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VALIDATION ASSESSMENT FOR MODELING THE THERMAL RESPONSE OF COMPONENTS EMBEDDED IN REMOVABLE EPOXY FOAM – EXPERIMENTS AND DATA ANALYSIS

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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.

Outline

- **Overview of Validation**
- **Experimental Hierarchy**
  - Hierarchy for validating models of system response in abnormal (high flux/high temperature) environments
- **Describe Experimental Apparatus for Foam in a Can (FIC)**
  - Exps to validate models for predicting the thermal response of objects embedded in foam
  - Test suite designed to study effects of orientation and temperature environment
- **Present Analysis of the Experimental Data**
  - Assess repeatability of experimental conditions
  - Study physical dependencies of the experimental data
  - Assess sample-to-sample variability

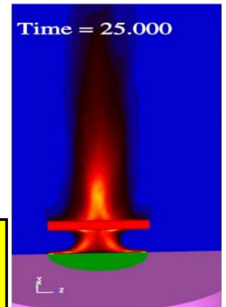
Validated models for predicting the thermal response of objects embedded in foam are needed

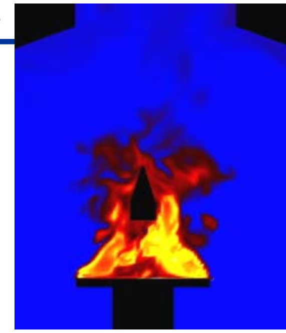
- **Experiments intended for the validation of models have additional requirements**
  - Want to assess the accuracy of the model as compared to discovery-type of experiments
  - Range of possible outcomes due to specimen-to-specimen variability
  - Study the accuracy over a suite of environmental conditions
- **Experiments need to be well-characterize**
  - Boundary conditions need to be measured with uncertainty characterized
  - Critical to know the specifics of an experiment
    - » TC locations, materials, experimental approach, impact ancillary materials, etc.
- **Topic of this talk is to demonstrate how to characterize validation quality experiments**

Validation Hierarchy Builds from Simple to Complex

Increasing Uncertainty

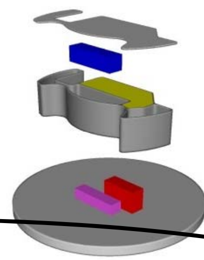
Validation of mockups in a Fire

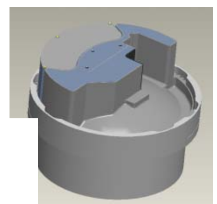


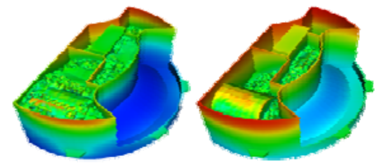


System Test (Qualification)

Validation Hierarchy specified with a PIRT (system in a Fire)

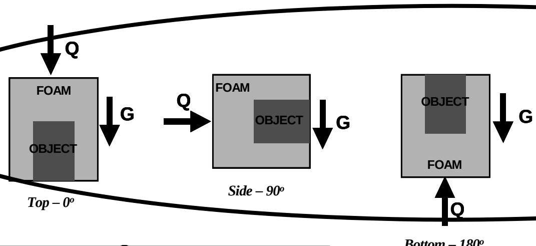




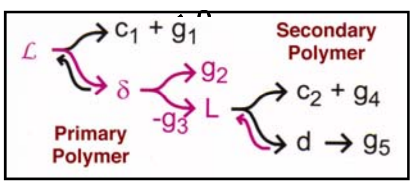


Validation with "as built"

Validation with mockups (multiple levels) in controlled environments (BCs)



Validation of foam recession



Validation of foam decomposition chemistry

Validation for each activity addresses uncertainty and estimates an appropriate uncertainty to carry to the next activity

Increasing Complexity

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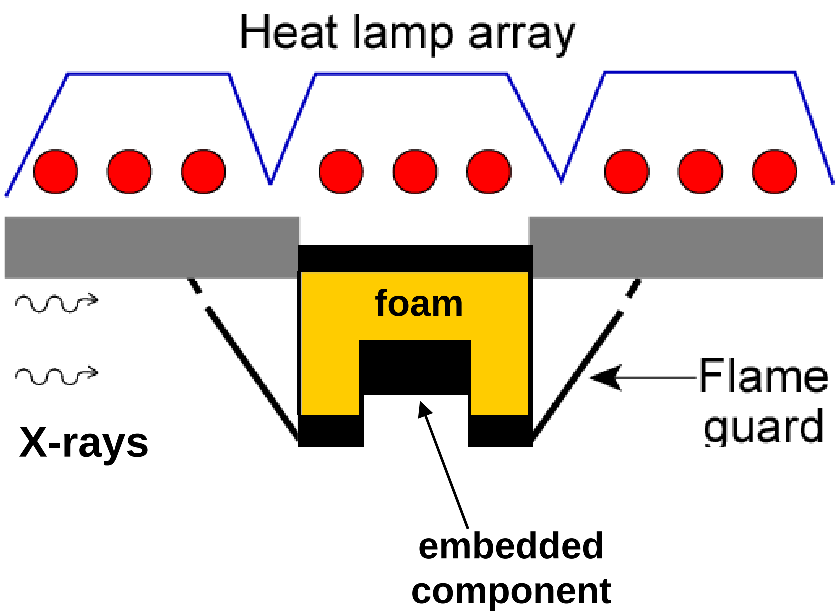
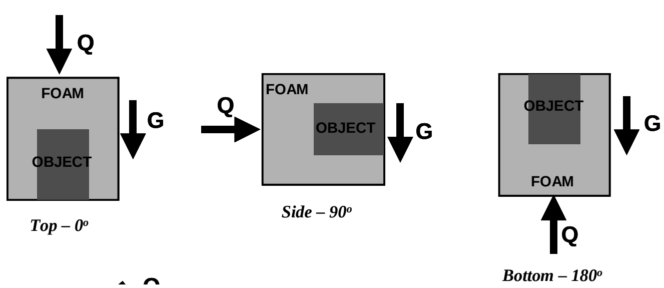
Foam in Can (FIC) tested in controlled radiant environment

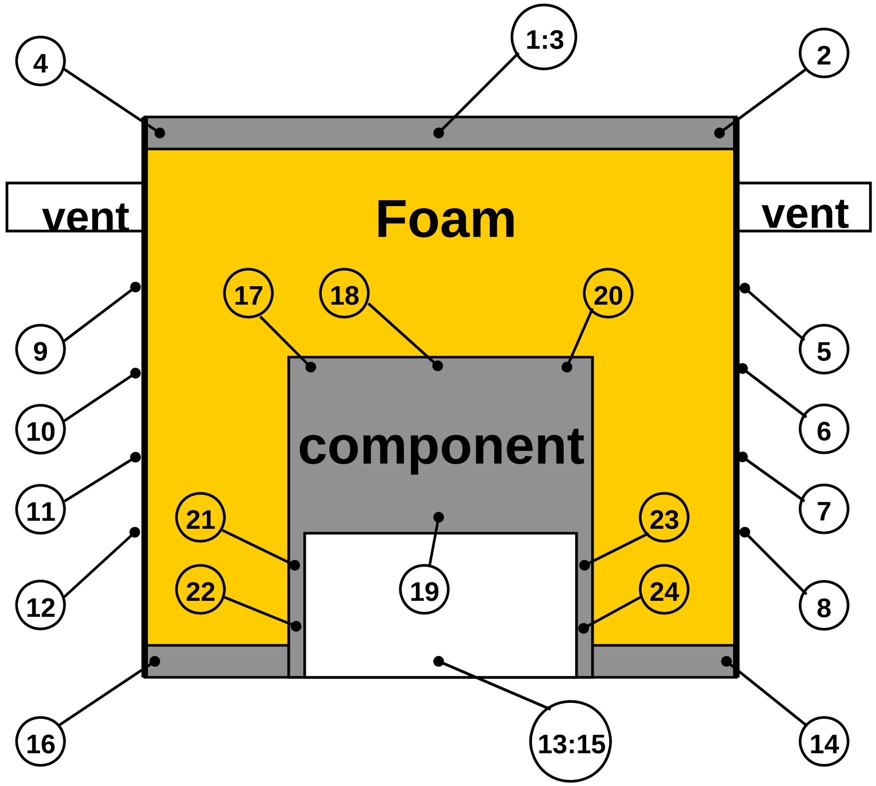


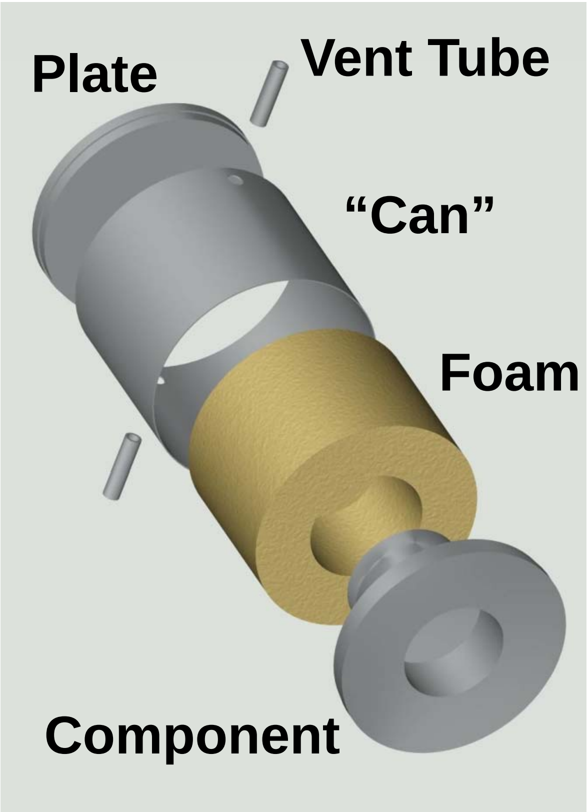


FIC Exp Apparatus

Apparatus rotated to study orientation effects and assess model's accuracy

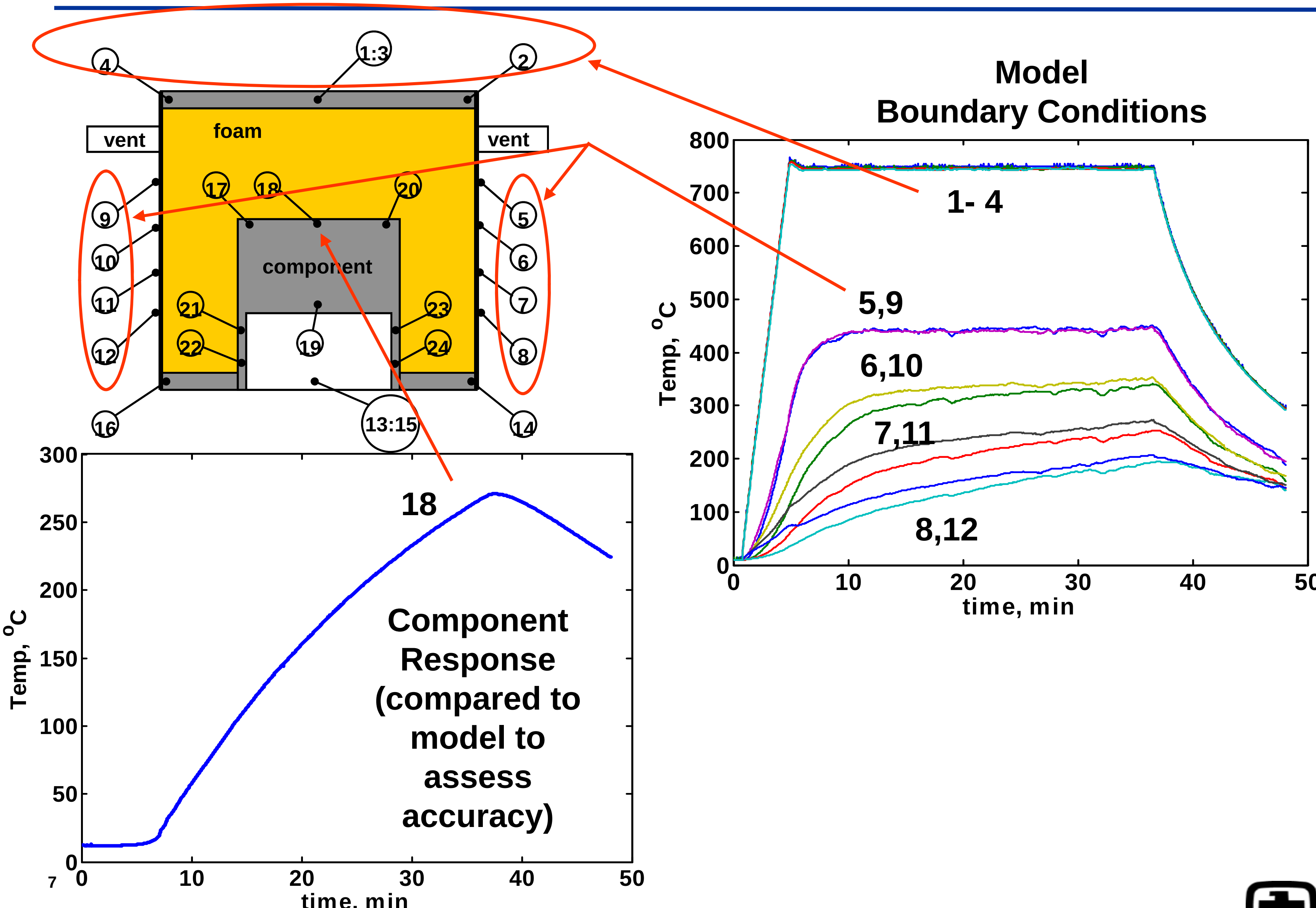
Assembly instrumented with 24 thermocouples for validation-quality data



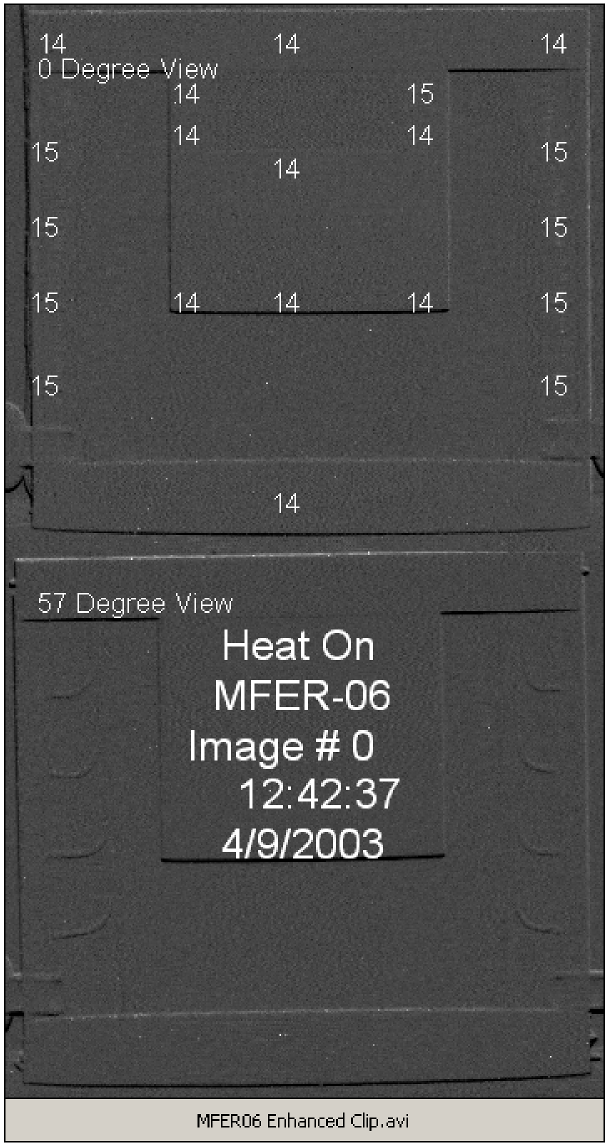


Material tested was a Removable Epoxy-based Foam (REF)

Typical measured temperature data

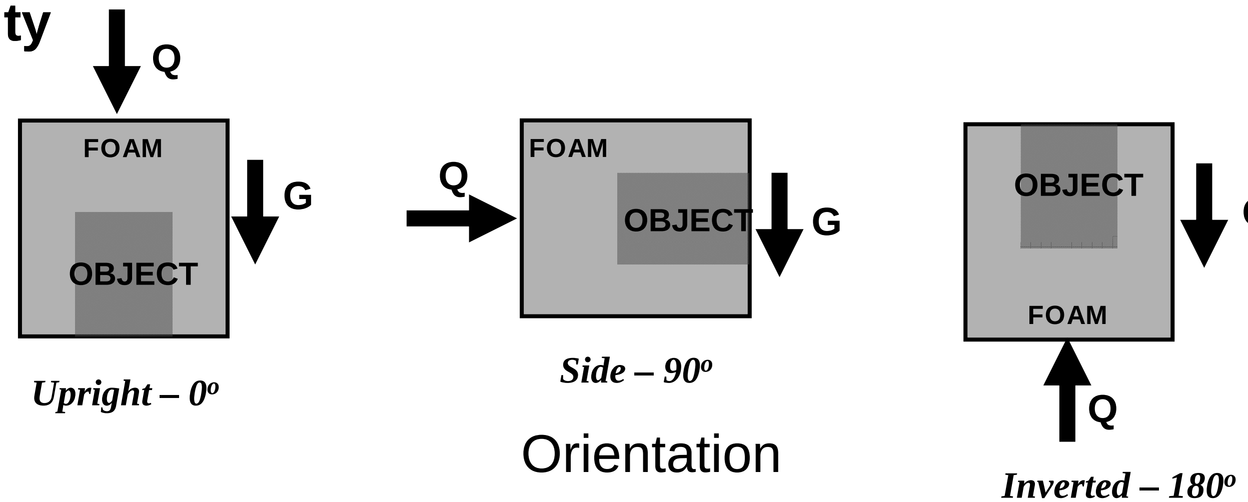


X-ray/T-response of



Test Suite designed to assess dependence on orientation and temperature

- **Intended application has foam in various orientations and T env.**
- **Experimental budget was to perform 16 experiments**
- **12 experiments conducted initially (2 T-level x 3 Orientations, with replication)**
- **Additional samples tested at 750ºC to better estimate sample-to-sample variability**



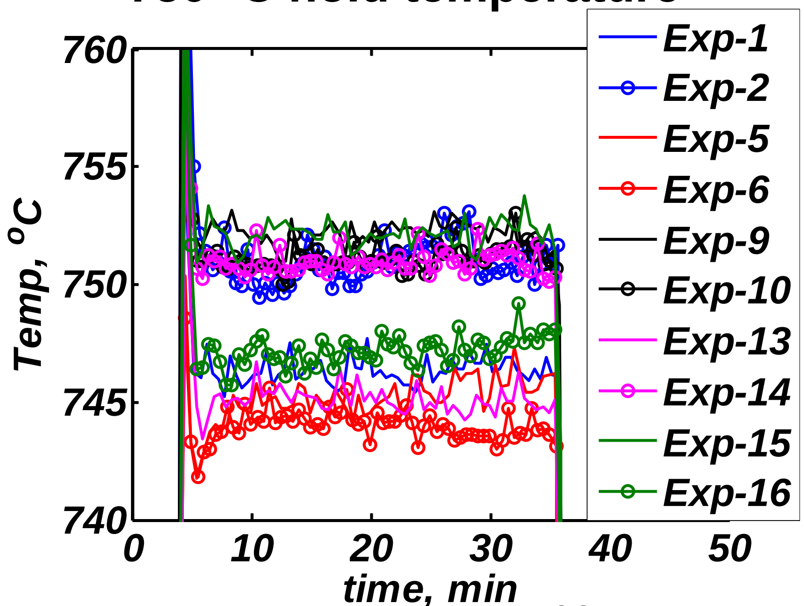
Hold Temp (ºC)	Orientation: Upright	Side	Inverted
750	2 + 2	2 + 2	2
900	2	2	2

Validation quality experiments have additional requirements

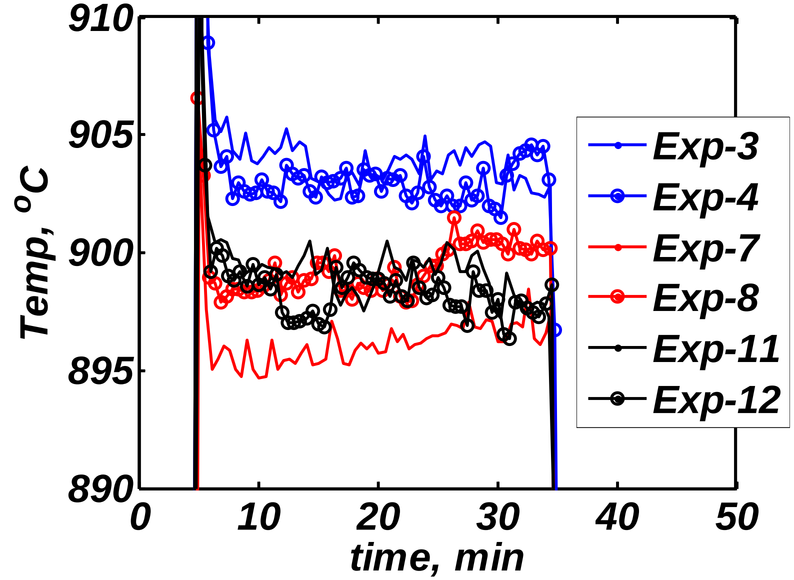
- **Repeatable and well-known boundary conditions**
  - Repeatable boundary conditions needed to directly compare outcome from experiments to assess effects of sample-to-sample variability
- **Assessments should be performed for application relevant measures**
  - Temperature response of objects embedded in foam
  - Time-to-temperature of objects embedded in foam (time to reach critical temperature)
- **Foam manufacturing processes have inherent variation**
  - Experimentally characterize the effect of sample-to-sample variation
  - Understand the impact of experimental variation on model validation (accuracy)

Boundary condition at the heated plate was repeatable in radiant environment

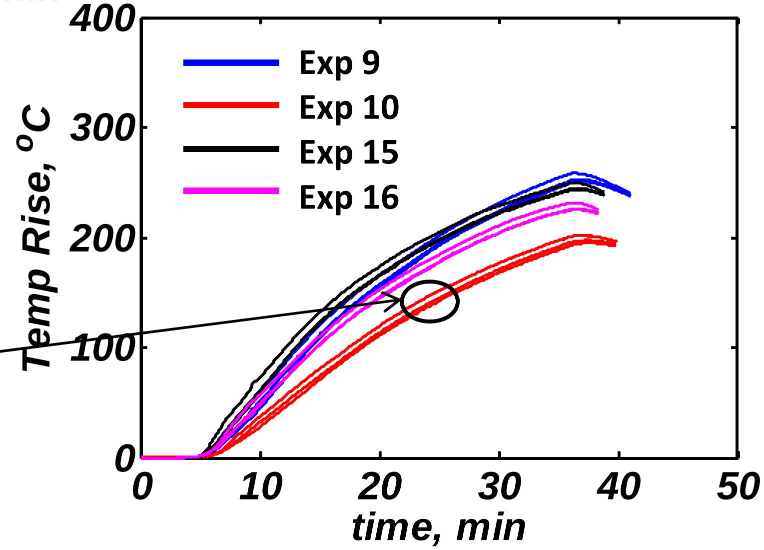
750 ºC hold temperature



900 ºC hold temperature



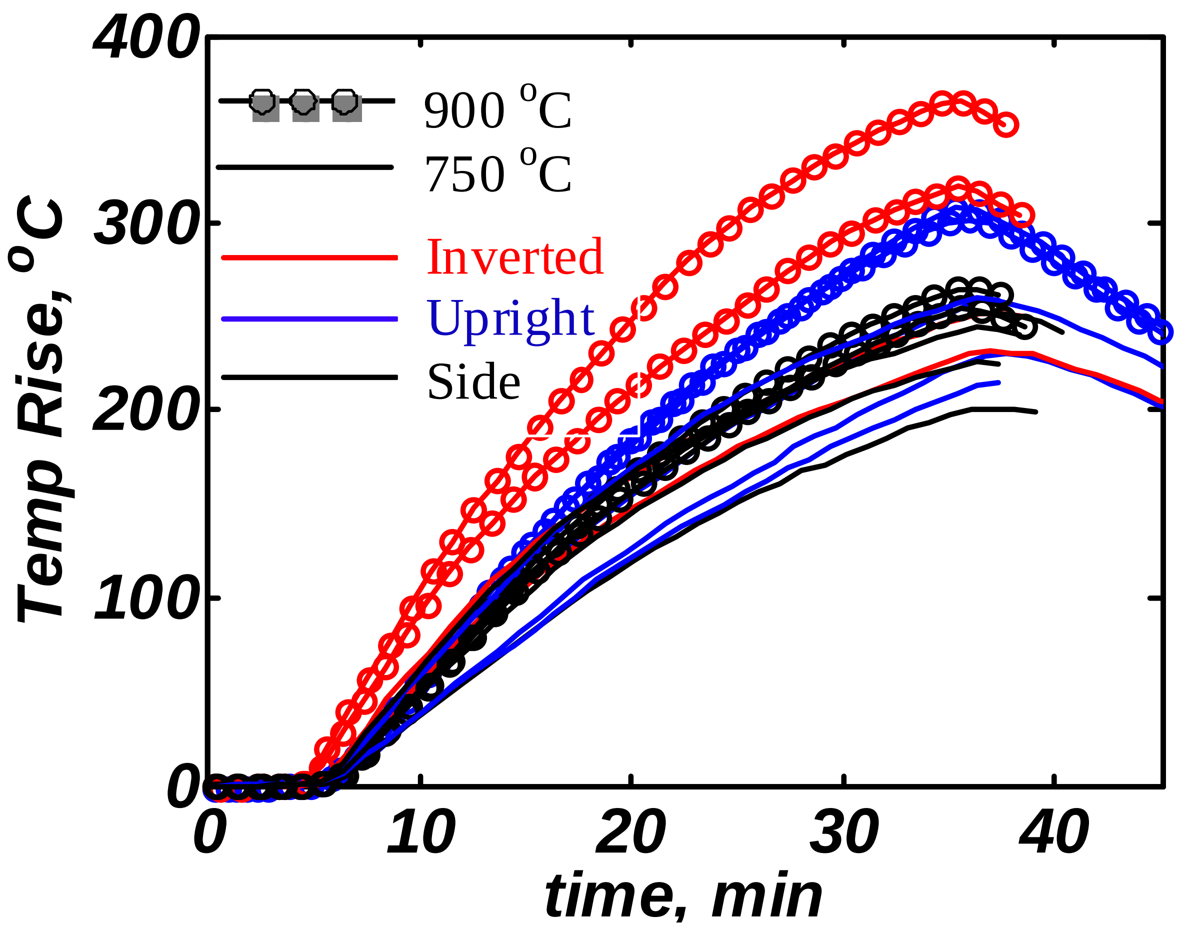
Component had small gradients in surface Temperature (TCs 17, 18, and 19)



Temperature Responses of 16 experiments over test suite (TC 18)

Replicate experiments can be compared if adjusted for:

1. Different initial temperatures and
2. Different initiation of heating



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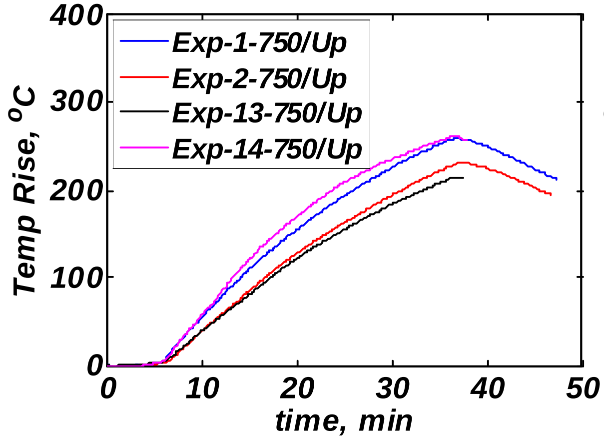
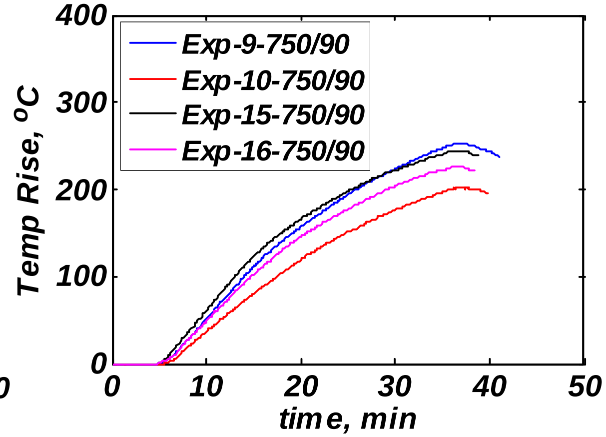
Thermal response of embedded component (TC 18)

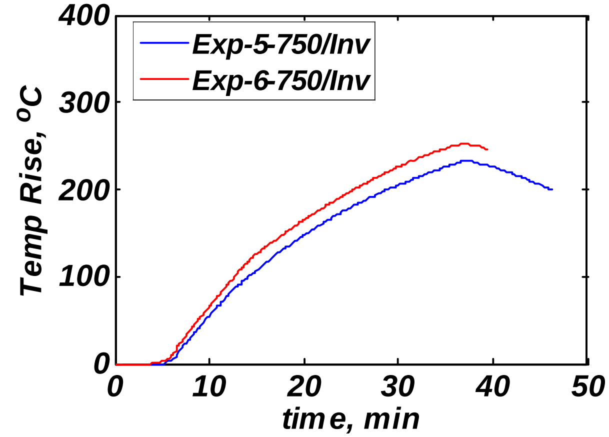
750 ^oC/Upright



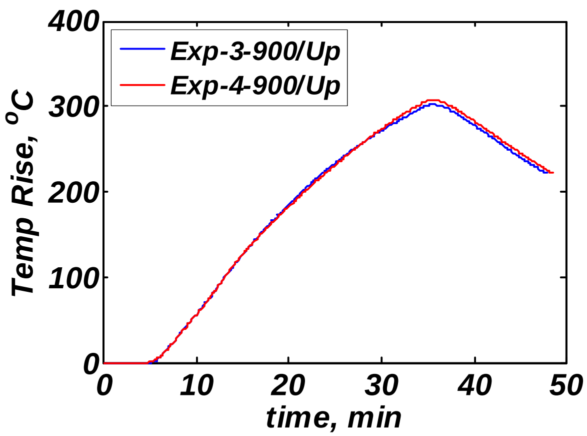
750 ^oC/Side



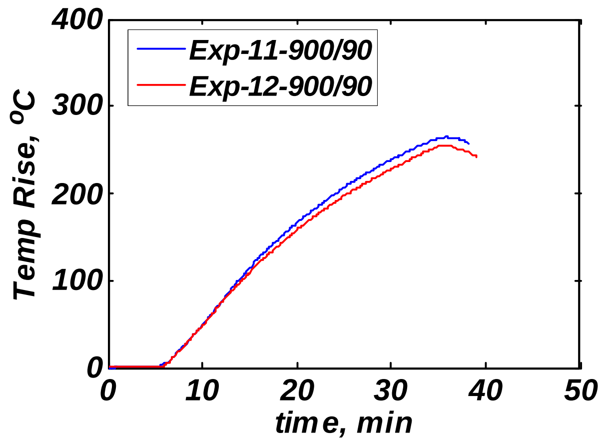
750 ^oC/Inverted



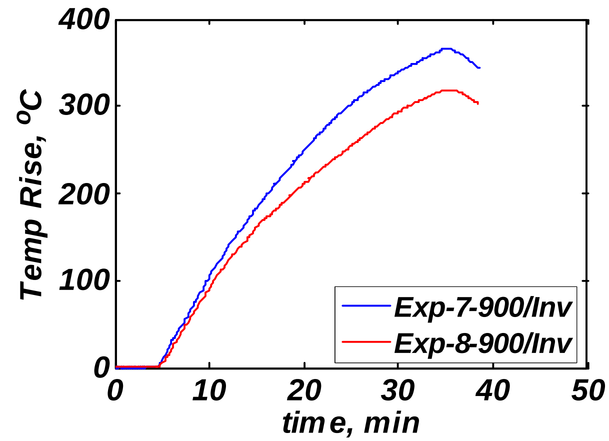
900 ^oC/Upright



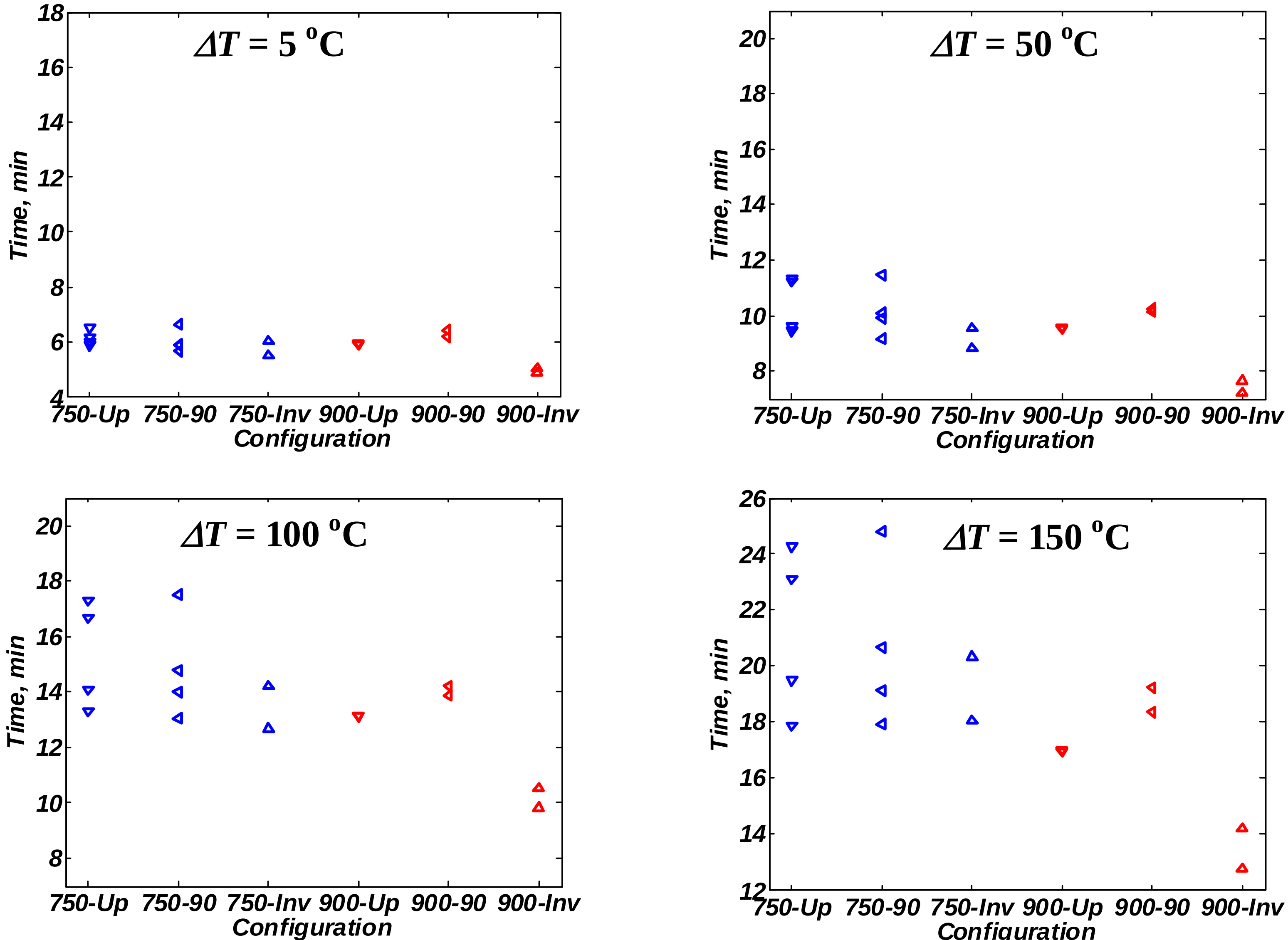
900 ^oC/Side



900 ^oC/Inverted



Assessment of time-to-temperature over the test suite



Experimental assessed for dependence on Temperature/Orientation

Analysis of Variance (ANOVA)

Source	Sum Sq.	d.f.	Mean Sq.	F	Prob>F
ΔT = 5°C					
Temp	0.15666	1	0.15666	1.13	0.3085
Orientation	1.43579	2	0.7179	5.18	0.0239
Error	1.66216	12	0.13851		
Total	3.43525	15			
ΔT = 50°C					
Temp	2.1998	1	2.19983	3.24	0.0969
Orientation	8.5586	2	4.2793	6.31	0.0134
Error	8.143	12	0.67858		
Total	20.4684	15			
ΔT = 100°C					
Temp	14.2587	1	14.2587	6.23	0.0281
Orientation	17.5634	2	8.7817	3.84	0.0515
Error	27.4616	12	2.885		
Total	64.8317	15			
ΔT = 150°C					
Temp	51.663	1	51.6629	9.26	0.0102
Orientation	25.646	2	12.823	2.3	0.1428
Error	66.927	12	5.5772		
Total	157.054	15			

Experimental assessed for dependence on Temperature/Orientation (2)

Analysis of Variance (ANOVA) excluding 900°C/Inverted

Source	Sum Sq.	d.f.	Mean Sq.	F	Prob>F
ΔT = 5°C					
Temp	0.00273	1	0.00372	0.03	0.8774
Orientation	0.14738	2	0.07369	0.68	0.5303
Error	1.08967	10	0.10897		
Total	1.26136	13			
ΔT = 50°C					
Temp	0.42692	1	0.42692	0.64	0.4421
Orientation	1.88375	2	0.94187	1.41	0.2881
Error	6.66587	10	0.66659		
Total	8.64573	13			
ΔT = 100°C					
Temp	5.8881	1	5.8881	2.37	0.1551
Orientation	4.2894	2	2.14472	0.86	0.4516
Error	24.8932	10	2.48932		
Total	33.0181	13			
ΔT = 150°C					
Temp	24.3313	1	24.3313	4.01	0.073
Orientation	4.9233	2	2.4616	0.41	0.6768
Error	60.6375	10	6.0638		
Total	86.0116	13			

Foam demonstrated a dependence on Orientation and Plate Temperature

- Early time-to-temperature responses (5 and 50 ^{o}C) depended on orientation
- Later time-to-temperature responses (100 and 150 ^{o}C) depended on plate temperature
- 900^{o}C/Inverted case was clearly different from other cases
- Excluding 900^{o}C/Inverted from the analysis indicated a dependence on plate temperature emerges at later time (150 ^{o}C and higher)
- Specimen-to-specimen variability ranged from 8-20%
- Effects of orientation and plate temperature were larger than variability

Summary

- Presented an experimental application for validation thermal response models for foam
- Described an approach to characterize validation quality date
  - Assessed repeatability of the heated boundary condition
  - Studied dependencies of the experimental data of test conditions (Orientation and Plate Temperature)
  - Analyzed data to quantify the dependencies and specimen to specimen variability
- Significant effect of orientation at 900 ^{o}C (Inverted)
- Plate temperature dependence emerges at later time in the experiments
- Significant sample-to-sample variation

Post-test

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Validation Assessment for Modeling the Thermal Response of Components Embedded in Removable Epoxy Foam – Numerical Modeling and Comparison

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Outline

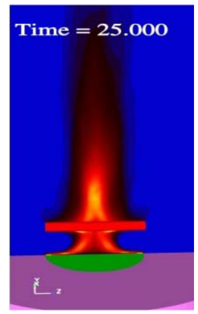
- Experimental Setup
- Numerical Modeling
- Comparison of Predicted Results and Experimental Data
- Uncertainty Quantification and Solution Verification
- Summary & Conclusions

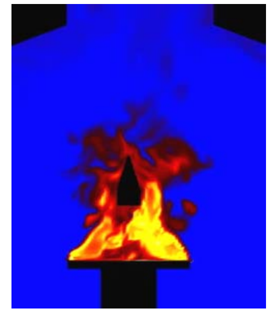
Validation hierarchy builds from simple to complex

Increasing Uncertainty

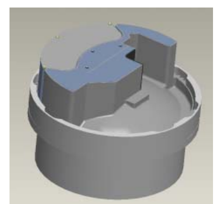
Validation hierarchy specified with a PIRT (system in a fire)

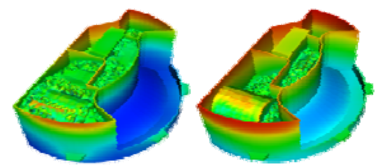
Validation of mockups in a fire



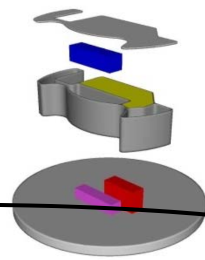


System Test (Qualification)

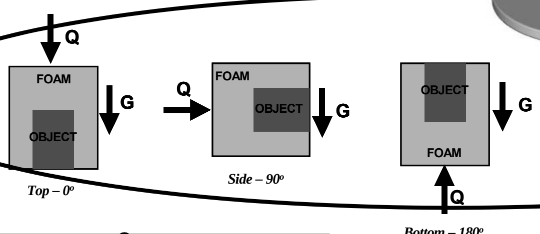




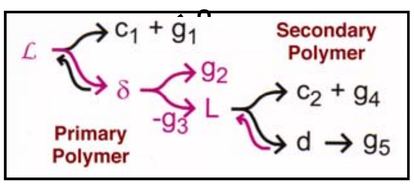
Validation with "as built"



Validation with mockups (multiple levels) in controlled environments (BCs)



Validation of foam recession



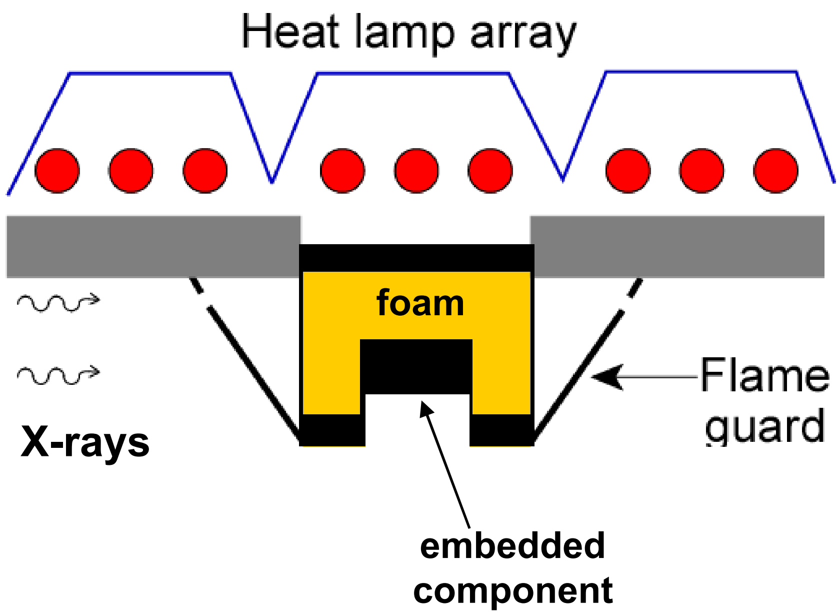
Validation of foam decomposition chemistry

Increasing Complexity

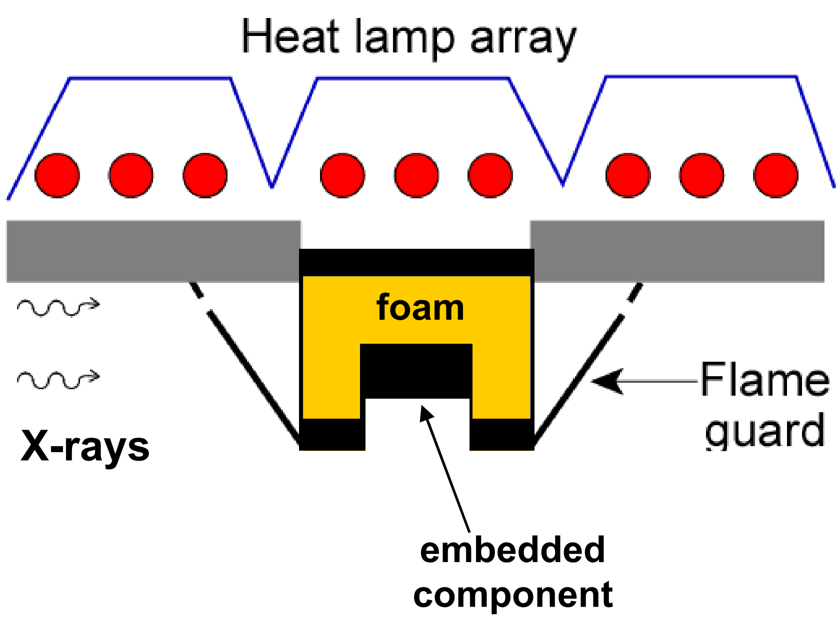
Validation for each activity addresses uncertainty and estimates an appropriate uncertainty to carry to the next activity

Experimental Setup

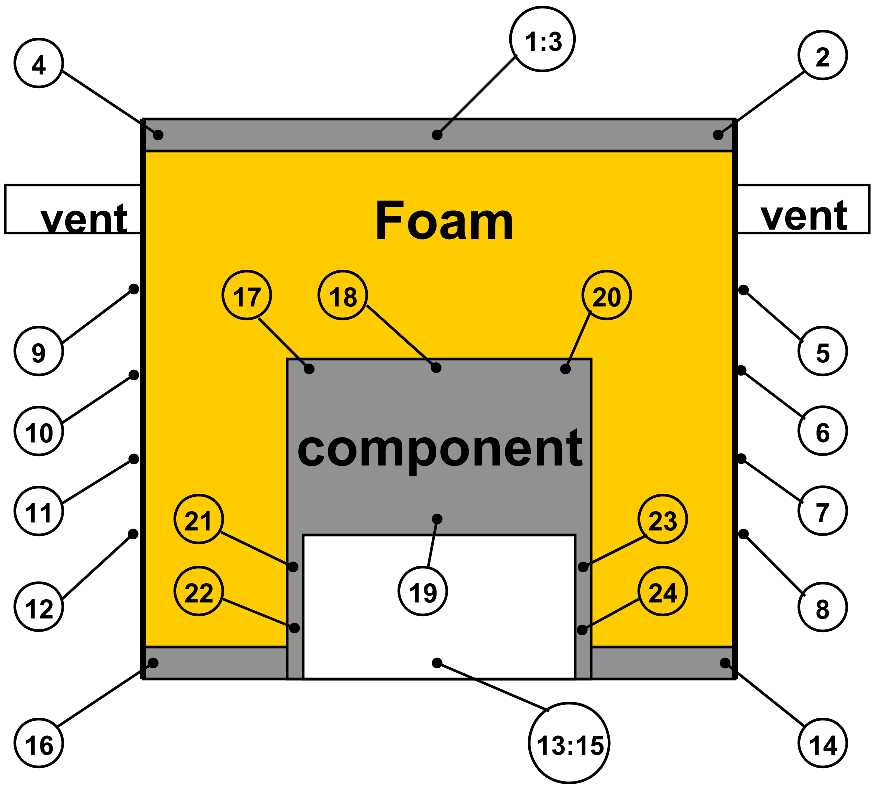
Foam in Can (FIC) tested in controlled radiant environment

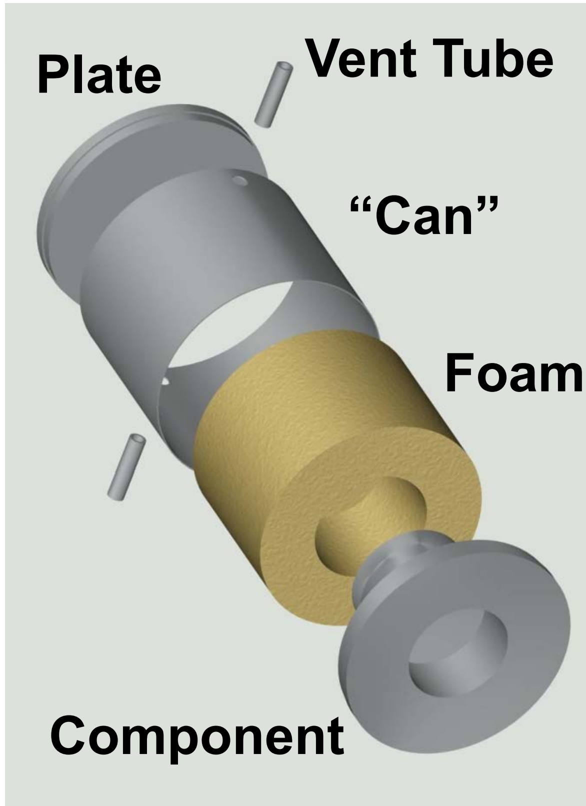


Foam in Can (FIC) tested in controlled radiant environment

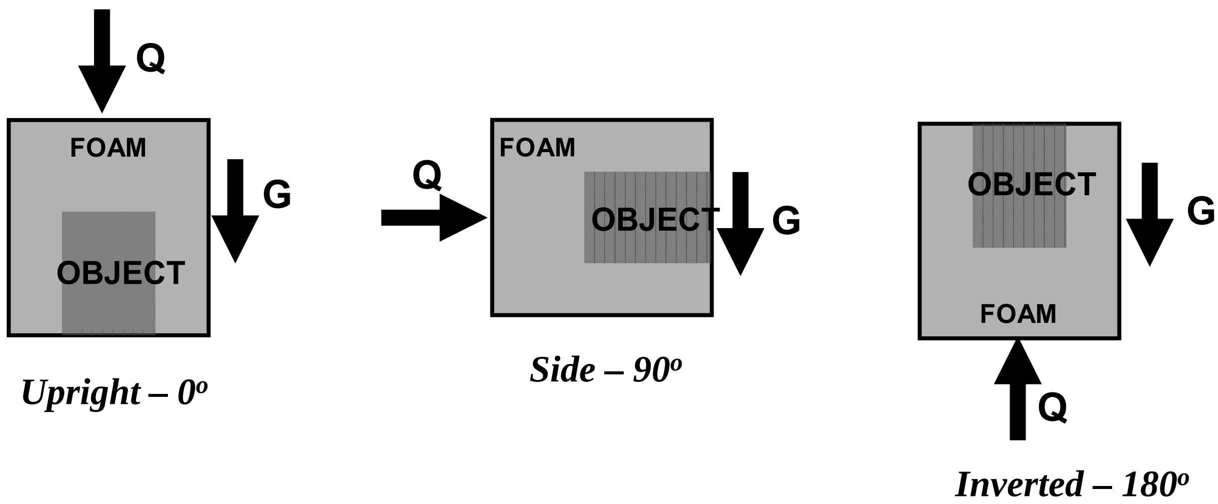


Assembly instrumented with 24 thermocouples





Foam in a Can test matrix (16 samples)



Orientation

Hold Temp (ºC)	Upright	Side	Inverted
750	4	4	2
900	2	2	2

Numerical Modeling

Numerical modeling

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

- Heat conduction
- Reactive materials
- Enclosure radiation through transparent media
- Dynamically evolving enclosures

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 liquid phase
- Other physics not represented by Calore

Description of the mathematical model

- Heat conduction with reactive energy generation

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

- Chemical reaction and energy generation in the reactive material

For the REF chemistry, 4 reactions &11 species

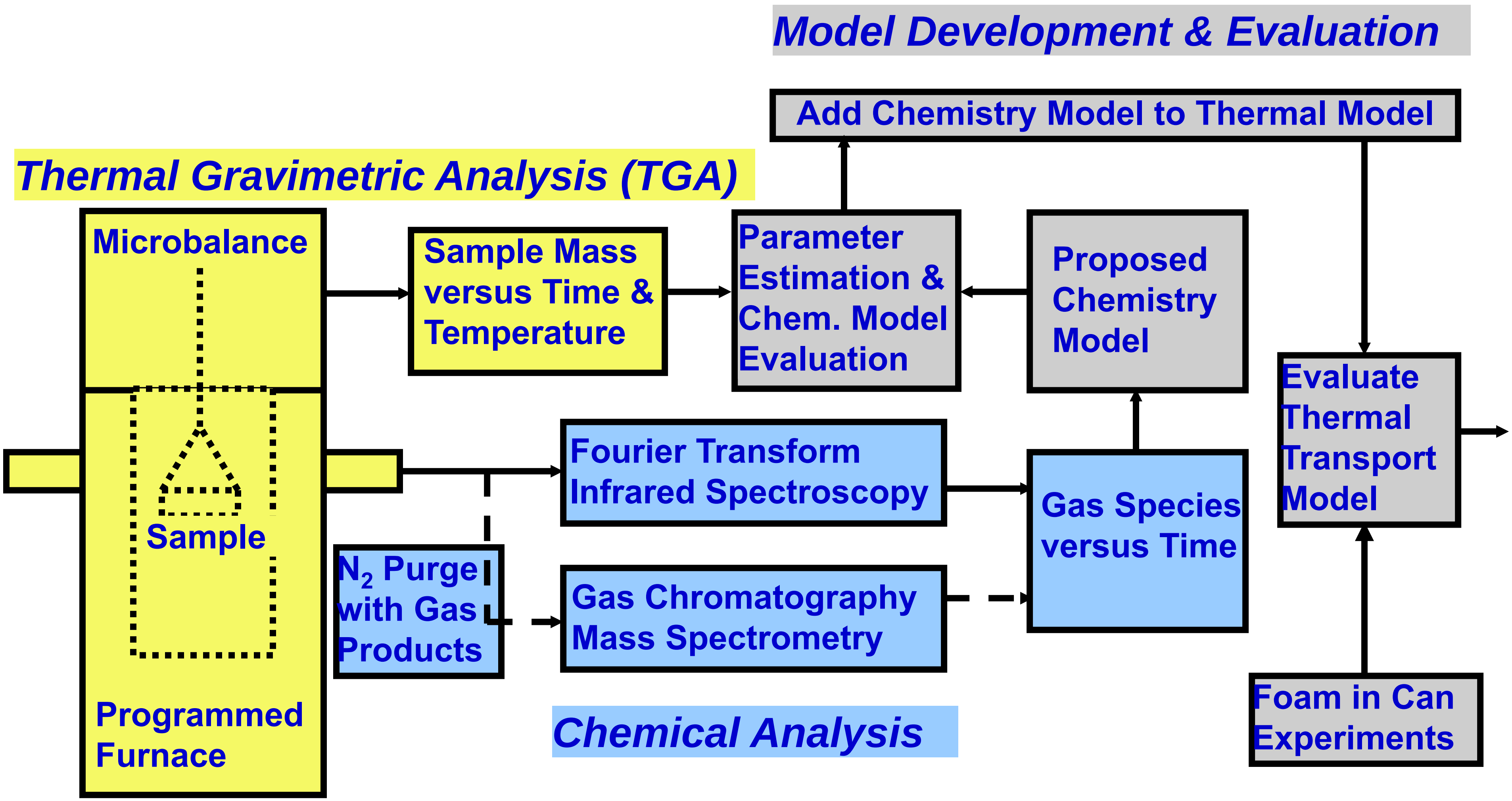
$$\sum_{i=1}^{I} \nu'_{ij} M_i \rightarrow \sum_{i}^{I} \nu''_{ij} M_i \quad j = 1, \ldots, J \qquad \frac{d}{dt}[N_i] = \sum_i (\nu''_{ij} - \nu'_{ij}) r_j \quad i = 1, \ldots, I$$

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

- Diffuse-gray radiation through a transparent enclosure

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

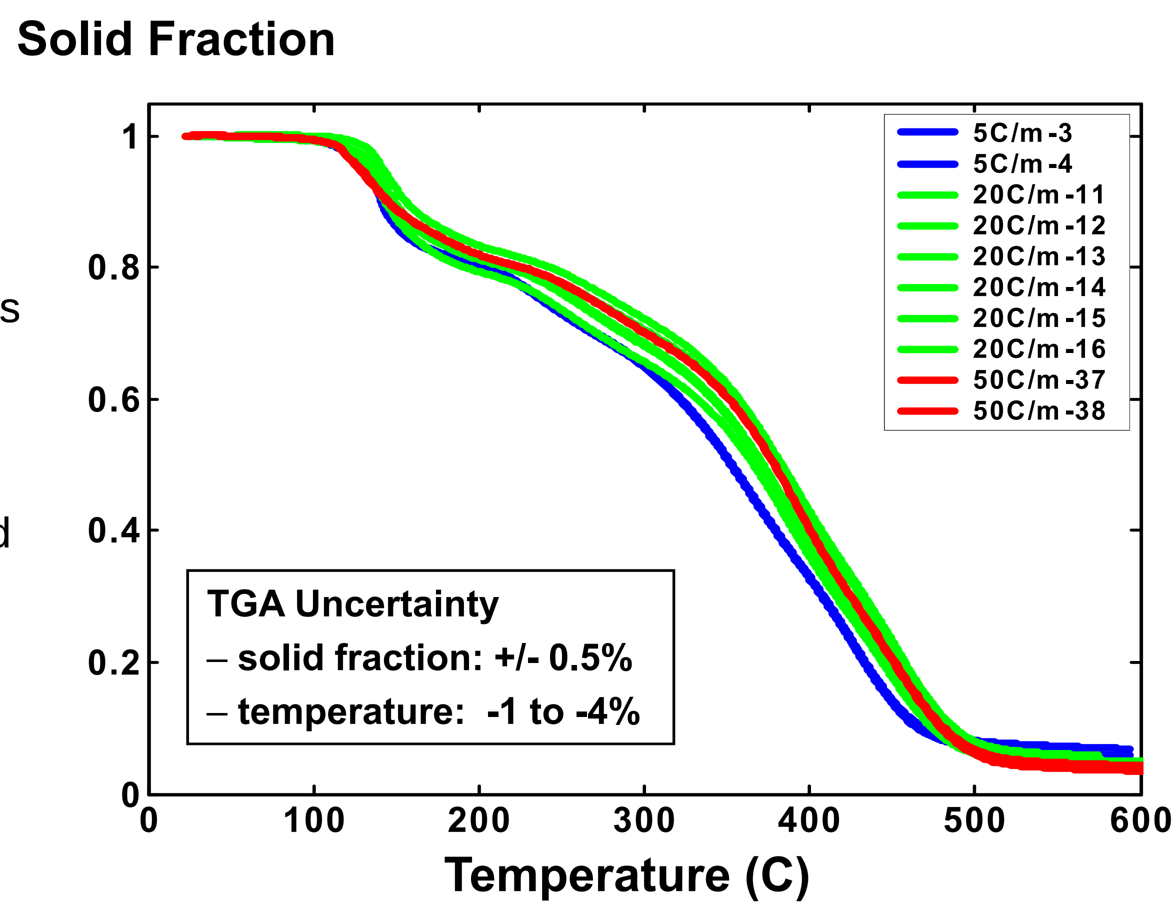
Experimental approach used to develop decomposition model



"Solid fraction" describes extent of foam reaction

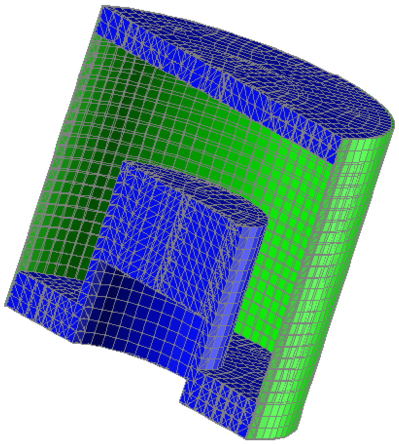
Solid Fraction (S_f)

- defined as the ratio of mass at time "*t*" to initial mass
- variable in foam chemistry kinetics model
- characterizes mass of solid as foam decomposes

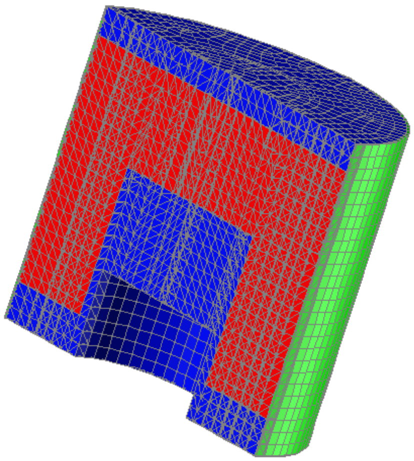


Decomposing REF Modeled using an "element-death" concept

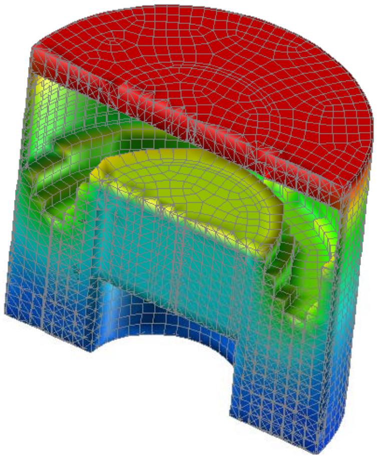
- State of the reacting foam is computed (solid fraction)
- Once the chemical state suggests that the element has completely reacted, foam elements are removed
- A transparent void is assumed to exist within the can



Mesh of can without foam

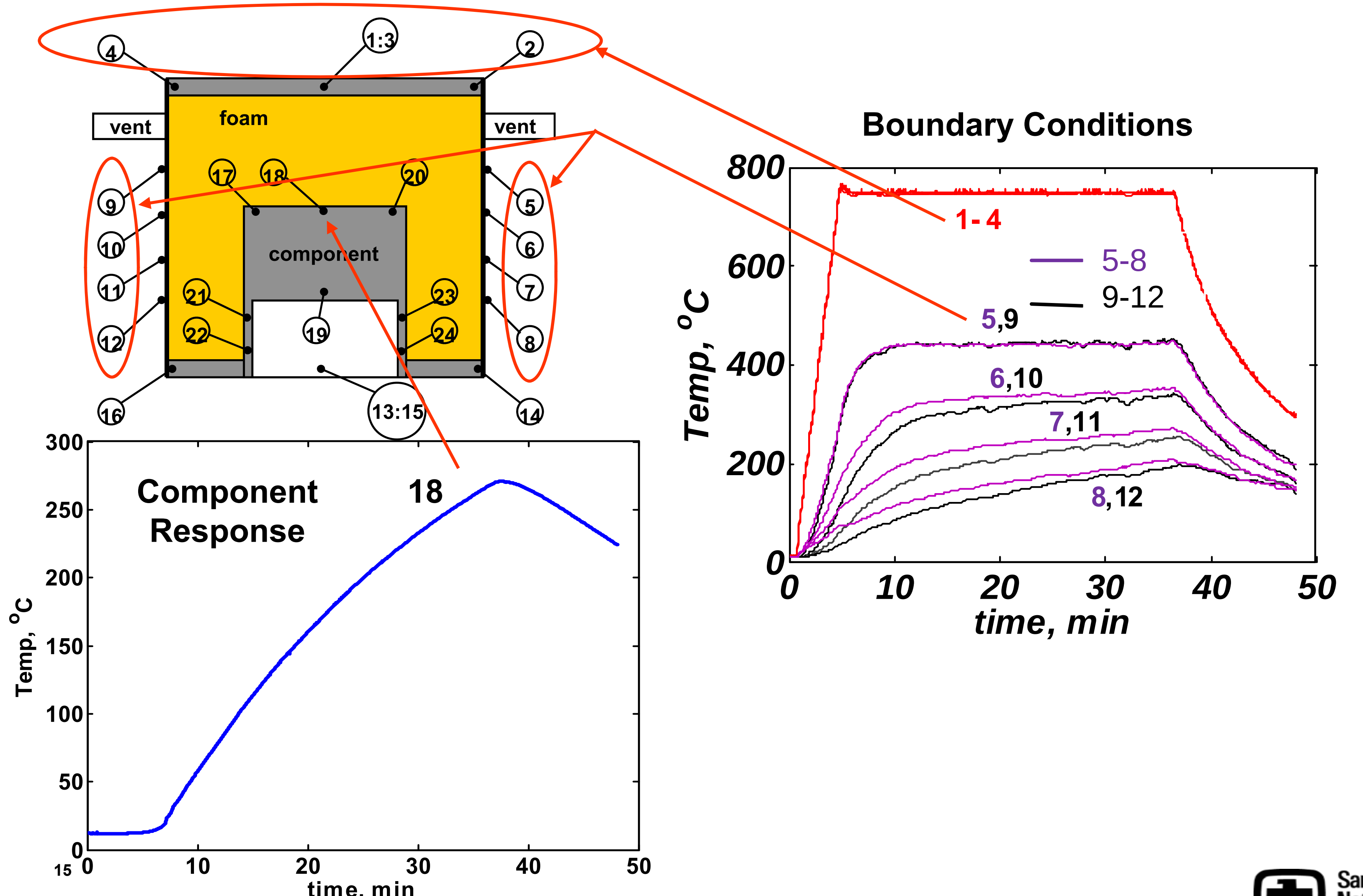


Mesh of can and foam



Mesh of can with foam decomposing

Boundary conditions applied using measured temperature data

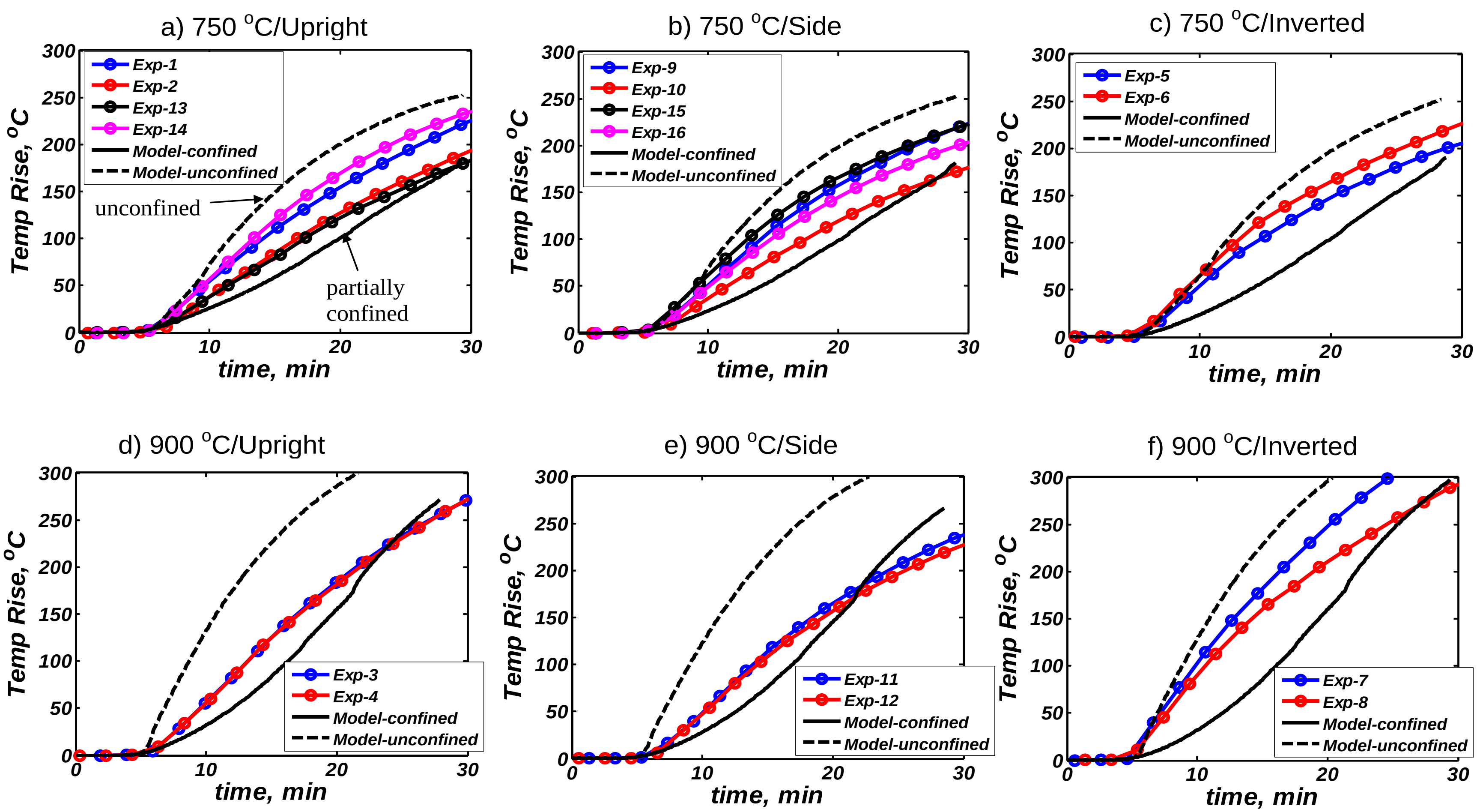


Comparison of Predicted Results and Experimental Data

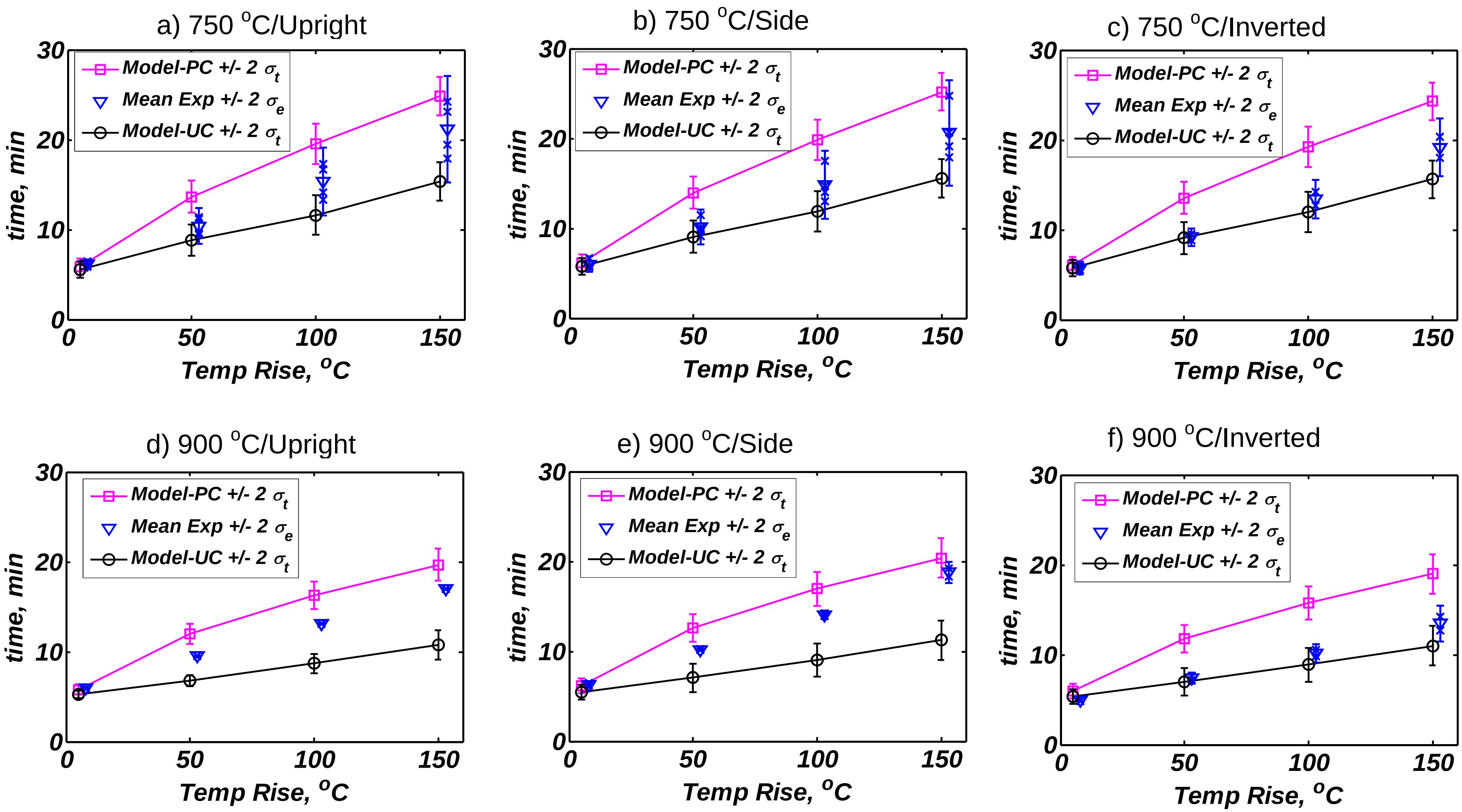
Comparison of model predictions and experimental data

- Multiple metrics could be selected
  - Temperature history
  - Time-to-temperature-rise
- For many of our applications, we are interested in the "time-to-temperature-rise" as a metric
- Uncertainty in predictions computed by propagating the uncertainty in model parameters through the numerical model

Comparison of predicted temperature rise and data



Comparison of predicted “time-to-temp” and data



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Uncertainty Quantification and Solution Verification

Model parameters were varied to assess uncertainty in predictions

Uncertainty assessed using both mean-value and Latin hypercube sampling methods

- Heat Conduction/Enclosure Radiation
  - Stainless Steel: C_p, k, ε (3 params)
  - Environment: T_{env} *(1 param)*
  - Foam: k, ρ, C_p, ε (4 params)
  - Death criterion, s_f (1 param)
- Foam Chemistry
  - Activation Energy, E_i, σ_{Ei}, h_r (9 params)
  - Confinement parameter
- Parameter Uncertainty Estimates
  - TGA: E_i, σ_{Ei}
  - FIC: Confinement parameter
  - Engineering Judgment/estimate: all others

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Uncertainty in predicted response quantified

- Response gradients computed using mean-value central-differences

$$\frac{\partial t(x)}{\partial p_i} \approx \frac{t(x, p_i + \delta p_i) - t(x, p_i - \delta p_i)}{2\delta p_i}$$

- Standard deviation in the predicted response

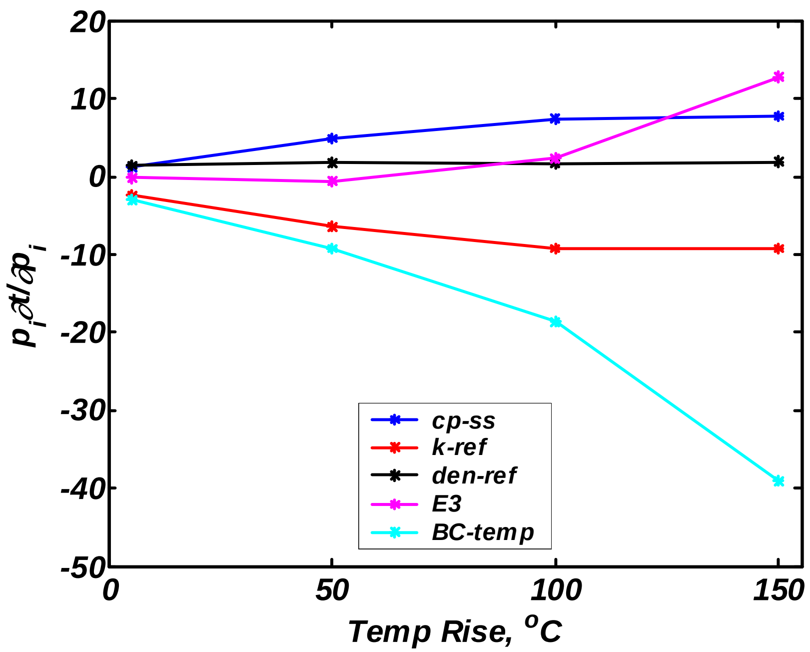
$$\sigma_r = \left[\sum_{i=1}^{n_p} \left(\sigma_{p_i} \frac{\partial r}{\partial p_i} \right)^2 \right]^{1/2}$$

- Importance factors allow comparison of relative importance

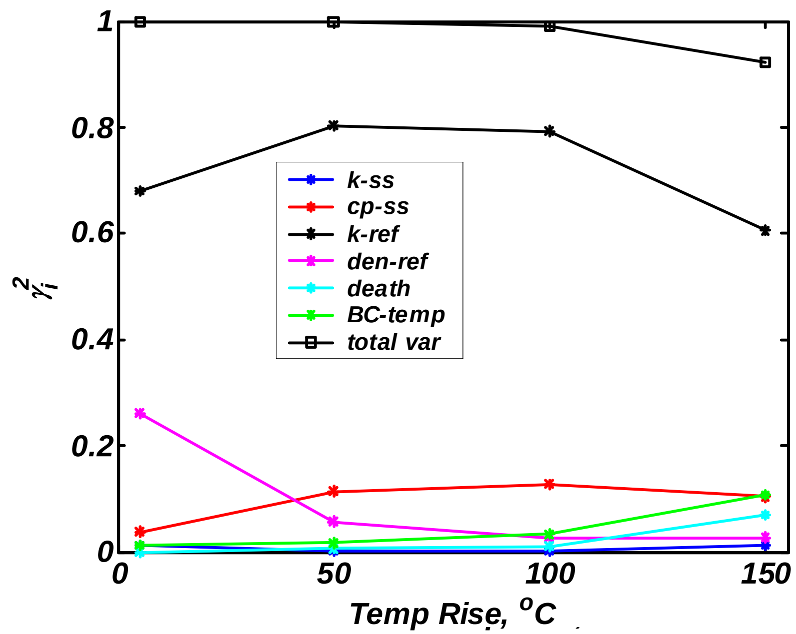
$$\gamma_i^2 = \frac{1}{\sigma_r^2} \left(\sigma_{p_j} \frac{\partial r}{\partial p_i} \right)^2$$

Thermal conductivity of the REF foam dominates the thermal response

Scaled Sensitivity Coefficients



Importance Factors



$$\sigma_r = \left[\sum_{i=1}^{n_p} \left(\sigma_{p_i} \frac{\partial r}{\partial p_i} \right)^2 \right]^{1/2}$$

$$\gamma_i^2 = \frac{1}{\sigma_r^2} \left(\sigma_{p_j} \frac{\partial r}{\partial p_i} \right)^2$$

Parameters used in assessing solution sensitivity to model parameters

Elem size “h” (cm)	Timestep (Δt) (sec)	$\Delta t/h^2$	Elems (K)	Nodes (K)	CPUs	Time (cpu-hrs)
0.6	4	11.11	3.4	4	4	1
0.6	2	5.56	3.4	4	4	1.2
0.6	1	2.78	3.4	4	4	1.8
0.6	0.5	1.39	3.4	4	4	2.7
0.3	1.0	11.11	20	22	32	34
0.3	0.5	5.56	20	22	32	62
0.3	0.25	2.78	20	22	32	100
0.3	0.125	1.39	20	22	32	150
0.15	0.5	22.22	151	160	48	500

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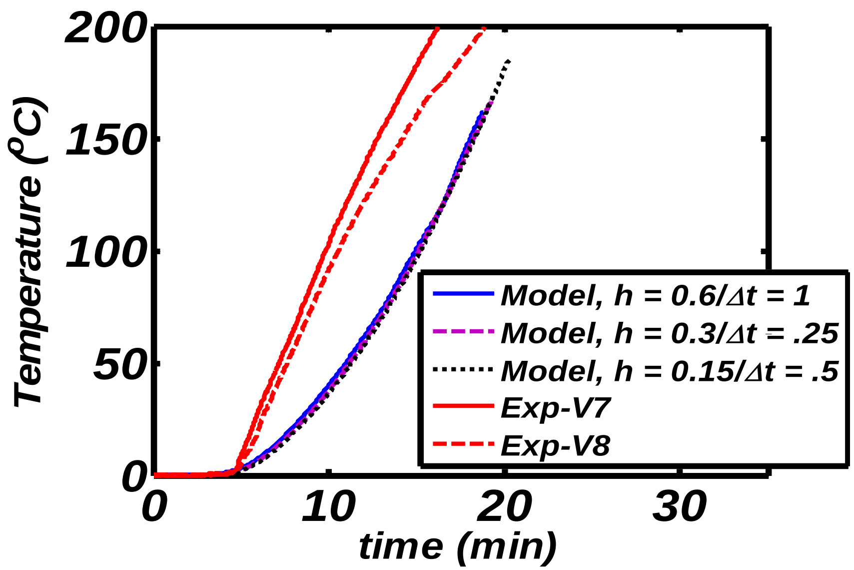
Assessment of solution convergence for differing mesh resolutions

- Temperature response for three mesh resolutions with fixed time step integration



- Coarse mesh (h=0.6) with an adaptive time step algorithm were used for all analyses

Irregular bubble-like char formed during experiments

Char formed inconsistently and impacted radiant heat transfer to encapsulated objects.

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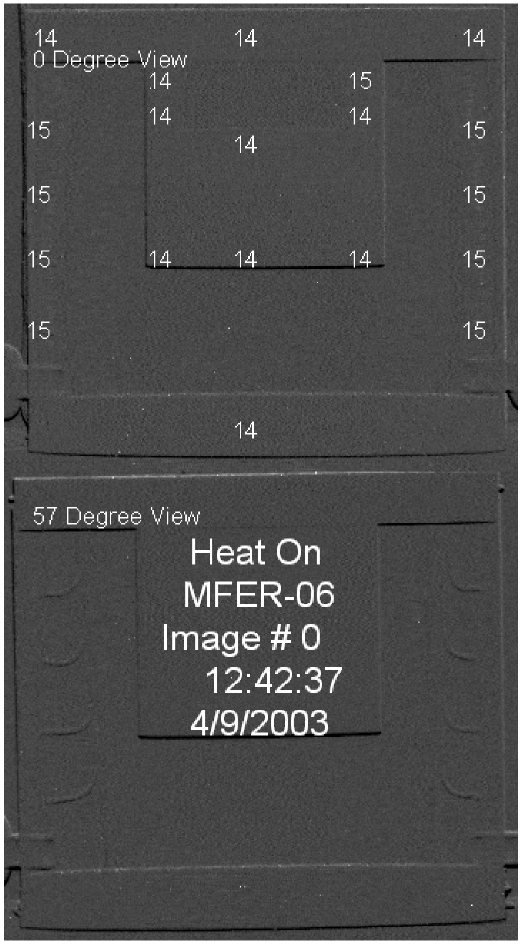
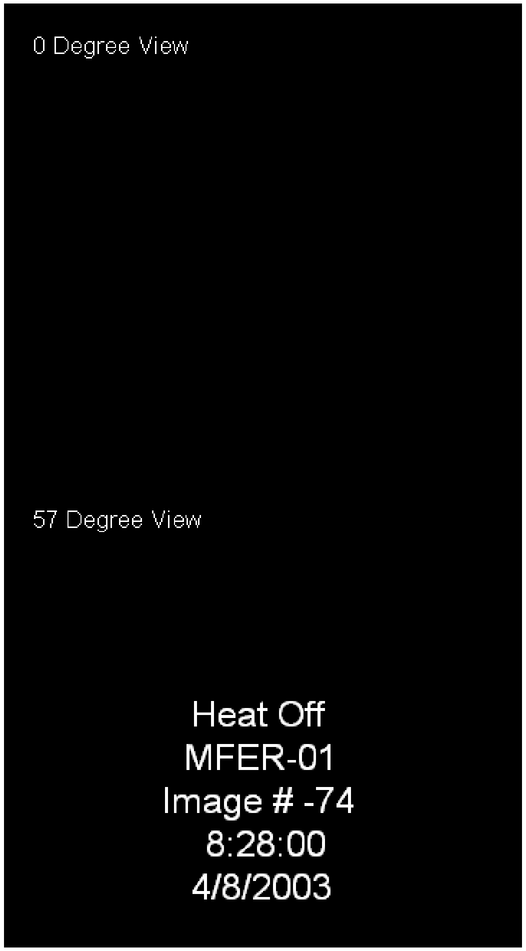
Irregular bubble-like char formed during experiments

Inverted Orientation

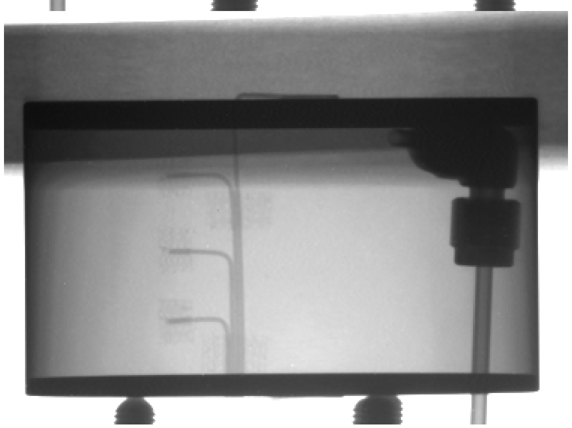


Upright Orientation

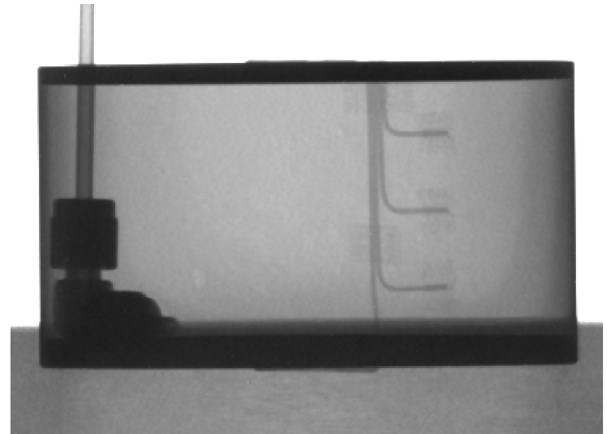


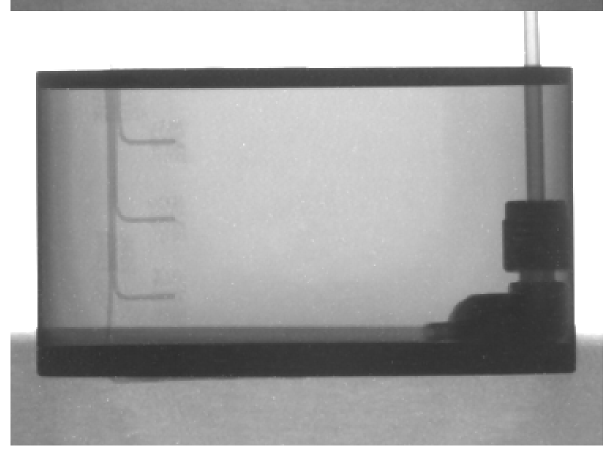
Erosive channeling and pressurization occurred with sealed samples

Inverted Orientation



Upright Orientation





Removable Epoxy Foam (REF): 320 kg/m^3 (20 lb/ft^3)

Plate temperature 1173 K   Heating Rate: 3.33 K/s

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Summary & Conclusions

Summary and Conclusions

- Predictions and data agreed better during early times
- Component responded more quickly than data for "unconfined" chemistry model
- Shape of response (concave downward) for "unconfined" chemistry matched data better than for the "confined" chemistry
- Variability in experiments (plate temperature and heating orientation) was larger than explainable by just variations in model parameters

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Summary and Conclusions (cont)

- Presence of solidified layers of crust within the decomposition void may have impacted the heat transfer to the component
  - Model assumed that a “clean” transparent void would evolve as the foam decomposed and turned to gas
  - Layers would act as a radiation “shield” between the hot plate and the component
  - Additional analysis is on-going to better understand the importance of these layers
- Model predictions with “confined” and “unconfined” chemistry model bounded the experimental data
- Future calculations will vary the confinement parameter to account for uncertainty in the decomposition model

END