Numerical Modeling of Heat Transfer in Foams in Fire Environments

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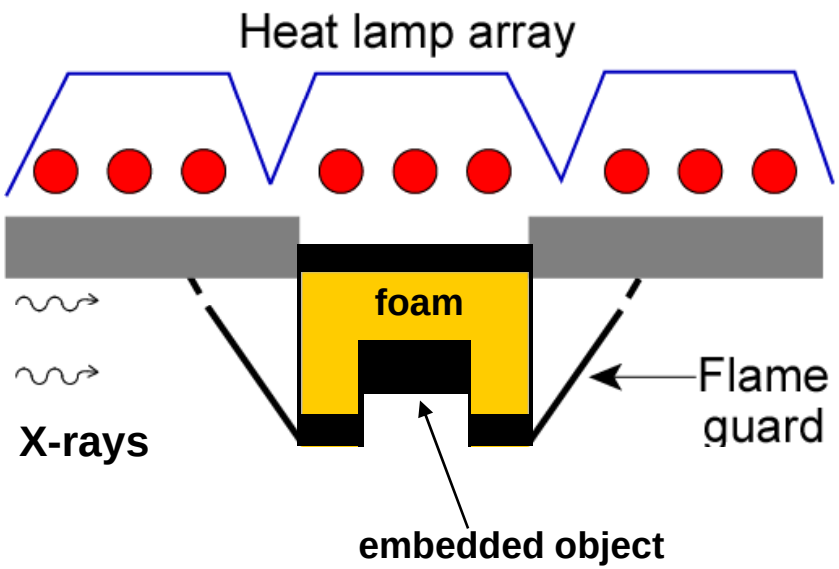
Outline

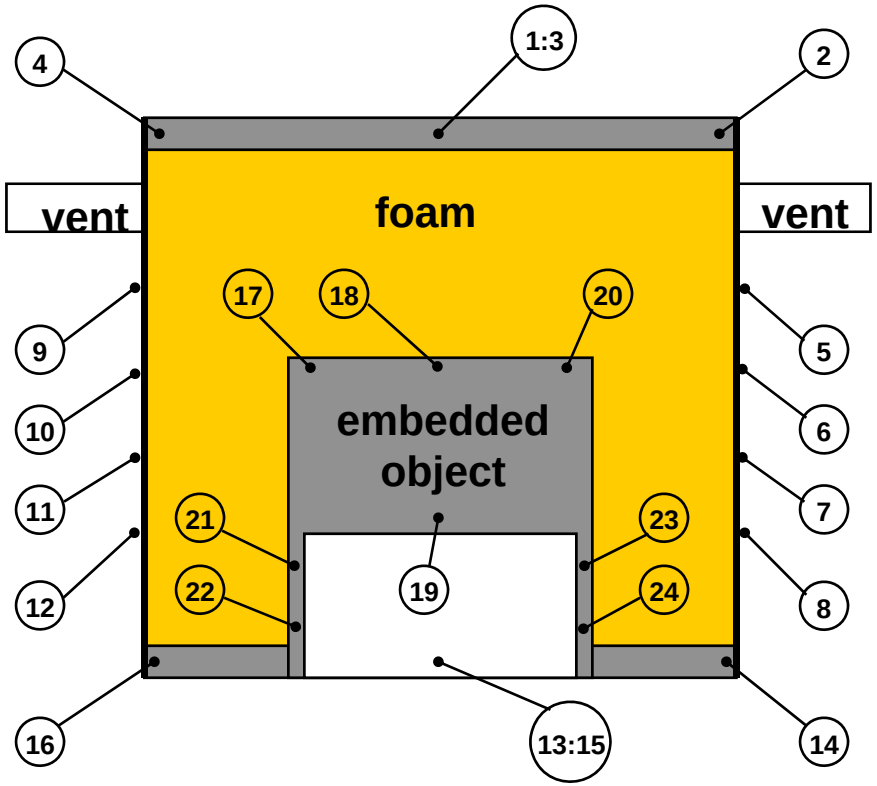
- Overview of Experimental Setup
- Overview of Mathematical Formulation
- Numerical Modeling of Removable Epoxy Foam (REF)
- Numerical Modeling of High-Char Foam
- Future Work

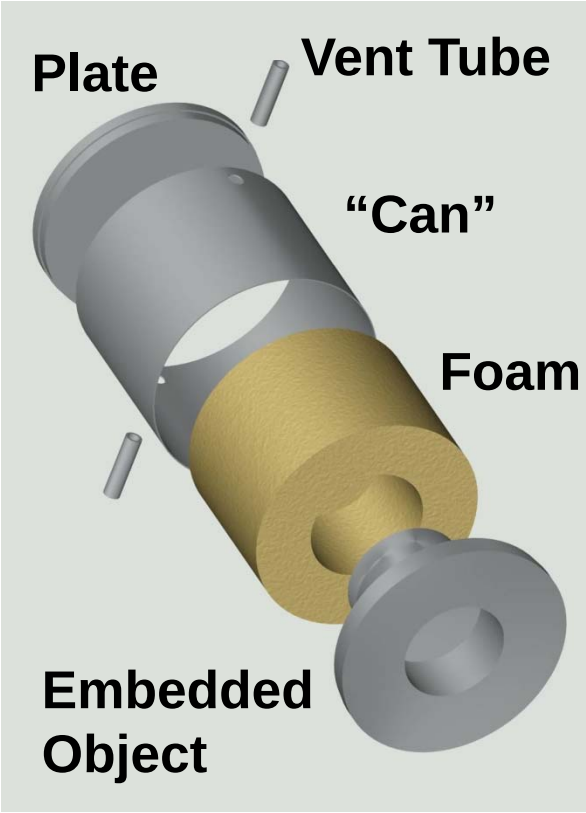
Overview of Experimental Setup

Foam in Can (FIC) tested in controlled radiant environment



FIC assembly instrumented with 24 thermocouples





Overview of Mathematical Formulation

General description of the mathematical model

- Heat conduction with energy generation due to reactions

$$\rho C_p \frac{\partial T}{\partial t} - \nabla\left(k \nabla T\right) = Q_c \qquad Q_c = \sum_j r_j q_j$$

- Material properties can be expressed as a function of decomposition state
- Chemical reaction and energy generation in the reactive material

For the REF chemistry, 4 reactions &11 species

$$\sum_{i=1}^{I} \nu'_{ij} M_i \rightarrow \sum_{i}^{I} \nu''_{ij} M_i \quad j = 1, \ldots, J \qquad \frac{d}{dt}[N_i] = \sum_i (\nu''_{ij} - \nu'_{ij}) r_j \quad i = 1, \ldots, I$$

$$r_j = k_j(T) \prod_i [N_i]^{\mu_{ij}} \quad j = 1, \ldots, J \qquad k_j = A_j \exp\left(\frac{-E_j + \sigma_{E_j}}{RT}\right)$$

Numerical modeling

Analyses were done with Sandia thermal analysis software based on heat-conduction – Sierra/Calore

- Heat conduction
- Reactive materials
- Radiative transfer (model formulation is foam dependent)

Foam decomposition may involve:

- Chemical reactions as a function of temperature, pressure, and mass transfer
  - » vented verses closed systems
  - » confined verses unconfined chemistry model
- Liquefaction and flow of decomposing foam
- Channeling of hot gases
- Other physics not represented by Calore

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Decomposition behavior of REF and high-char foams are different

Decomposing REF

- Early testing of decomposing REF foam showed that a void opened as the REF decomposed
- Decomposition appeared to occur with a uniform regression front
- More recently, the foam-in-can experiments showed that additional layers of char-like structures developed within the void

Decomposing high-char foam

- Decomposing high-char foam was developed to decompose in a more predictable manner
- Early testing showed that a continuous porous solid structure remained after decomposition.
- Observed decomposition behavior was more consistent than REF

Formulation for the radiative transfer depends on the physical behavior of the decomposing foam

- REF → enclosure radiation with element death based on chemistry
- High-char foam → diffusion approximation for optically thick media

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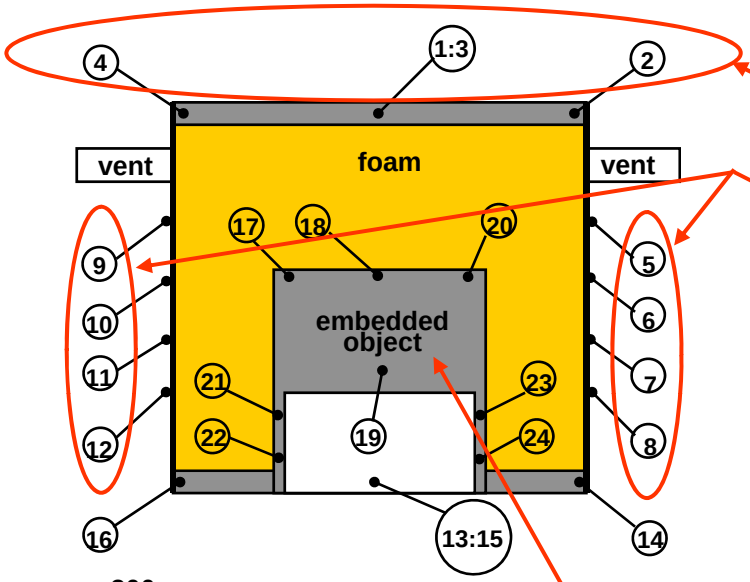
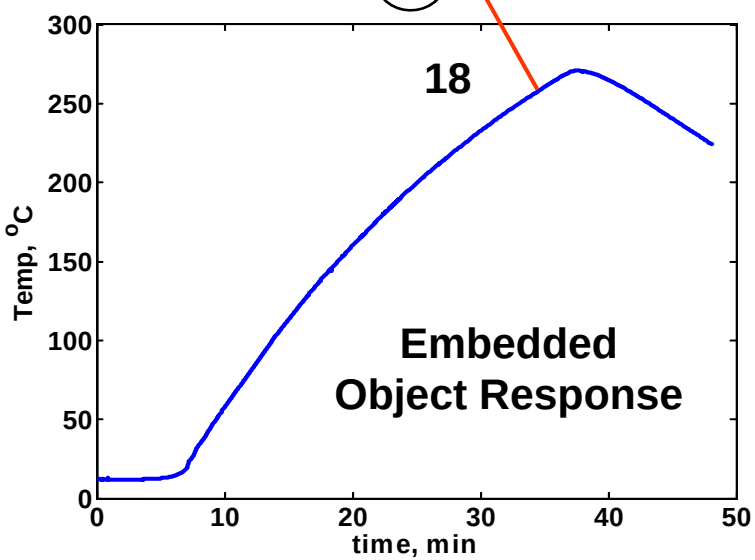
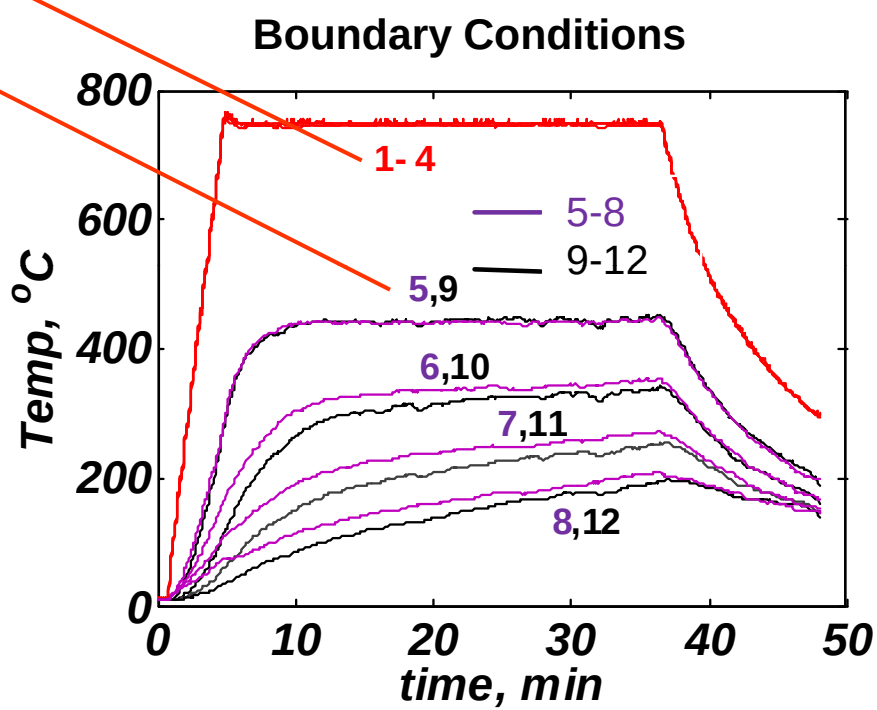
Comparison of model predictions and experimental data

- Focus of these comparisons are on the heat transfer to an embedded object
  - Pressure evolution (mechanical loading) is also important
- Multiple metrics could be selected
  - “Temperature history” or “Time-to-temperature-rise”
- For many of our applications, we are interested in the “time-to-temperature-rise” as a metric (thermal race)
- Validation & Verification of model predictions
  - Uncertainty in predictions computed by propagating the uncertainty in model parameters through the numerical model
  - Mesh sensitivity and convergence was demonstrated

Boundary conditions applied using measured temperature data







Numerical Modeling of REF

Formulation of radiative transfer in decomposing REF

Idealized decomposition behavior for REF

- As chemical state of foam elements approaches “complete reaction,” the decomposed elements are removed from the conduction calculation using an “element death” approach
- As elements are removed, a transparent void evolves in which radiative transfer is modeled using enclosure radiation (diffuse, gray surfaces)

$$\sum_{j=1}^{N}\left[\frac{\delta_{kj}}{\varepsilon_j} - F_{k-j}\left(\frac{1-\varepsilon_j}{\varepsilon_j}\right)\right]\frac{Q_j}{A_j} = \sum_{j=1}^{N}\left(\delta_{kj} - F_{k-j}\right)\sigma T_j^4$$

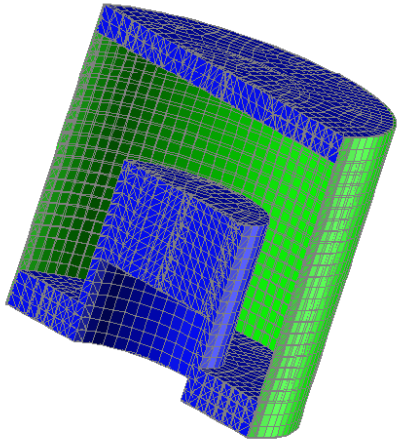
- Topology of the radiation enclosure is dynamic and requires that the viewfactors be recomputed at each time step
- Radiative fluxes are boundary conditions to the conduction equation

$$\rho C_p \frac{\partial T}{\partial t} - \nabla\left(k\nabla T\right) = Q_c$$

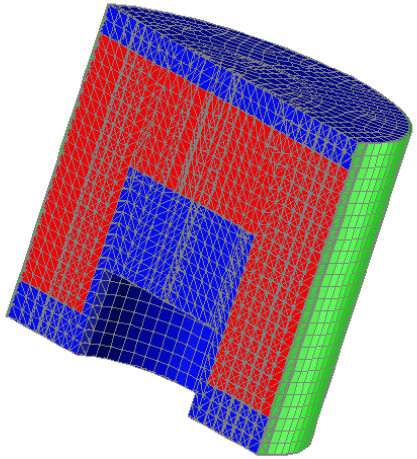
Decomposing REF modeled using an “element-death” concept

$$\rho C_p \frac{\partial T}{\partial t} - \nabla\left(k \nabla T\right) = Q_c$$

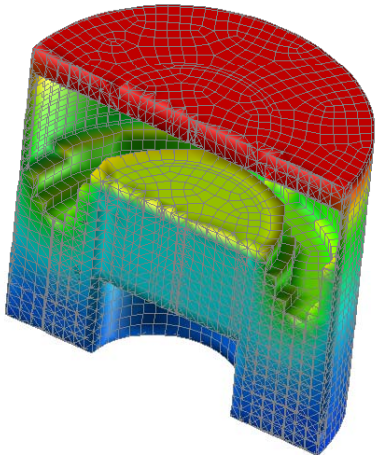
$$\sum_{j=1}^{N}\left[\frac{\delta_{kj}}{\varepsilon_j} - F_{k-j}\left(\frac{1-\varepsilon_j}{\varepsilon_j}\right)\right]\frac{Q_j}{A_j} = \sum_{j=1}^{N}\left(\delta_{kj} - F_{k-j}\right)\sigma T_j^4$$



Mesh of can without foam



Mesh of can and foam

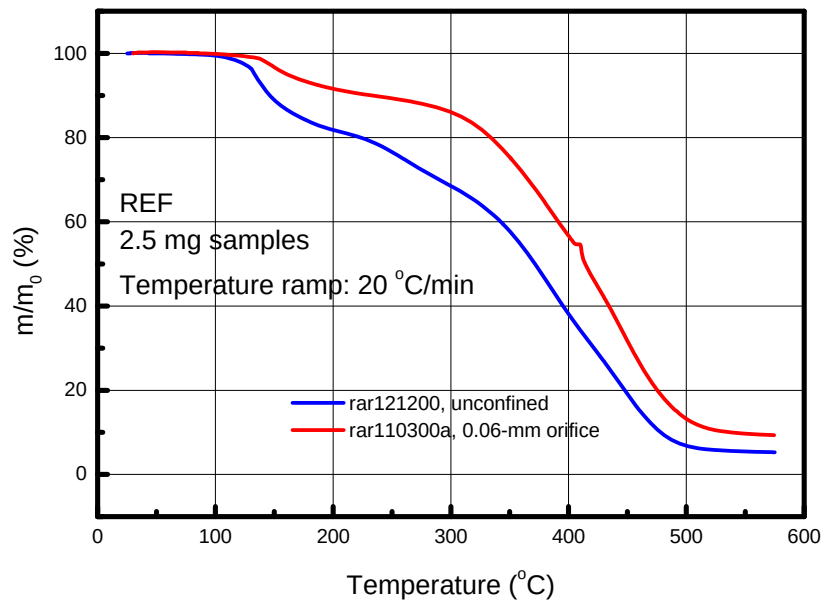


Mesh of can with foam decomposing

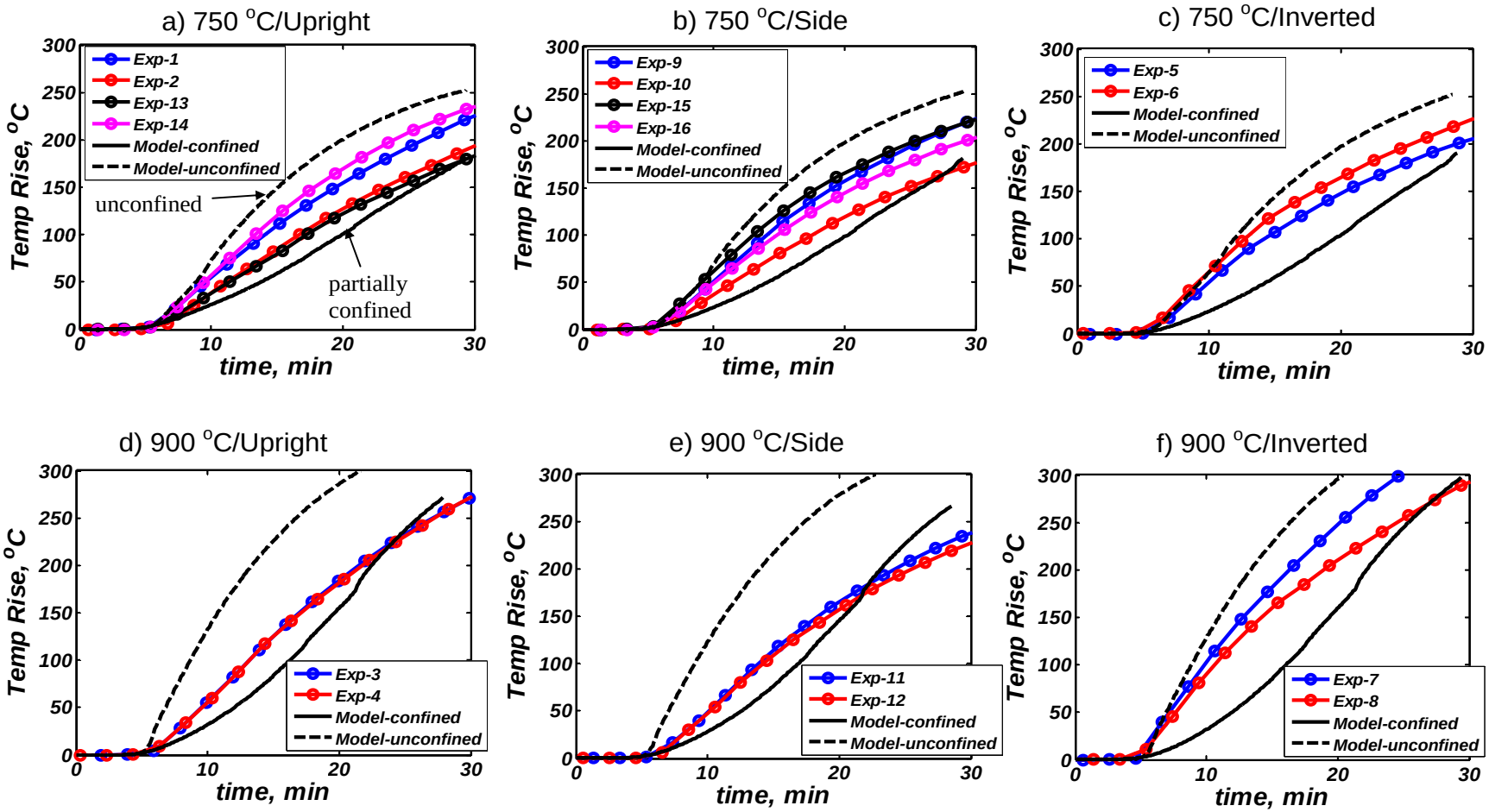
TGA-FTIR used to obtain reaction rate data

- Foam decomposition rates dependent on mass transfer effects that were characterized using a concept of “confinement”
- Confinement parameter was incorporated into the model to represent the bounds in restricting the role of mass transfer of decomposition products away from the decomposing material

- Evolved gases are monitored real-time with FTIR and periodically sampled for GC/MS
- Composition of evolved gases and vapors are relatively insensitive to confinement
- Decomposition rates are sensitive to confinement



Comparison of predicted temperature rise and data for vented REF



Post-test assessment of decomposed REF in FIC tests

Physical behavior of decomposing REF

- Incomplete reaction of foam due to complex behavior
  - Liquefaction, boiling, residue formation
- More residue formed than anticipated
- Model assumed that a “clean” transparent void would evolve as the foam decomposed and turned to gas
- Layers act as a radiation “shield” between hot plate and component
- Additional analysis to better understand impact of layers is on-going

Char layers formed inconsistently and impacted radiant heat transfer to encapsulated components

Summary and conclusions for REF

- With “unconfined” chemistry model
  - Component responded more quickly than data
  - Shape of response (concave downward) is consistent with data
- With “confined” chemistry model
  - Component responded more slowly than data
  - Shape of response (concave upward) is inconsistent with data
- Model predictions with “confined” and “unconfined” chemistry model bounded the experimental data

Current safety analyses include pressurization threats:

- Need to improve physical understanding of pressure evolution
- Pressure affects the overall physical behavior during decomposition
- Pressure provides the mechanical loading on sealed systems

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Developing models for decomposing REF is extremely challenging

Modeling issues with REF:

- Physical behavior includes coupled decomposition, liquefaction, and flow
- Erosive channeling and/or pressurization occurs in sealed containers
- Irregular bubble-like char evolves inconsistently and unpredictably

One alternative is to develop highly charring foams that:

- Develop a char that decomposes uniformly/predictably
- Do not liquefy and flow during decomposition
- Have physical and chemical properties amenable to modeling with available radiation-conduction heat transfer codes

Numerical Modeling of High-Char Foam

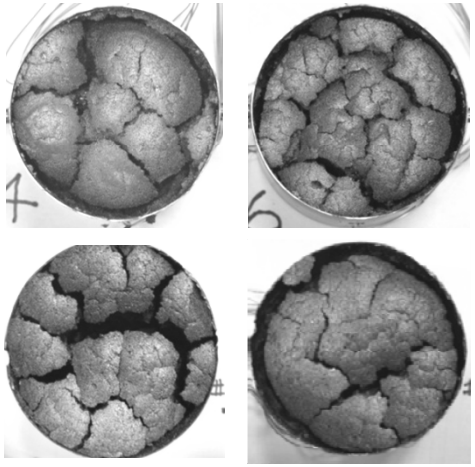
High-char foam is modeled using a diffusion approximation

Idealized decomposition behavior for high-char foam

- Foam is assumed to maintain structural integrity and overall volume as it decomposes
- Radiative transfer is modeled using a “diffusion” approximation appropriate for optically thick materials

$$\rho C_p \frac{\partial T}{\partial t} - \nabla\left(\left(k + k_e\right)\nabla T\right) = Q_c$$

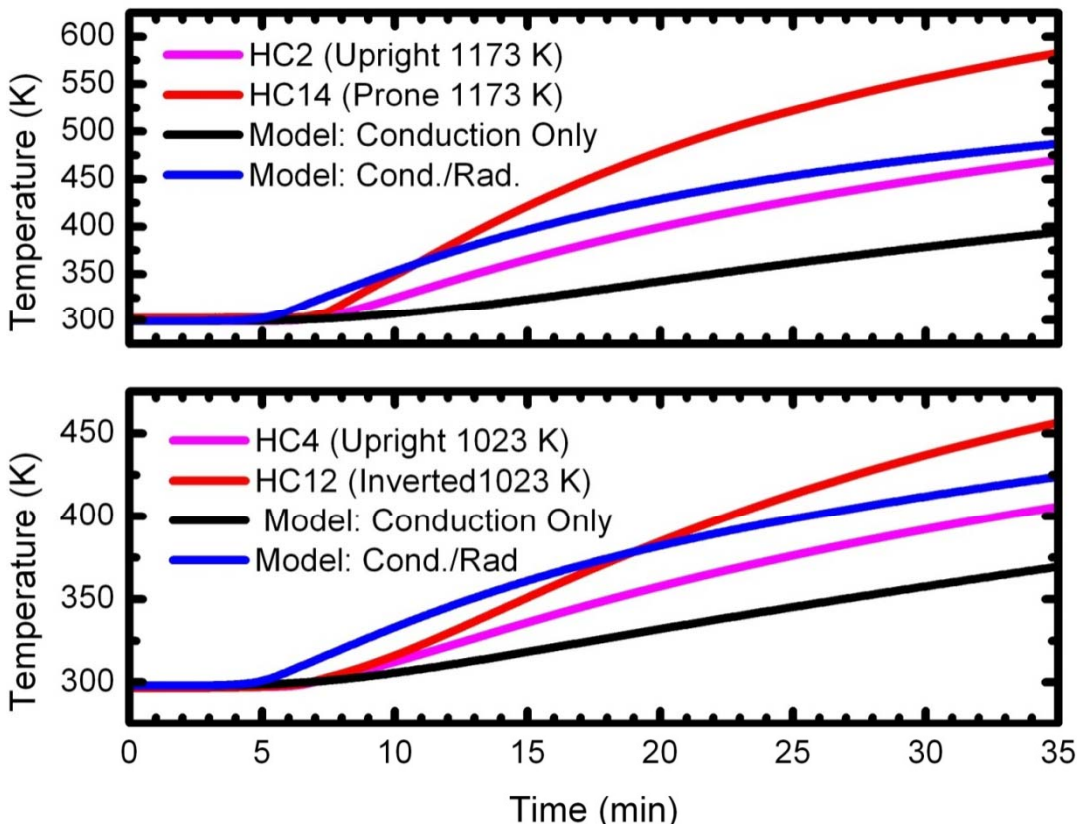
where $$k_e = \frac{16\sigma}{3\left(a + \sigma_s\right)} T^3$$



- Radiative diffusion coefficient determined from optical measurements (absorption and scattering coefficients) for un-reacted and reacted states

Comparison with experimental data for high-char foam was encouraging

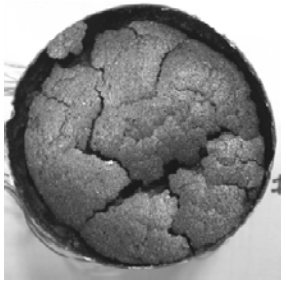
Model predictions for high-char model with diffusion approximation radiative transfer fall within experimental data for vented samples



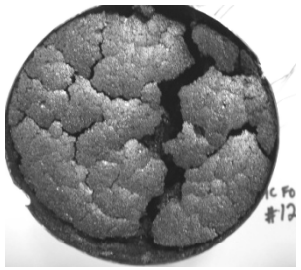
HC2

HC14

HC4



HC12



Post-test assessment of decomposed high-char foam in FIC tests

Comparisons of predictions and data:

- For vented samples
  - Large sample-to-sample variation in thermal response observed
  - Foam maintained it overall dimensions, but macro-cracks developed
  - Macro-cracks believed to be associated with voids during initial material processing and curing
- For sealed samples with pressurization
  - Smaller sample-to-sample variation in thermal response
  - Cracking was less prominent than for vented samples
  - Overall shrinkage was greater than for vented samples
- Presence of macro-scale cracks may have impacted the heat transfer to the embedded component
  - Model assumed radiative transfer could be represented using a diffusion approximation for a homogeneous medium
  - Macro-cracks provided path for radiative transfer through voids

Summary and conclusions for high-char foam

High char foams show promise:

- Experiments have demonstrated that high-char foam has the potential to decompose more consistently than REF
- Physical behavior is more amenable to modeling with conduction-based software

Additional development is needed to improve the material processing and consistency of decomposition:

- Improve foam uniformity by improving initial processing and curing
- Continue assessing foam formulations with improved physical behavior
- Need to improve physical understanding of pressure evolution
- Need similar experiments and characterization as done for REF

Future Work

It is important to include pressurization in future analyses

- Most of the past work has been directed towards understanding the heat transfer to embedded objects
- Focus has been on the predicting the thermal response and not the pressurization aspects
- Predicting pressurization depends on understanding the heat transfer "to the foam," in addition to "to the object"
  - Need to include the effects of liquefaction and flow
  - Need to consider a variety of discovery and model development experiments to characterize the pressure in these environments
  - Need small-scale as well as larger-scale experiments to resolve different physical behaviors

Future work is being directed on pressurization, with an emphasis on polyurethane foams

- Pressurization research could leverage our current collaboration with VNIIA on foam decomposition and "heat transfer to objects"

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Thank You