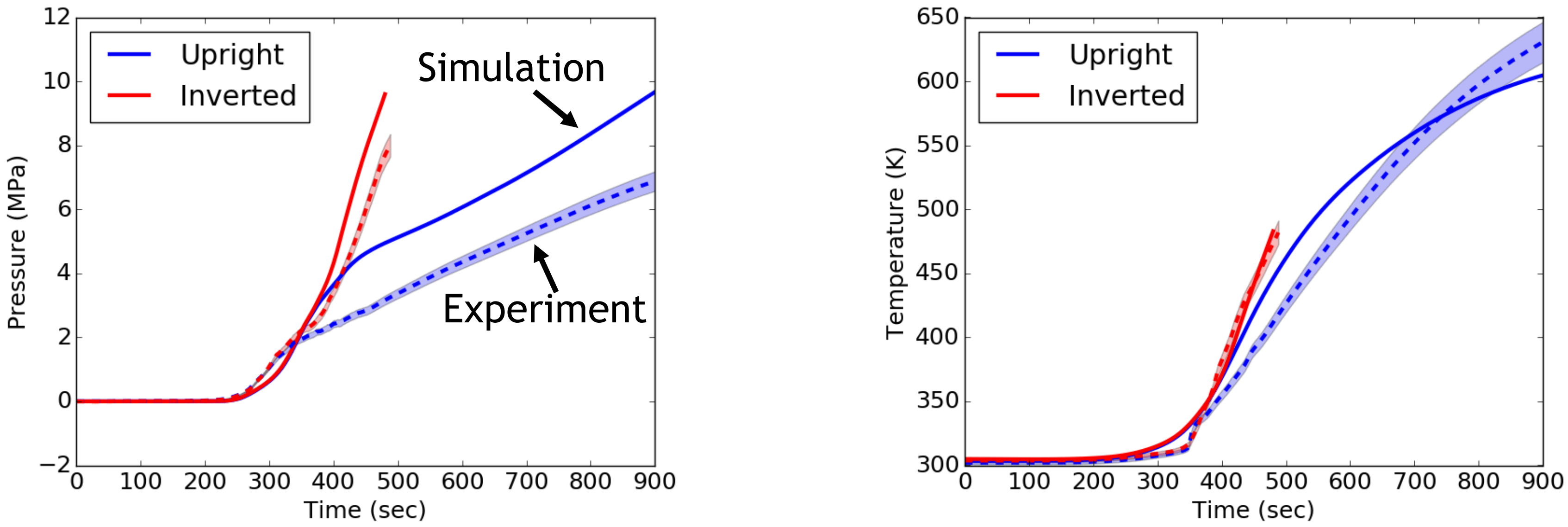
X-Rays to view can interior

Experiments run to breach


Model Validation and Uncertainty Quantification

How Do We Validate This Model?

We have both experimental and simulation data – can we just compare them?



However, to run this simulation, **31** foam properties were used.

Nominal Properties

		Virgin	*Liquid*	*Char*
Foam (virgin, liquid, char)	Bulk Density (kg/m^3)	320	1000	64
	Solid Density (kg/m^3)	1500	1050	1500
	Rosseland Coefficient (mK)	1990	100000	340
	Bulk Conductivity (W/mK)	0.098-0.8	0.15	0.098-0.8
	Specific Heat Capacity (J/kgK)	1269-2203	1000	2203
	Permeability (m^2)	5.25×10^{-12}	5.25×10^{-12}	1.45×10^{-8}
Reactions	Heat of Reaction (J/kg)	0		
	Activation Energy (MJ/kg)	179		
	Mass Fractions	$0.45\ FOAM \xrightarrow[k_1]{} 0.252\ CO_2 + 0.198\ organics$ $0.15\ FOAM \xrightarrow[k_2]{} 0.15\ organics$ $0.40\ FOAM \xrightarrow[k_3]{} 0.2\ organics + 0.2\ char$		
Gas Products	Specific Heat Capacity (J/kgK)	1000		
	Mass Diffusivity (m^2/s)	2×10^{-5}		
	Viscosity (Pa s)	0.0005		
	Molecular Weight (g/mol)	85-107		
	Saturation Pressure (Pa)	$10^{\left(9.3-\frac{1661}{T-74}\right)}$		

How To Determine a Range?

Example 1: Virgin Foam Bulk Conductivity

- Have multiple data sets for the conductivity at several densities over a temperature range of 300-523 K
- A range of ±**35%** encapsulated the measured values (with measurement error included)

Example 2: Char Radiative Conductivity

- Radiative heat transfer is accounted for by an effective conductivity calculated by the diffusion method for an optically thick media
- Have no experimental data, had previously calibrated this parameter
- Chose to have the char radiative conductivity have twice the uncertainty of the virgin foam, ±**70%**.

Sensitivity

How do we assess the sensitivity of each response to each parameter?

- **Pearson correlation coefficient** is a number between 0 and 1, where 0 means there is no correlation and 1 means there is a high correlation

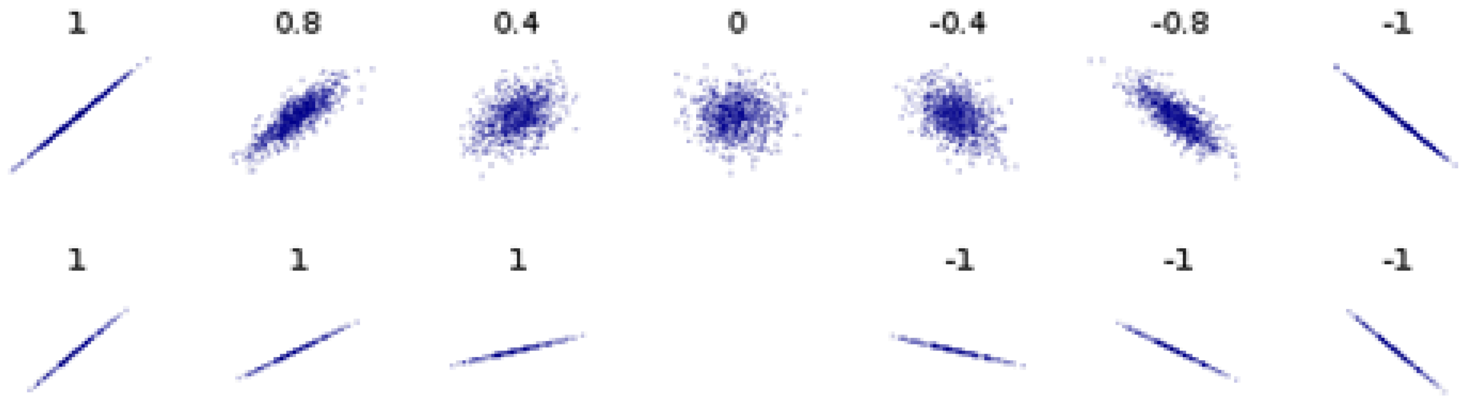
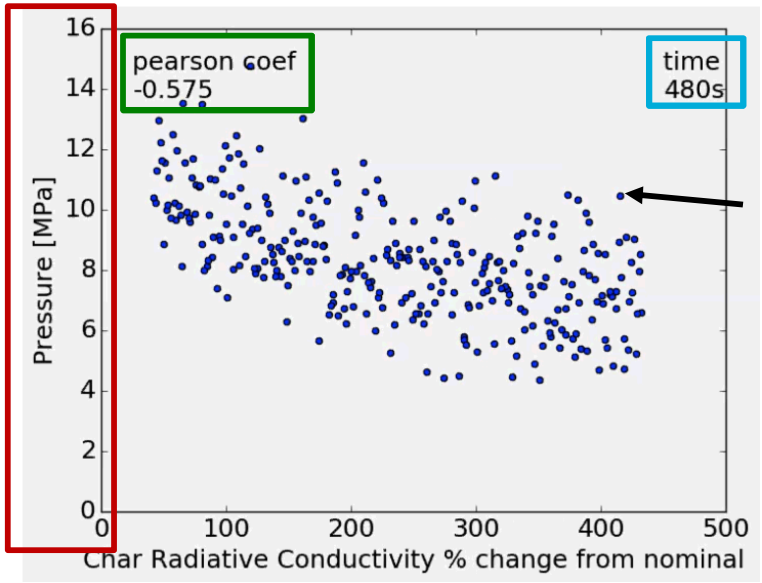
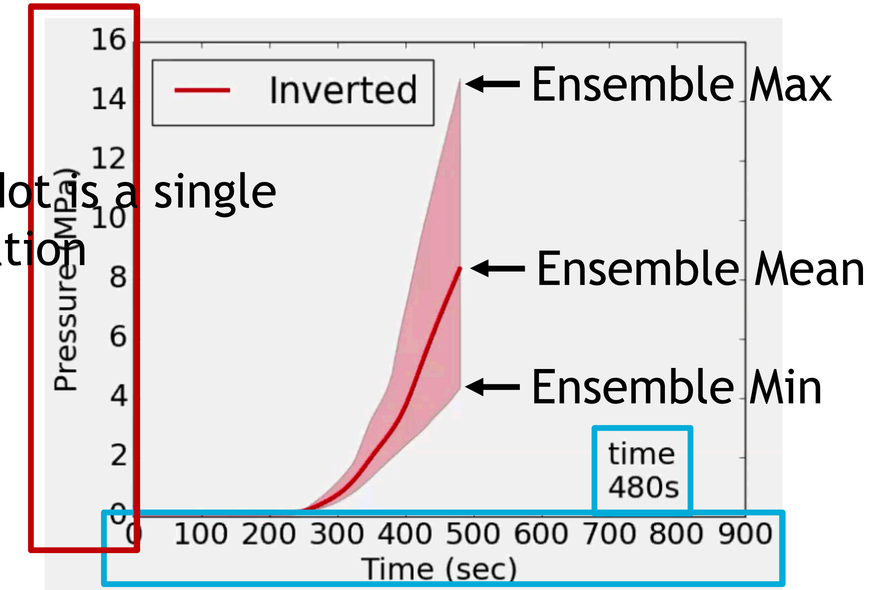


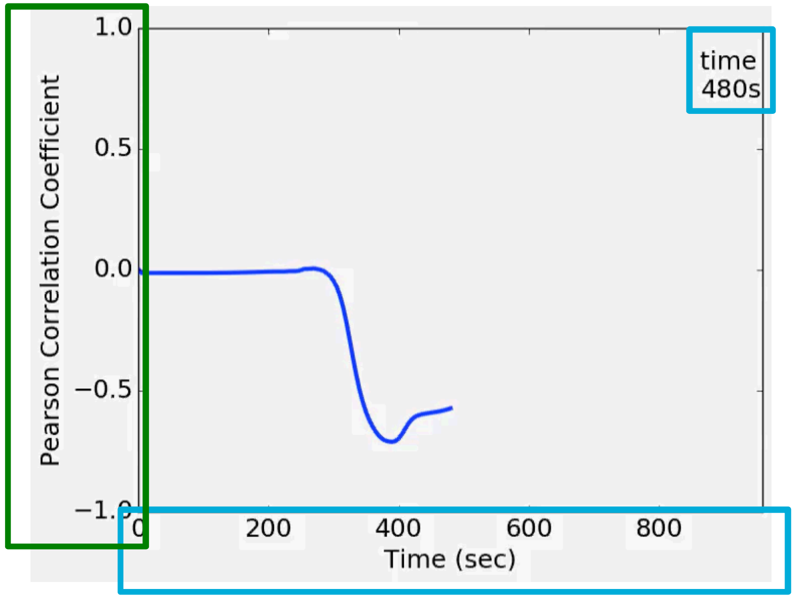
Image: https://en.wikipedia.org/wiki/Pearson_correlation_coefficient

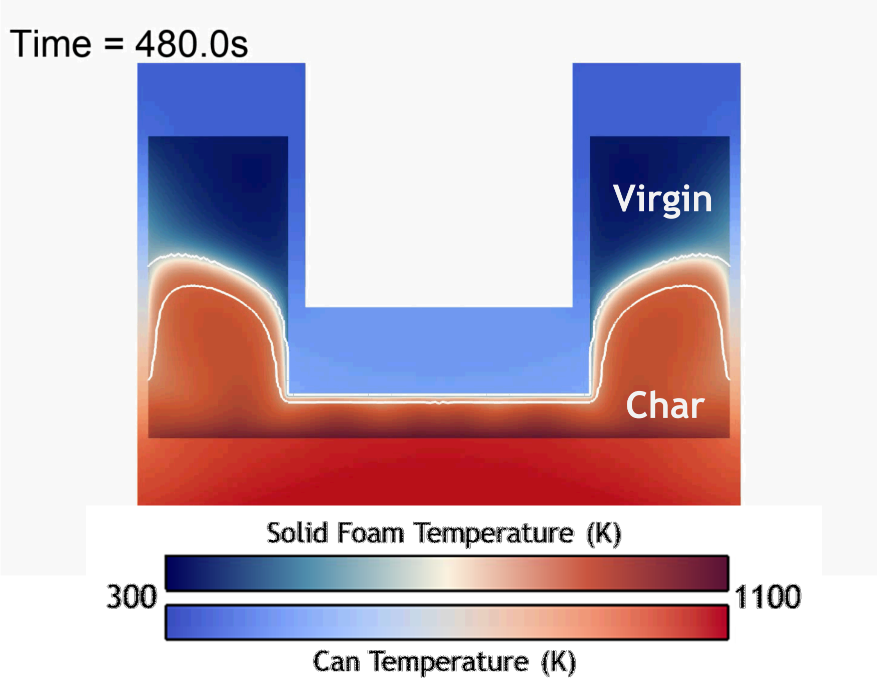
Parameter: Char Radiative Conductivity



Each dot is a single simulation







Top Three Parameters