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Verification, Validation, and Uncertainty Quantification of a Thermal-Mechanical Pressurization and Breach Application

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Outline

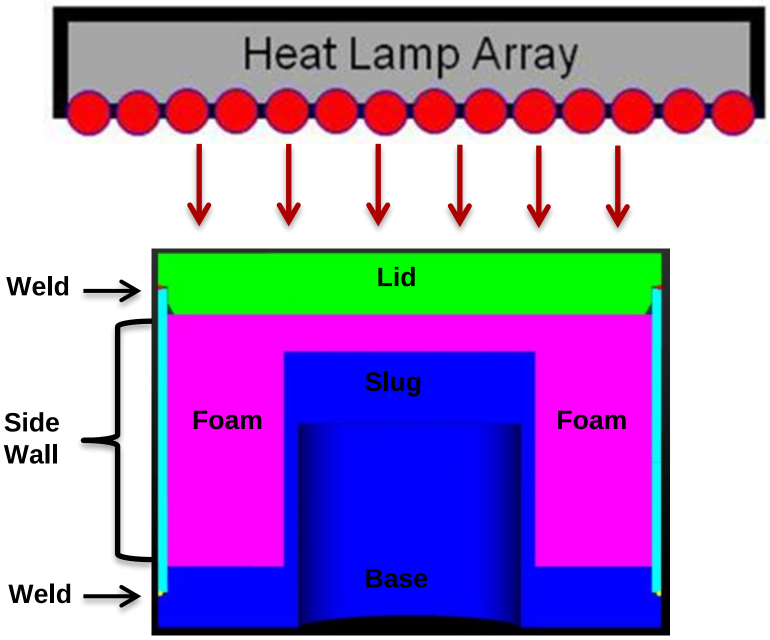
- Introduction
- Thermal-Mechanical Breach Validation Experiments
- Thermal-Mechanical Breach Simulations
- Solution Verification Assessment
- UQ Approach
- Validation Assessment
- Insights & Conclusions

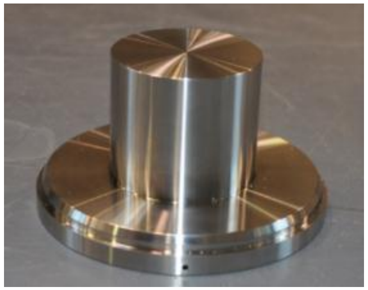
Characterization of T-M Breach

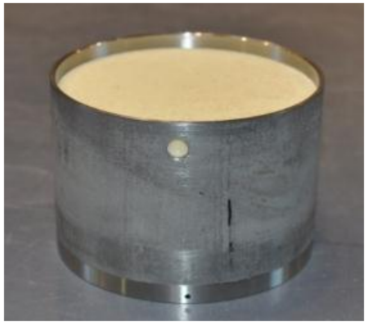
- Qualification of a weapon system requires safety assessments in abnormal environments such as a hydrocarbon fuel fire scenario
- Thermal loads resulting from a fire can cause foams to decompose resulting in the pressurization and breach of sealed regions
- A multi-physics approach was used to numerically model:
  - heat transfer and thermal response
  - foam decomposition and pressurization
  - mechanical deformation and weld failure
- Abnormal breach experiments and material characterization tests were conducted to validate the multi-physics modeling capability

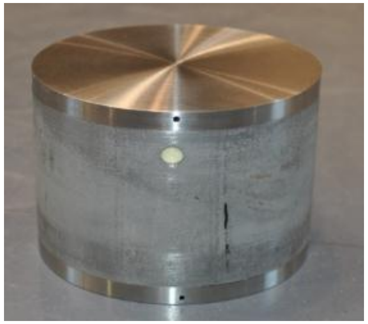
T-M Breach Validation Experiments

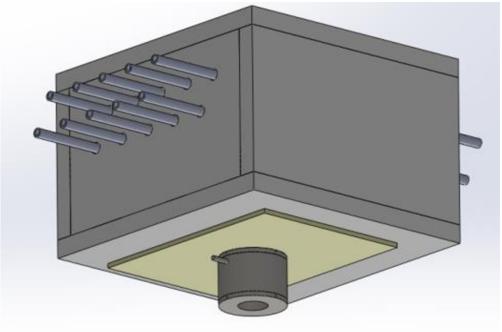
- Test Variables: Can Orientation and Heating Rates
- Response Quantities:
  - Thermocouples (Temperature)
  - Pressure Gauges (Pressure)
  - X-Ray Imaging (Displacements & Foam Decomposition)
  - Time to Breach
- 5 upright tests at 150ºC/min to 800ºC Lid Temperature







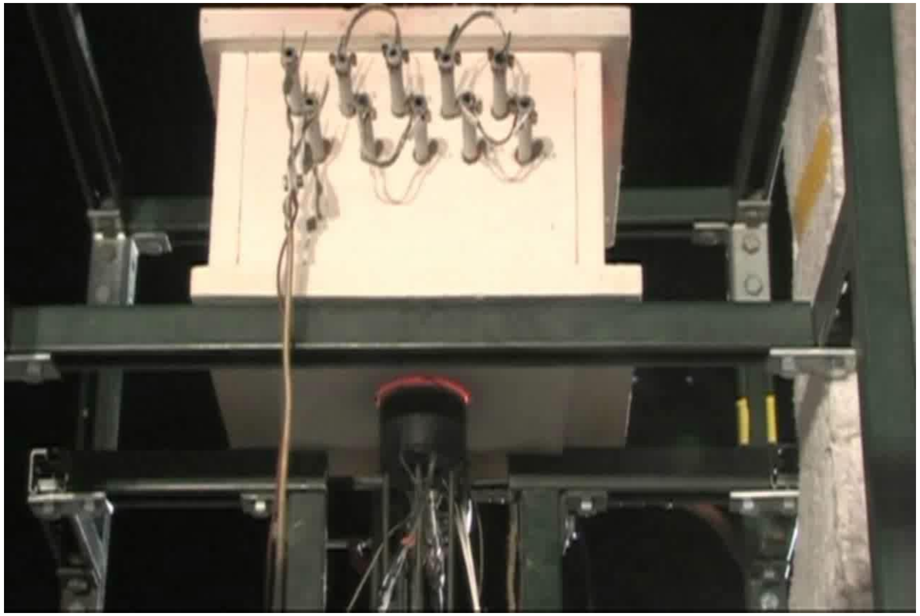




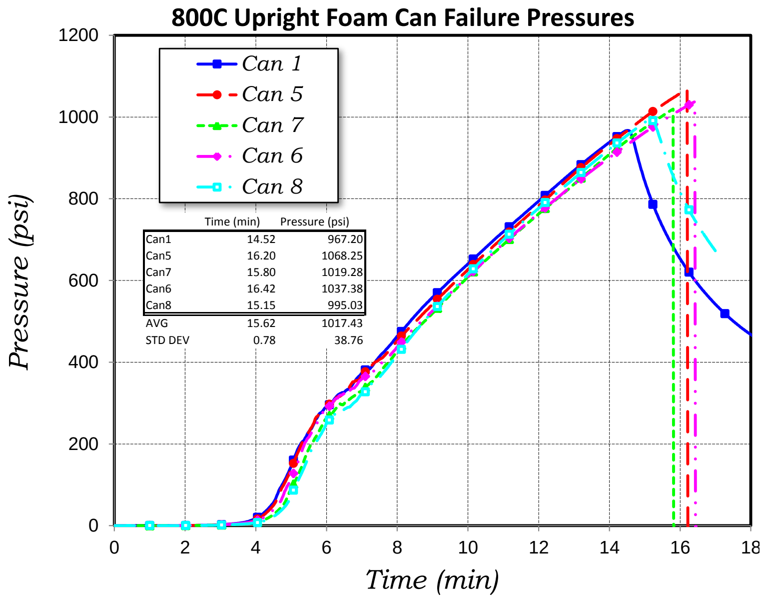
Comparison of Upright 800C PMDI Results

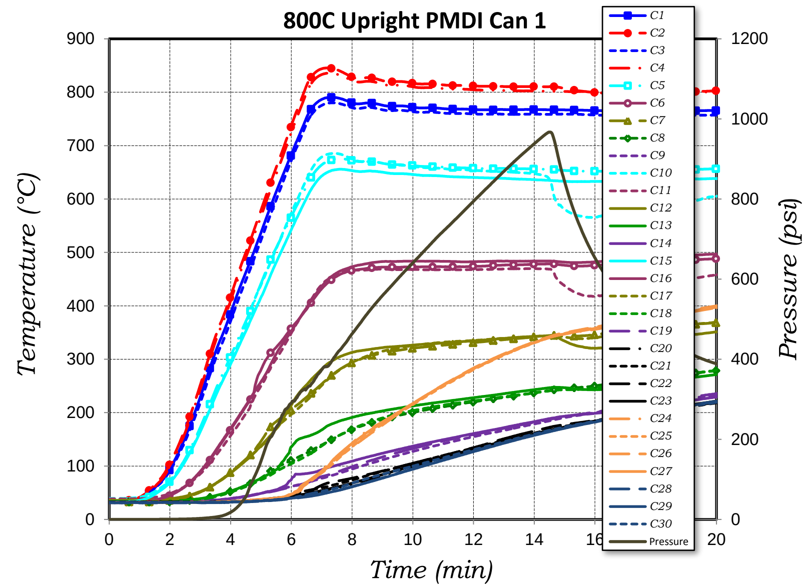
(Suo-Anttila, Dodd, Jernigan)

- Failure pressure of 1017 ± 39 psi
- Time to failure of 15.6 ± 0.8 min
- Weld temperature at failure, 650°C < T < 750°C
- Two failure modes observed, venting or abrupt weld failure



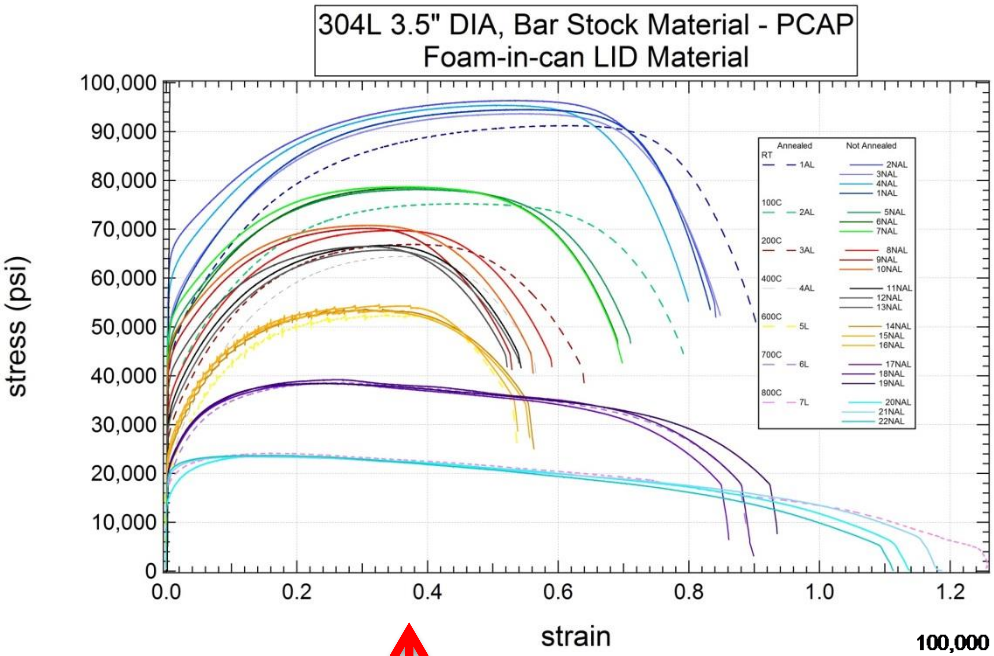
Can 5 Upright 800C Video





Material Characterization of Lid and Wall

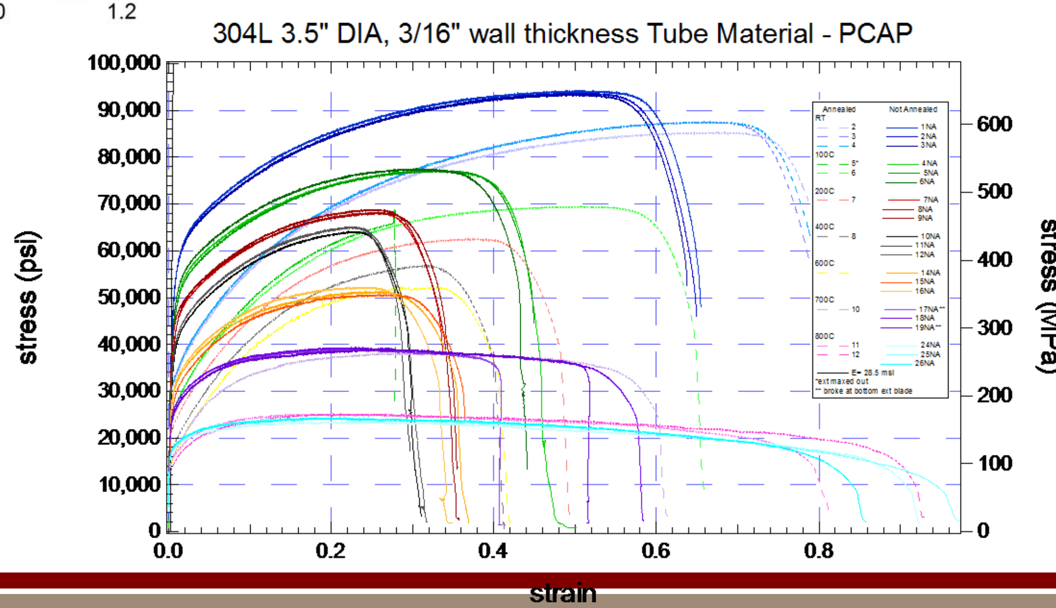
(Antoun & Connelly)



- Temperatures =
  20, 100, 200, 400, 600, 700, 800°C
- Material Characterization Tests
  - Lid Tensile Tests = 8 temps x 3 repeats = 24
  - Wall Tensile Tests = 8 temps x 3 repeats = 24

304L Lid Material

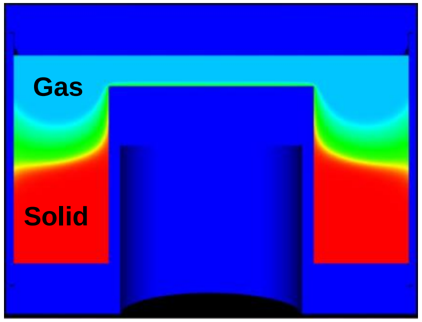
304L Wall Material

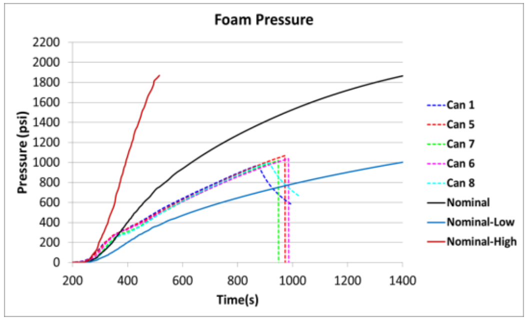


T-M Simulation Problem Description

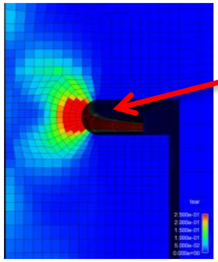
- Thermal-Mechanical Simulations, 1-1/2 way coupled
- Heat flux boundary condition specified on lid based on experimental lid temperature
- Convection and radiation boundary conditions specified on walls and base
- Effective radiative conductivity model used to represent heat transfer in free volume portion of foam
- Multi-Linear Elastic Plastic (MLEP) material model used to represent canister material behavior
- Weld failure criteria was defined using two approaches:
  - Tearing Parameter Criteria (TP)
  - Equivalent Plastic Strain Criteria (EQPS)

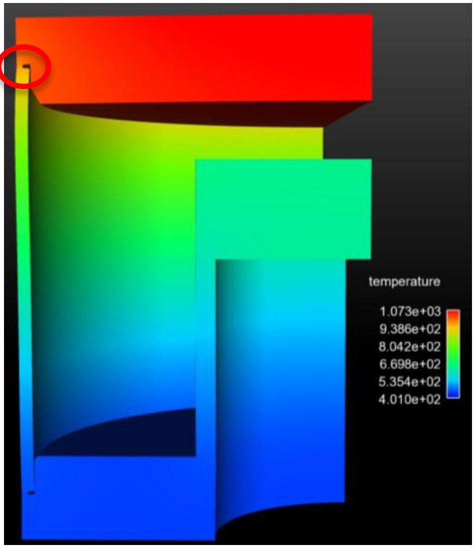
Thermal Heat Transfer Drives Foam Decomposition & Pressurization





Mechanical Deformation & Weld Failure





- **Applied temperature and pressure from thermal analysis drive mechanical response and failure**

Modeling Foam Decomposition

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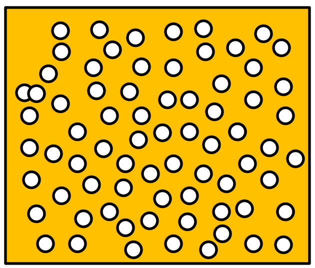
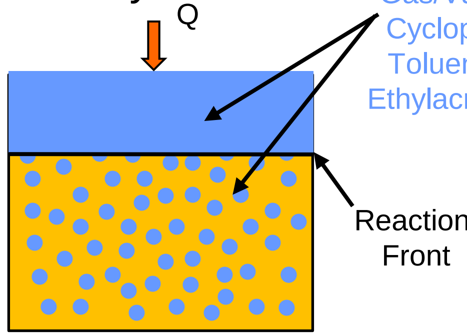
Initial Foam



Partially Reacted



Foam decomposition is predicted by Arrhenius-type model for reaction rate:

$$\frac{d[\mathrm{M}]}{dt} = Ae^{-E_a/RT}[\mathrm{M}]^n$$

- Activation energy and heat of reaction are calculated from ThermoGravitmetric experiments

Energy Equation

Based on diffusive approximation for optically thick material

$$\rho c \frac{\partial T}{\partial t} = \nabla \bullet (k + k_e)\nabla T + \sum_i \rho r_i(-\Delta H_i)$$

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

Effective radiative conductivity k_e depends on absorption coeff. a and scattering coeff. σ_s[1]

Pressure

Decomposition gases and temperatures are summed over the relevant region to calculate the pressure

$$P = \frac{n_g R}{\int_{V_g} \frac{1}{T} dV_g} = \frac{n_g R}{\left(\int_{V_{fv}} \frac{1}{T} dV_{fv} + \int_{V_B^0} \frac{\Phi}{T} dV_B^0\right)}$$

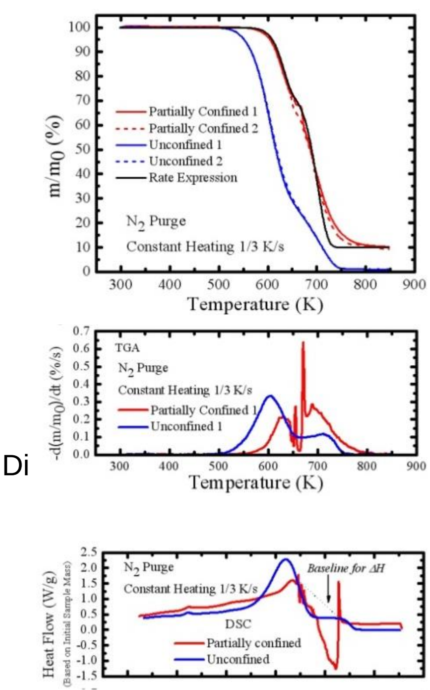
Moles of gas

Free volume/ temperature

Gas Volume: reacted area and pore space

Decomposition Model

ThermoGravimetric Analysis (TGA)



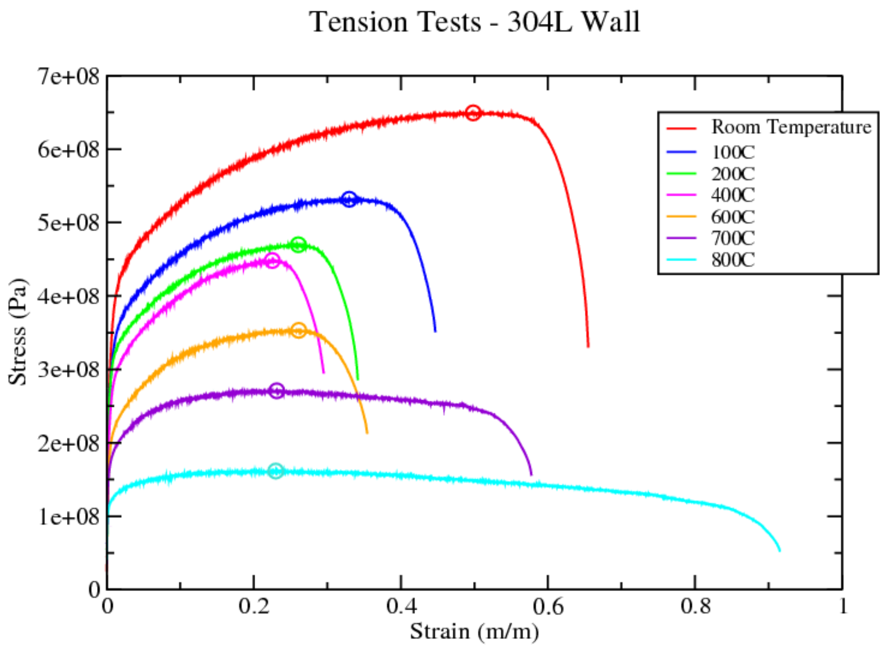
Di (DSC)

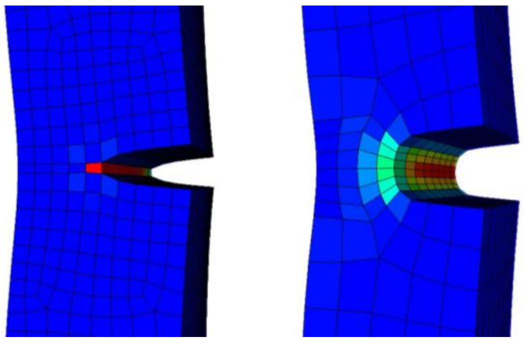
Weld Failure Prediction Method

- Determined critical values of tearing parameter and EQPS at maximum load from tensile tests at each temperature
- Considered 2 weld representations, 2 element types, and several levels of mesh size

Tearing Parameter (TP) relates the stress state to the plastic strain at failure by the evolution integral (developed at Sandia):

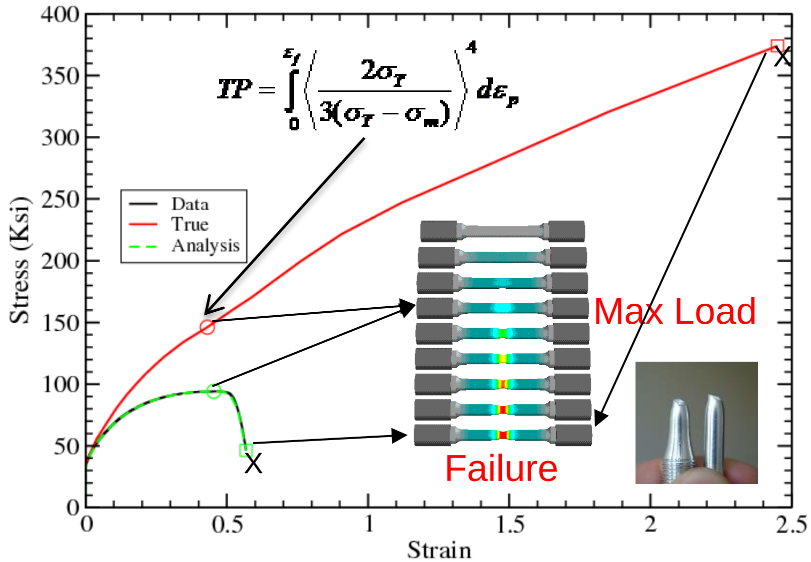
$$TP = \int_0^{\epsilon_f} \left\langle \frac{2\sigma_{max}}{3(\sigma_{max} - \sigma_m)} \right\rangle^4 d\epsilon_p$$

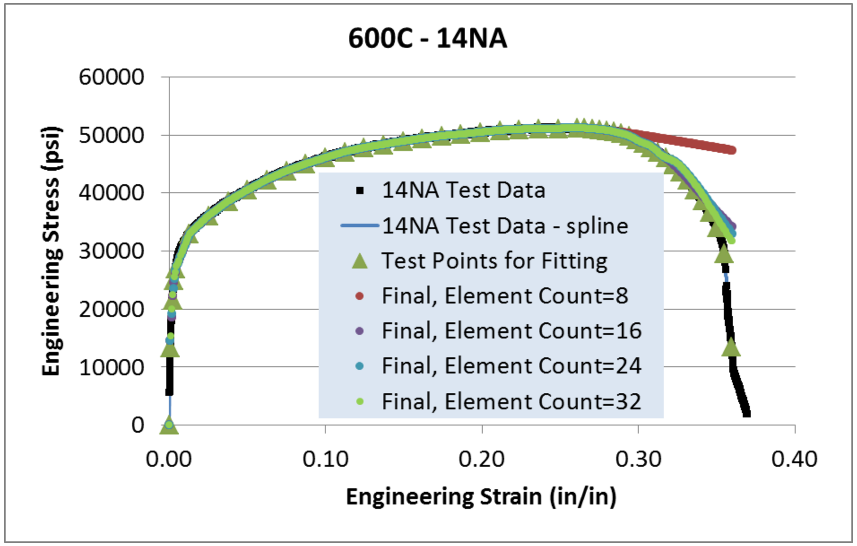




- Square notch vs. Curved notch
- Mean Quadrature vs. Selective Deviatoric elements

MLEP Model Calibration Based on Mesh Converged Models



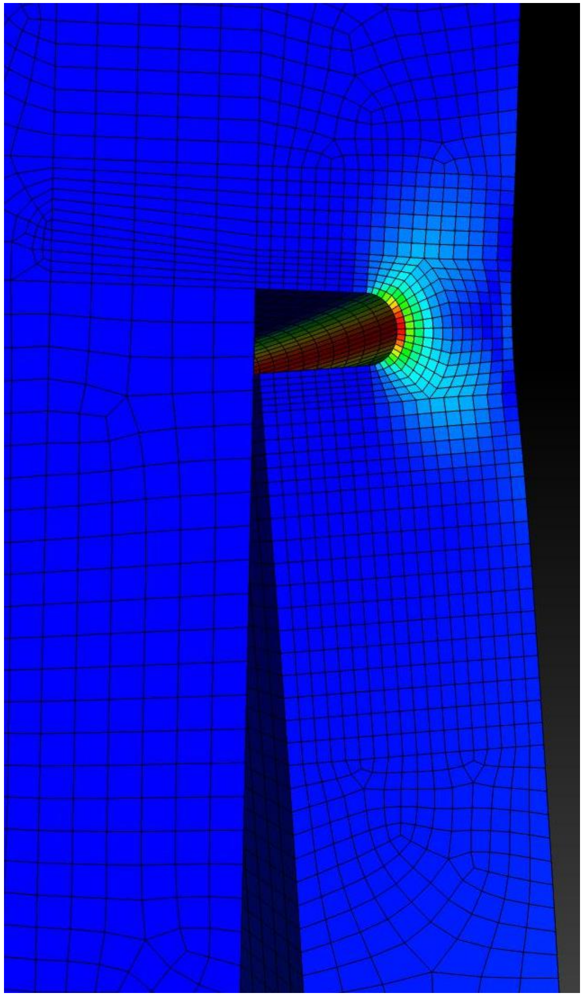


- Inverse calculations used to derive Cauchy stress-logarithmic strain curves
- Mesh independent up to max load (uniform stress/strain field)
- Very mesh sensitive past max load where necking occurs (strain-rates increase by orders of magnitude)
- Unable to get a converged solution for the last part of the data curve
- Tensile shape and material model form are incorrect past max load, likely due to strain-rate effects

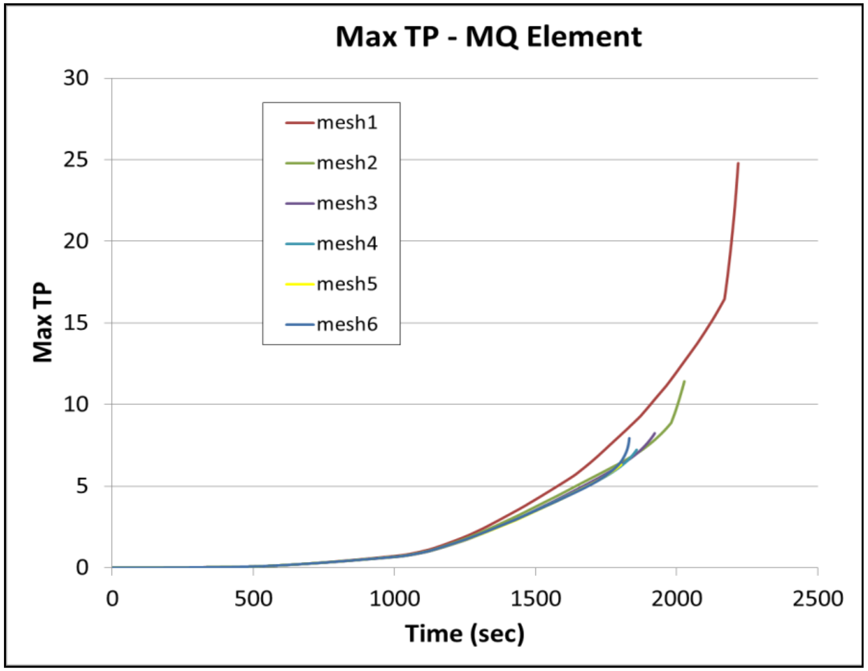
Solution Verification Study

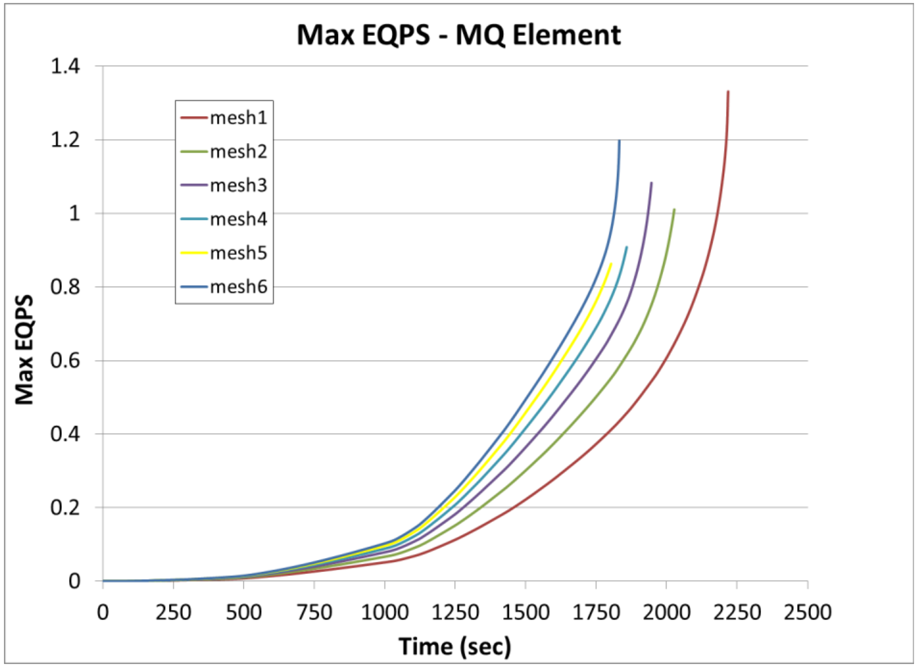
Mechanical Deformation and Breach

- Solver and residual tolerances were set to small values to reduce numerical noise
- Load Step (10.0, 1.0, 0.1)
  - Solver tolerances were set to small values, 1.0e-06
- Element Size: 6 meshes – ¼ symmetry geometry
  - Mesh 1 = 370,440; Weld block = 6,048 (6x6)
  - Mesh 2 = 694,936; Weld block = 10,752 (8x8)
  - Mesh 3 = 1,190,721; Weld block = 16,800 (10x10)
  - Mesh 4 = 1,850,944; Weld block = 24,192 (12x12)
  - Mesh 5 = 2,639,996; Weld block = 32,928 (14x14)
  - Mesh 6 = 3,684,285; Weld block = 43,008 (16x16)
- Element Type
  - Mean-Quadrature (MQ) Element - Uniform Gradient with Total Hourglass Formulation
  - Selective Deviatoric (SD) Element - Fully Integrated Gradient, Hourglass control isn't required



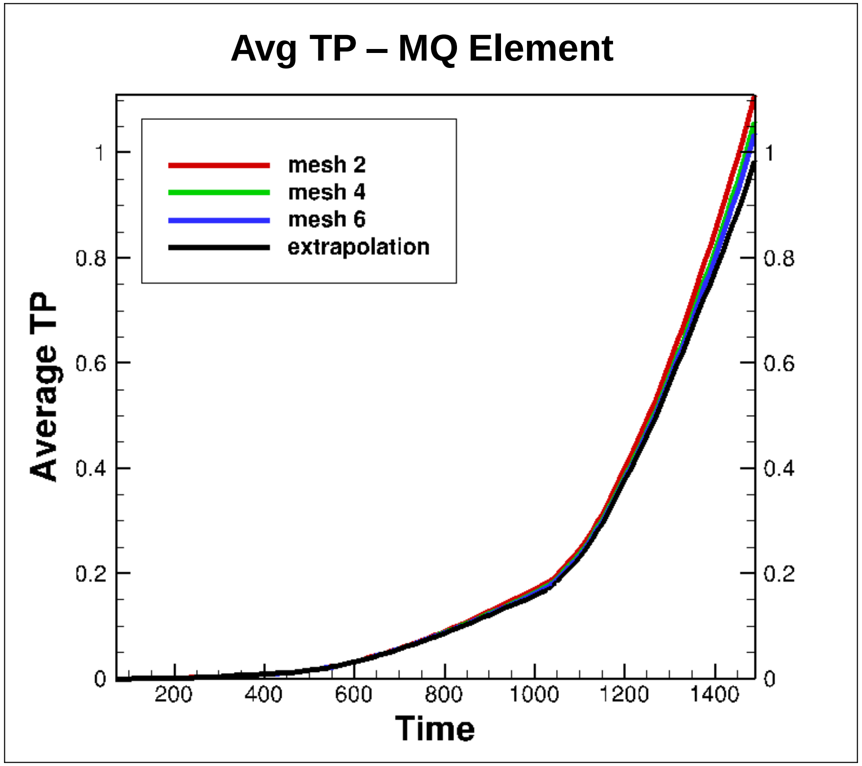
Mesh Sensitivity – Max TP & Max EQPS

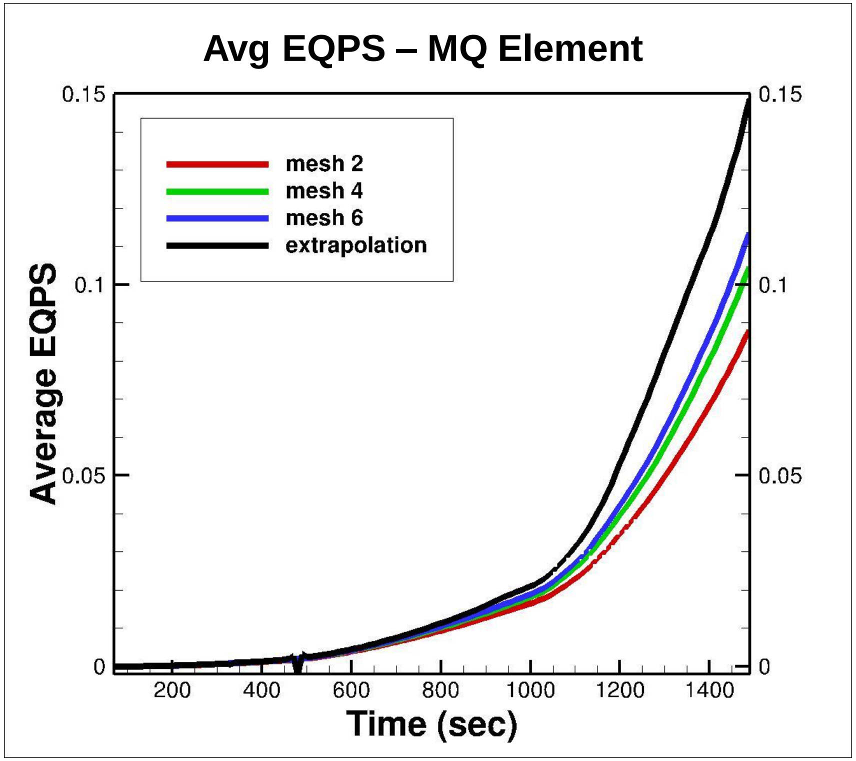




- Max TP results didn't show monotonic convergence but were very similar
- Max EQPS results showed better convergence with mesh refinement
- Maximum quantities convergence can be problematic because the physical location may change

Mesh Sensitivity – Avg TP & Avg EQPS





- Average values calculated in weld block only
- Average TP and Average EQPS show monotonic convergence with mesh refinement and extrapolated solutions are possible
- EQPS shows more sensitivity to mesh size than Tearing Parameter

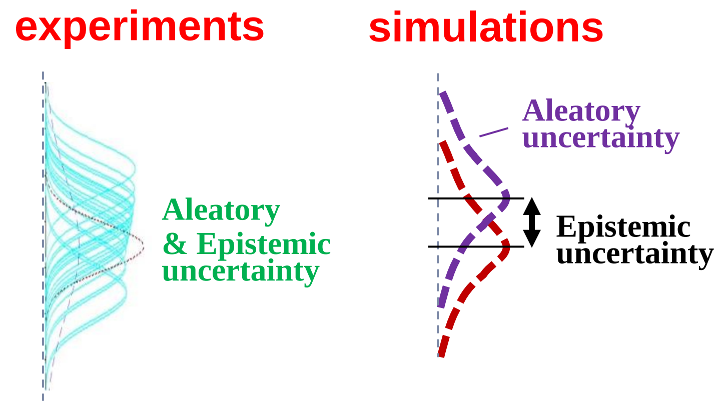
UQ Study

- Categorize Uncertainties
  - Aleatory, Epistemic, Traveling, Non-Traveling
- Characterize Uncertainties
  - Highly dependent on expert judgment
  - Accommodate different representations
    - Interval Tolerances
    - Discrete
    - Distributional
  - Quantify discretization and sparse data uncertainties
- Propagate Uncertainties
  - Staged mixed-order polynomial surrogate model
    - Linear UQ Propagation – all uncertainties
    - Linear Sensitivity Analysis – identify dominant factors
    - Higher-Order UQ Propagation – dominant factors
- Compare Experimental Results to Simulation Result

Real Space Comparison of Experiments and Simulation Results used in the Validation Study

Approximate Pbox representations segregate aleatory and epistemic uncertainties

- ***Aleatory*** – random uncertainty, stochastic variability, describes a set or population of multiple values
- ***Epistemic*** – systematic uncertainty, unknown single result within uncertainty range



Extrapolation from validation assessment to application assessment requires additional separation of traveling and non-traveling uncertainties

- ***Traveling*** – model quantities and uncertainties that "travel" from the validation study to applications of interest
- ***Non-Traveling*** – quantities and uncertainties that are specific to the validation experiment and study

➢ *For additional UQ details, refer to Vicente Romero's presentation this afternoon @ 3:10p.*

Traveling and Non-Traveling Uncertainties in Thermal-Mechanical Validation Problem

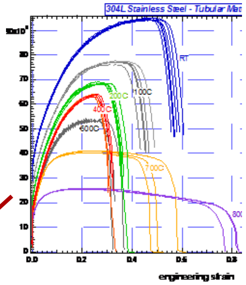
Non-Traveling Uncertainties

Experimental Aleatory
- lid TC measurement/redundancy test-test variations: I[±2%]
- ss304 emissivity can-can variations: I[±0.03]
- ambient temperature test-test variations I[±10C]
- pressure measurement/redundancy test-test variations: I[±2%]

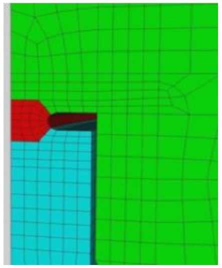
Experimental Epistemic
- ss304 emissivity effective value over time, space: 0.69 + I[±20%]
- effective temperature for radiative, convective losses: 29C + I[±15C]
- convection coeff. effective value over time, space: 10W/m^2-K + I[±40%]

Model Epistemic
- mesh size error
- solver error

Traveling Uncertainties



Model Aleatory
- material stress-strain curves for lid, weld, & wall
- lid thermal contact: I[20%, 90%] of distance between modeled extremes of no heat transfer and perfect-contact heat transfer
- wall thickness: I[0.062,0.0645]in.
- weld depth: I[0.023, 0.031]in.



Model Epistemic
- foam conductivity: *f(temp.)* + I[±20%]
- foam specific heat: *f(temp.)* + I[±20%]
- foam activation energy: value + I[±4%]
- foam pressure multiplier: I[0.5, 2.64]
- ss304 conductivity: *f(temp.)* + I[±20%]
- ss304 specific heat: *f(temp.)* + I[±20%]

SA/UQ Analysis for T-M Assessment

(75 thermal-mechanical runs for response surfaces + ~150 mechanical-only for σ-ε curve strength rankings)

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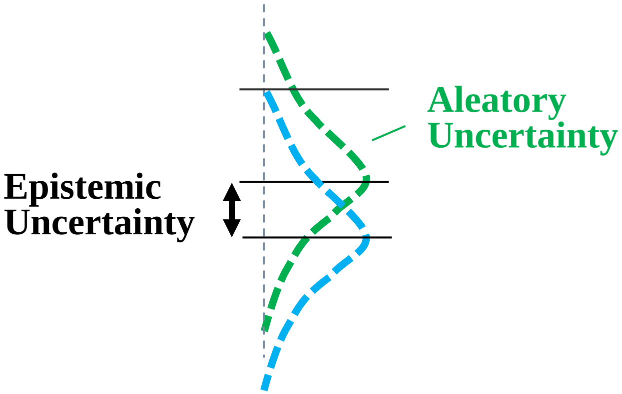
Experimental UQ processing



- *4 sims. to normalize results for known input differences in the 5 experiments*
  - *measured changes in foam dens. & lid TC temperatures from test to test*

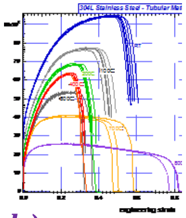
+

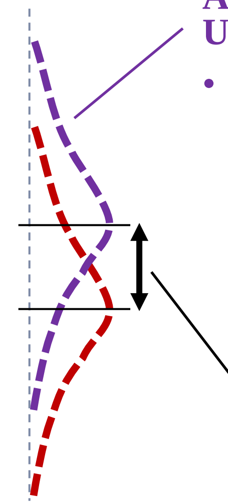
8 sims. to process data for random and systematic uncertainties in experiments

4 sources:
- *lid temperature*
- *convection coefficient*
- *emissivity*
- *ambient temperature*

Simulation UQ processing

~150 mechanical sims. for σ-ε curve strength rankings at each temperature





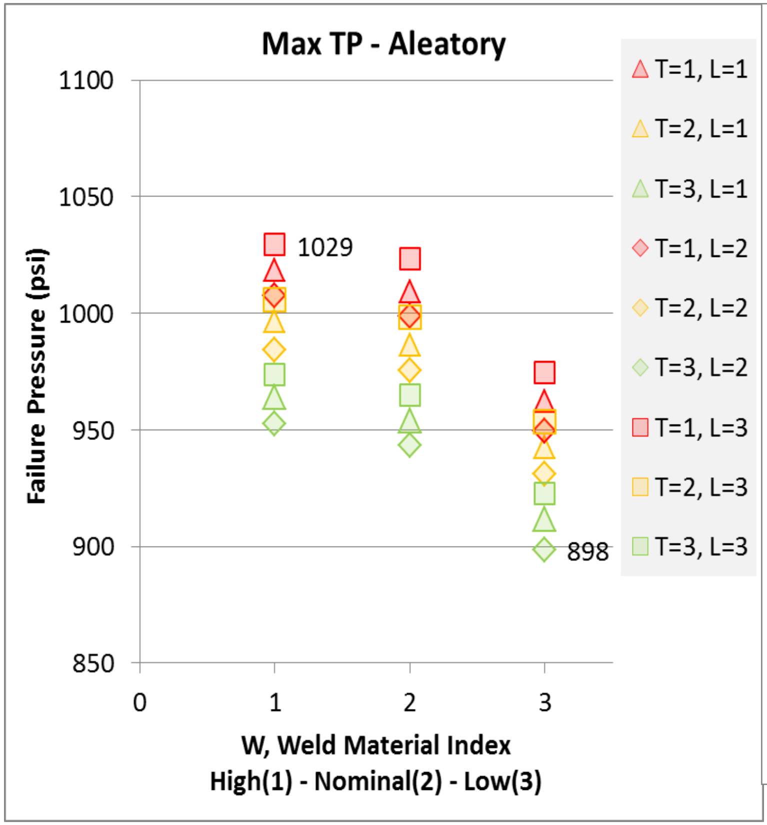
Aleatory Uncertainty

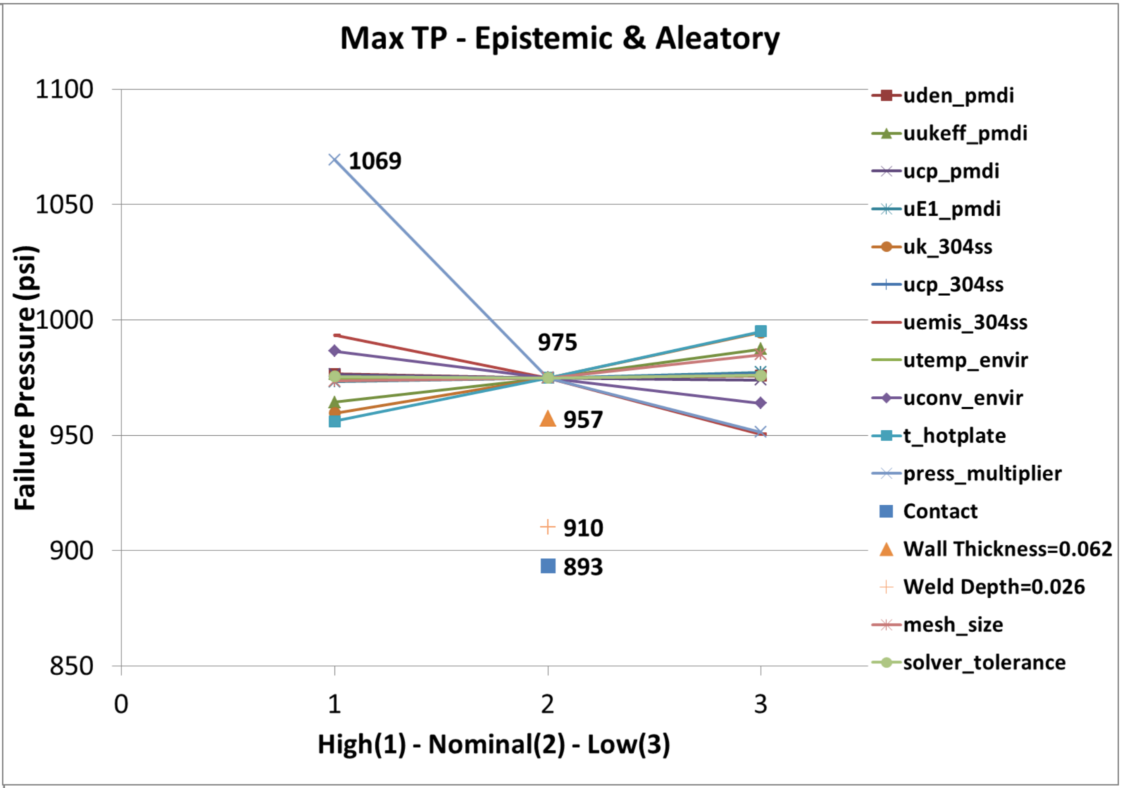
- *32 sims.*
  - *σ-ε curve variations for weld, lid, & wall*
  - *thermal contact (2 models)*
  - *wall thickness (2 models)*
  - *weld depth (4 models)*

Epistemic Uncertainty

- *31 sims. – staged adaptive polynomial Resp Surf. for 7 parametric sources*
  - *foam conductivity*
  - *foam specific heat*
  - *foam activation energy*
  - *pressure multiplier*
  - *ss304 conductivity*
  - *ss304 specific heat*
- *6 sims. for mesh & solver effects (3 meshes)*

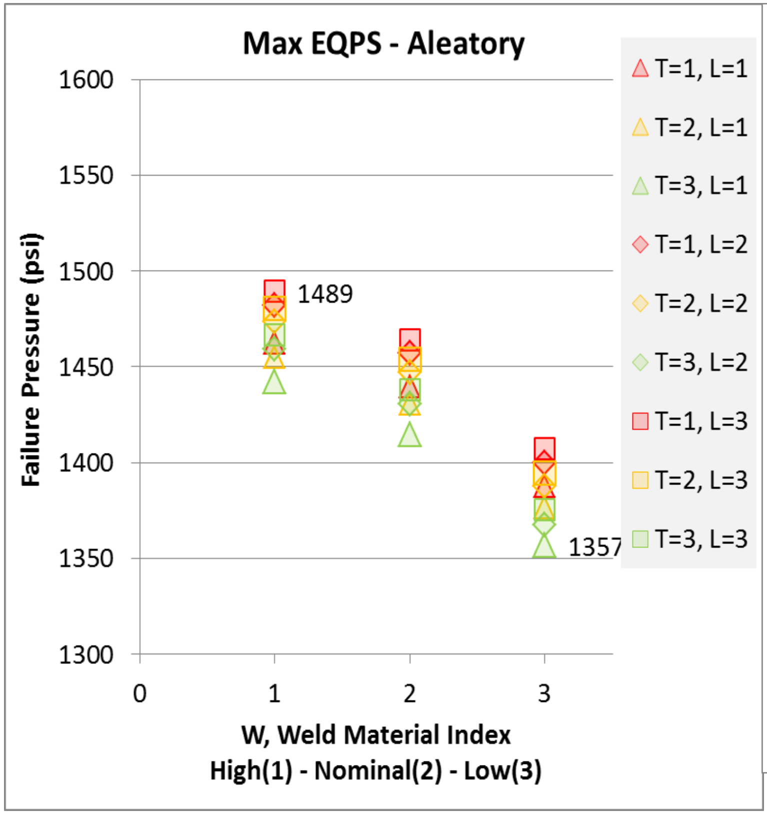
Parameter Sensitivity – TP Failure

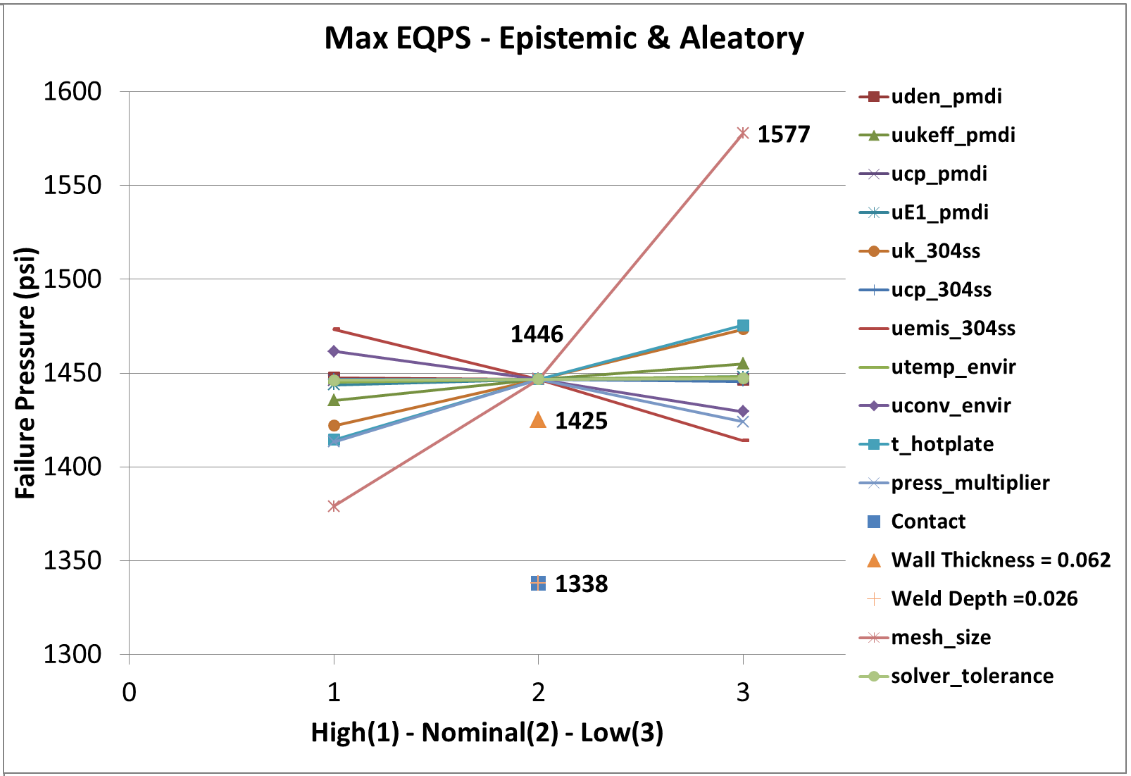




- Uncertainties due to repeat material curves and foam pressure multipliers are dominant factors

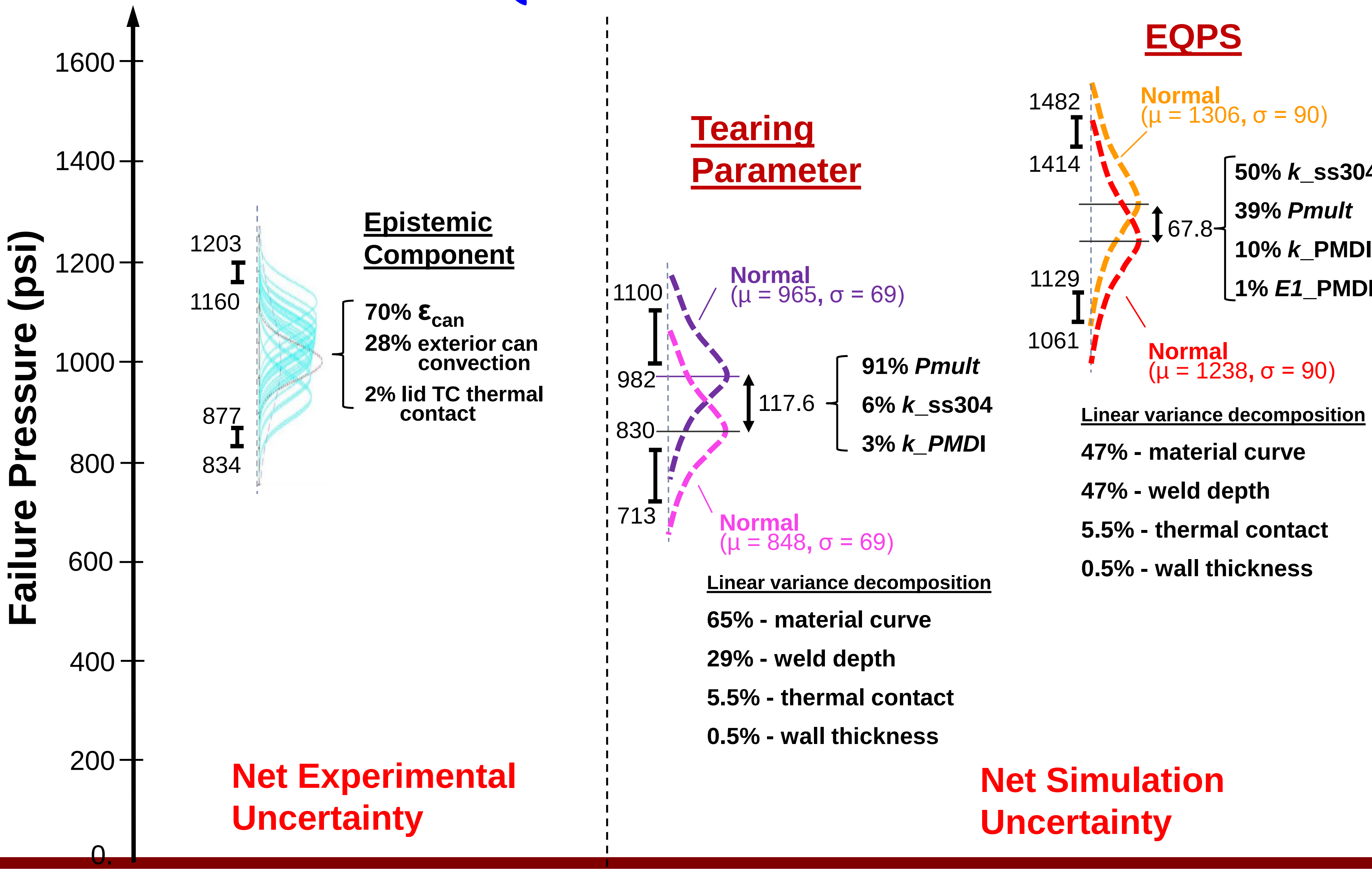
Parameter Sensitivity – EQPS Failure





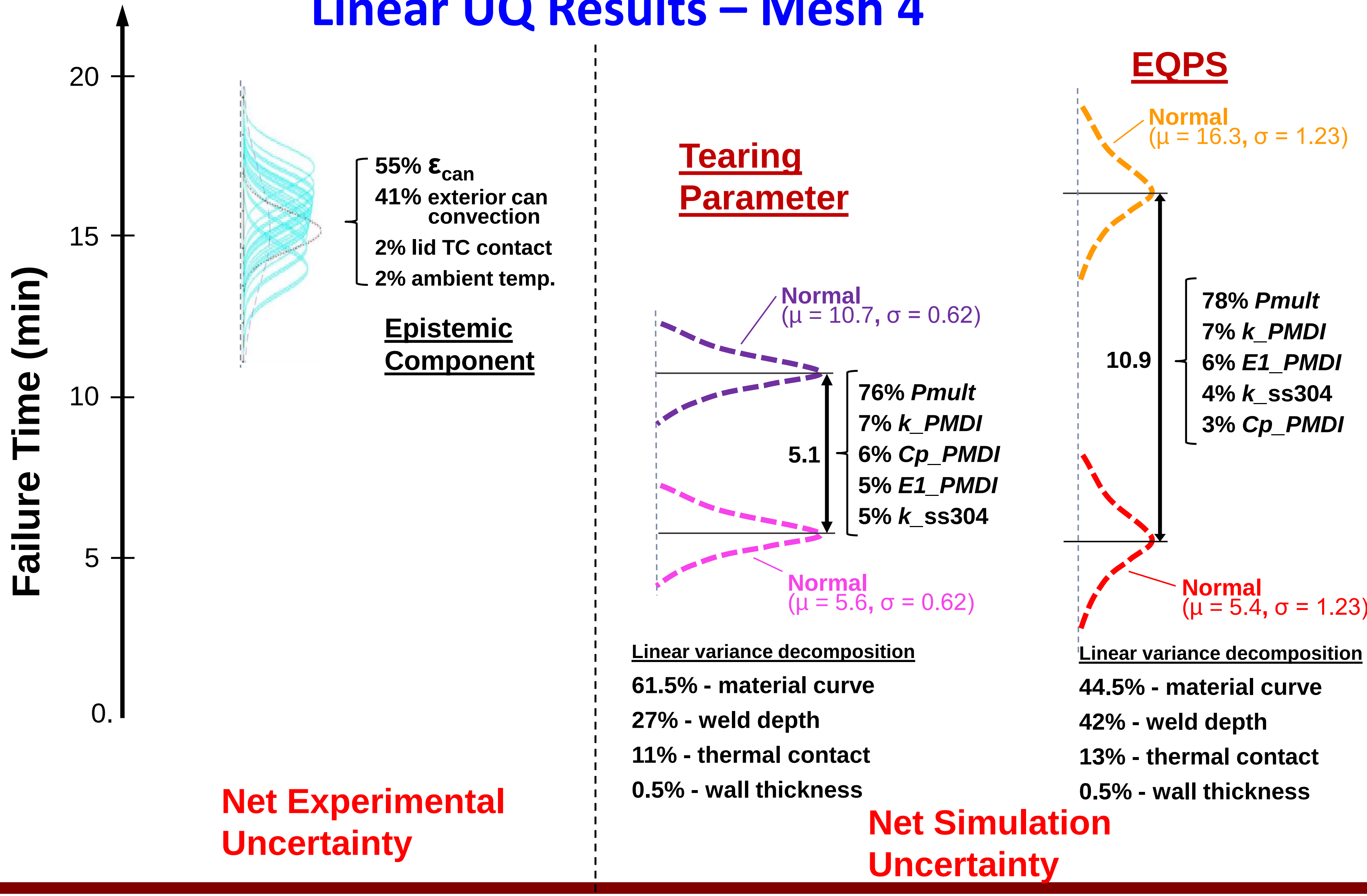
- Uncertainties due to repeat material curves and mesh size are dominant factors

T-M Validation Comparisons – Failure Pressure
Linear UQ Results – Mesh 4



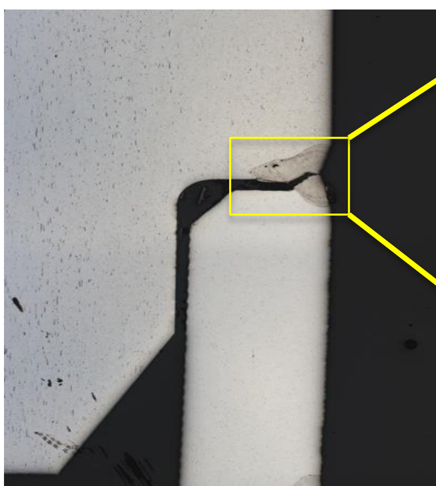
T-M Validation Comparisons of Failure Time

Linear UQ Results – Mesh 4

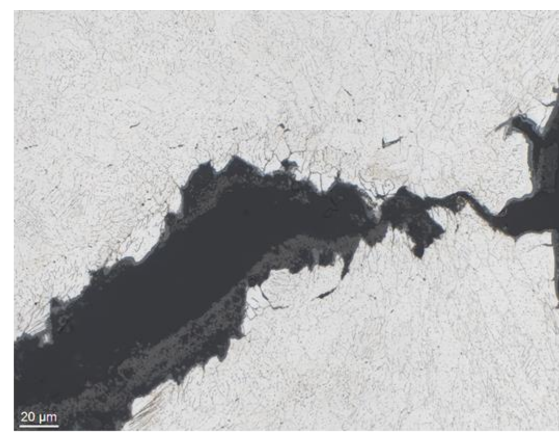


Thermal-Mechanical Breach Insights

- Different deformation mechanisms occur for higher temperature scenarios:
  - Low Temperature mechanism = void growth
  - High Temperature mechanism = grain slippage
- Cracking occurs in weld region and leads to breach
  - High temperature effect
  - Partial penetration weld with voids
  - Pressure loading from decomposing organic materials
  - Complicated stress state, including residual stresses in weld
  - Strain-aging at temperature, can cause material hardening and reduced ductility



(Charlie Robino, 1831)



Conclusions

- Abnormal thermal environments in combination with strain-rate effects introduced new material deformation mechanisms and failure modes
- Tearing Parameter criteria was conservative relative to experimental data but may not necessarily be predictive; mesh effects and strain-rate effects were reduced by setting critical values at max load conditions
- Material model provides the basis for all mechanical analysis and as such, including the correct form and data is critical to any assessment; e.g., strain rate effects are necessary to capture correct tensile shape past max load
- Weld modeling approach is a critical choice in any assessment and will determine the degree of accuracy and uncertainty
- Solution verification was necessary to quantify the numerical error and as such, provided a basis to evaluate the physics models and the modeling approach
- Uncertainty quantification approach prototyped the separation of aleatory and epistemic uncertainties, traveling and non-traveling uncertainties for extrapolation, and a higher order assessment for computationally-intensive simulations
- Fully-integrated process from experimental design through predictive assessment provided an opportunity to better characterize boundary conditions, reduce uncertainties, and generate repeat data sets for validation assessment