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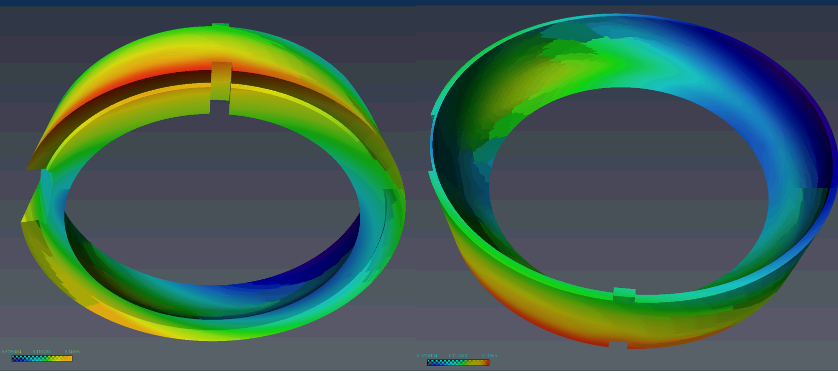

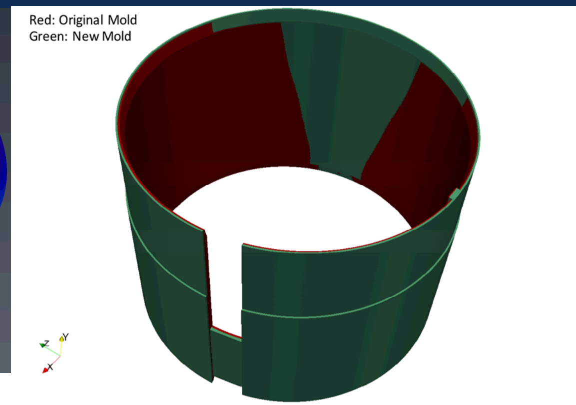

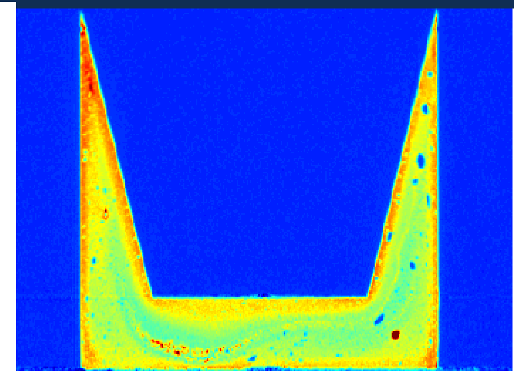

Inverse Mold Design To Accommodate Manufacturing Warpage in Chemically Blown PMDI Foams

Kevin Long[1], Rekha Rao[1], Christine Roberts[1], Melissa Soehnel[1], Shayna Begay[1], and James Tinsley[2]

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33rd Polymer Processing Society, Cancun, Mexico

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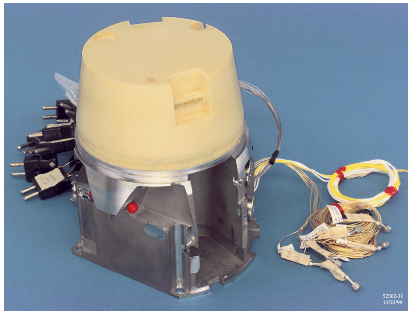
(pMDI) Polyurethane Foams Are Challenging!

Application Space

- PMDI is used as an encapsulant and as a structural material to mitigate against shock and vibration



(Mike Gerding, UUR)

Problems Arise From a Short Pot Life and High Exothermicity

- Void Defects, Density Variations, Residual Stress
- Short Term: Meet Tight Geometric Specifications
- Long Term: Long term shape change/loss of component function

The Current Design Approach Is Costly!

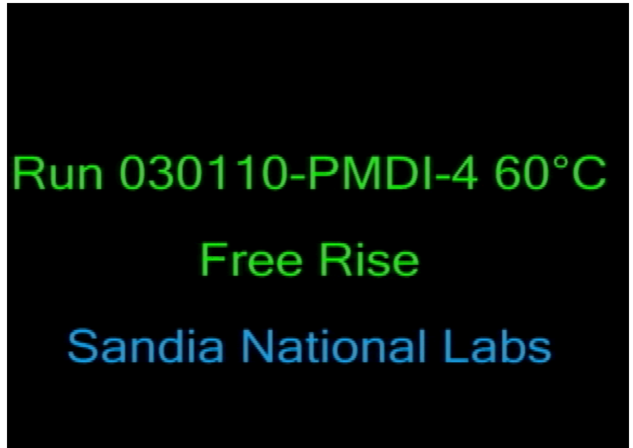
Manufacturing and Acceptance through Trial and Error
Modeling and Simulation Can Help!

The Challenge: Predicting How Manufacturing Conditions Impact Component Dimensional Stability

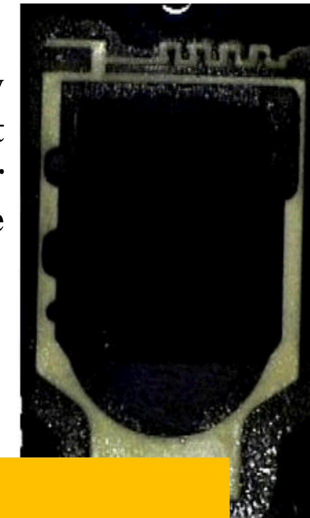
A Typical Manufacturing-to-Lifetime Process

Mix Resin

Injection, foaming and initial curing at lower T

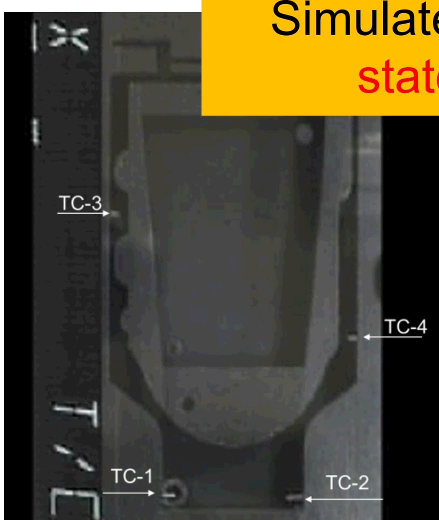


Secondary Cure at Higher Temperature



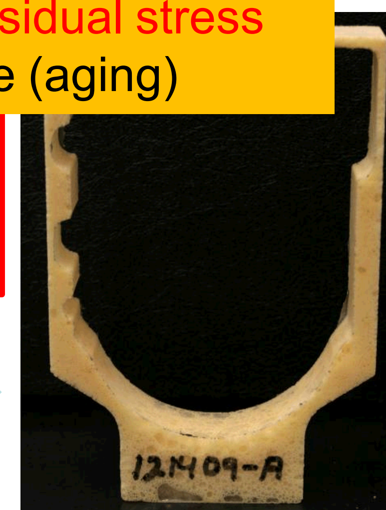
Objective

Simulate the manufacturing process, develop the residual stress state, and predict component warpage over time (aging)



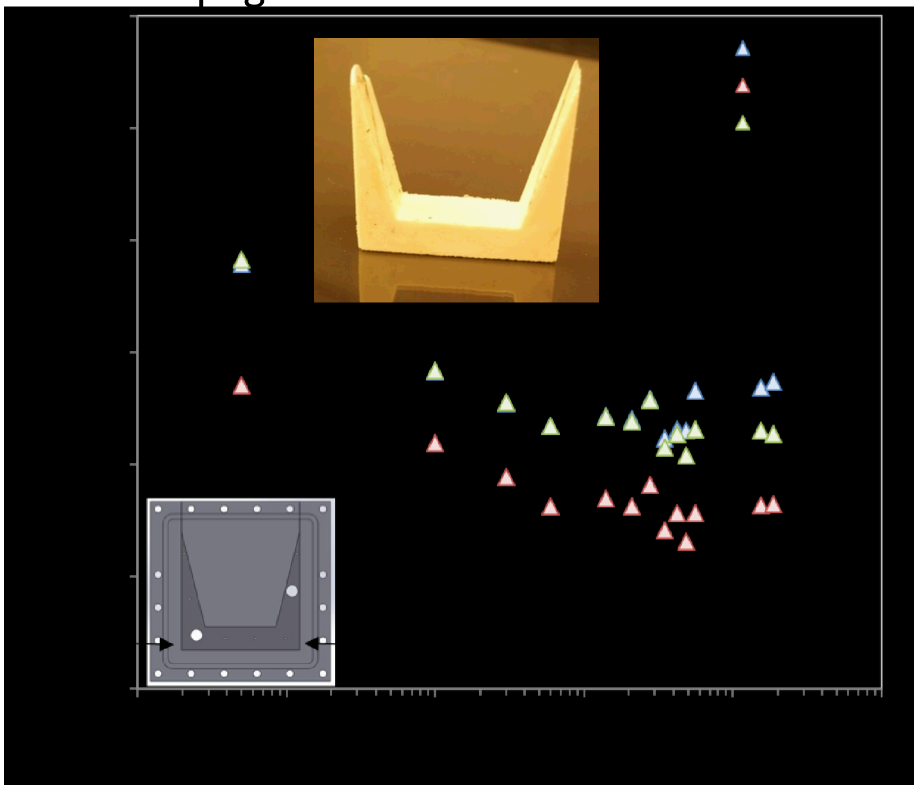
from mold – predict cure and thermal stresses

Predict shape and size over years

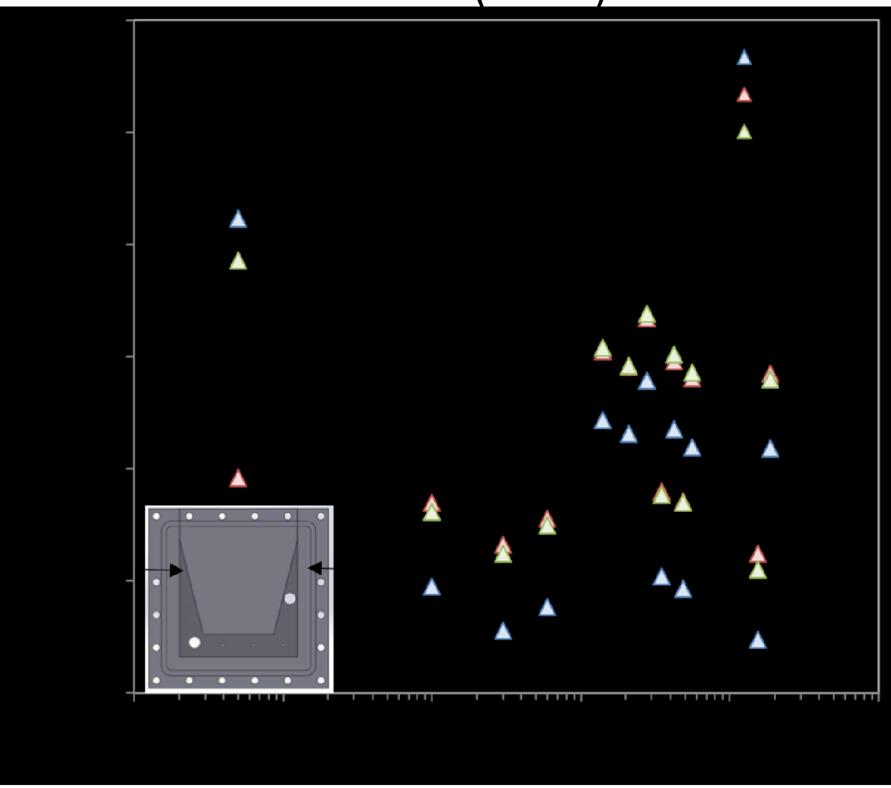


Experimental Motivation: Warpage and Aging Demonstration on the Sandia Staple

- PMDI 10 S packed to 12.5 PCF
- Cure Schedule: 30 C for 10 minutes, 4 hours at 120 C
- Warpage measurements with a Zeiss® Coordinate Measurement (CMM) Machine



Monotonic and Consistent Warpage Trend in Thick Regions



Non-Monotonic and Complex Warpage Trend On Thin Staple Arms

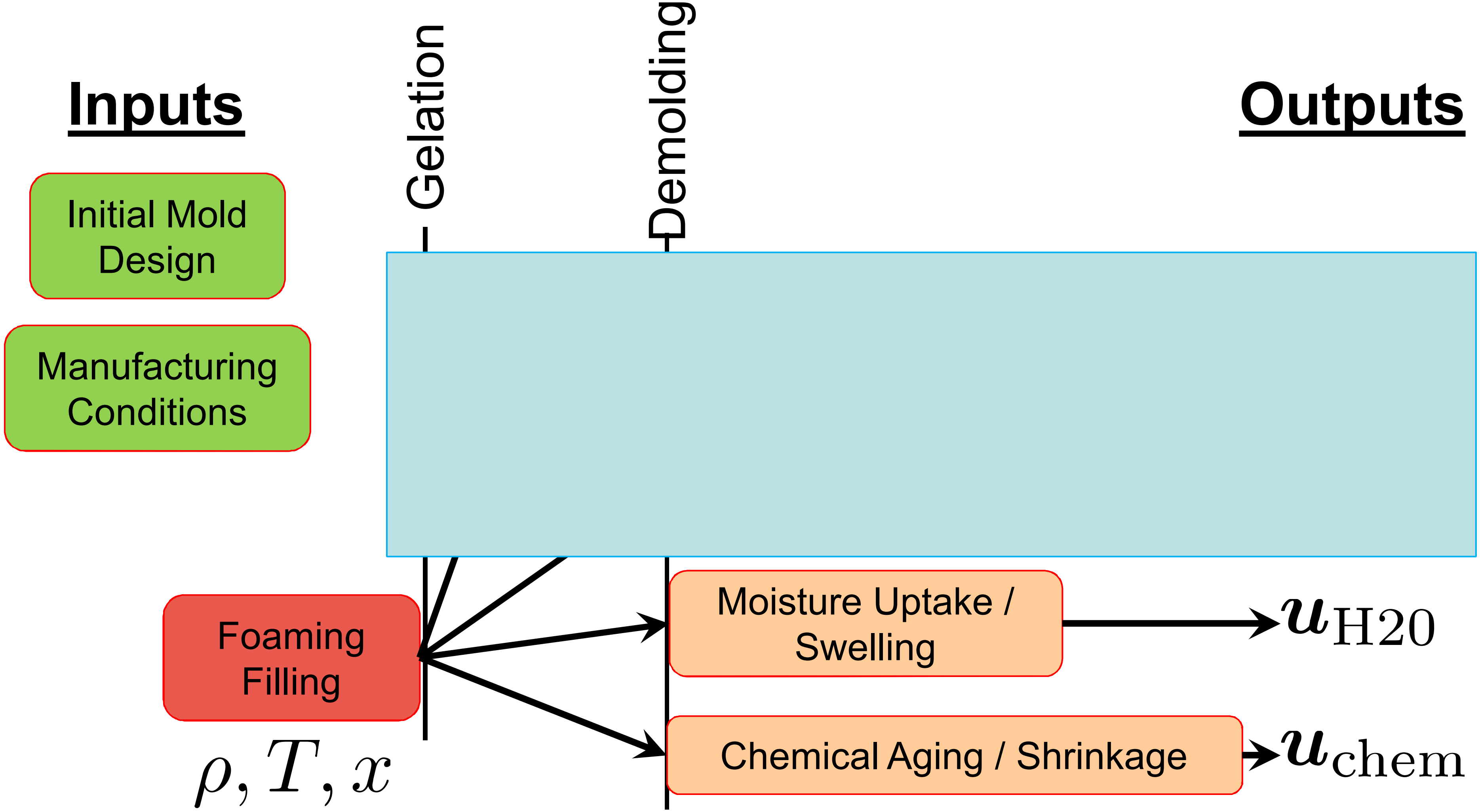
What are the key factors that make complex warpage behavior at the "staple arms"?

Presentation Outline

1. Problem Definition and Customer Needs
2. ”Cradle-to-Grave” Modeling and Simulation:
3. Parametric Studies on the Sandia Staple Mold from Resin Injection through 20 years of aging
4. Warpage Predictions on complex foam components
5. Summary and Key Findings

MODEL SUMMARY

Cradle-to-Grave Simulation Process



$$\boldsymbol{u} = \boldsymbol{u}_{\mathrm{visco}} + \boldsymbol{u}_{\mathrm{dep}} + \boldsymbol{u}_{\mathrm{H20}} + \boldsymbol{u}_{\mathrm{chem}}$$

Inverse Mold Design Process

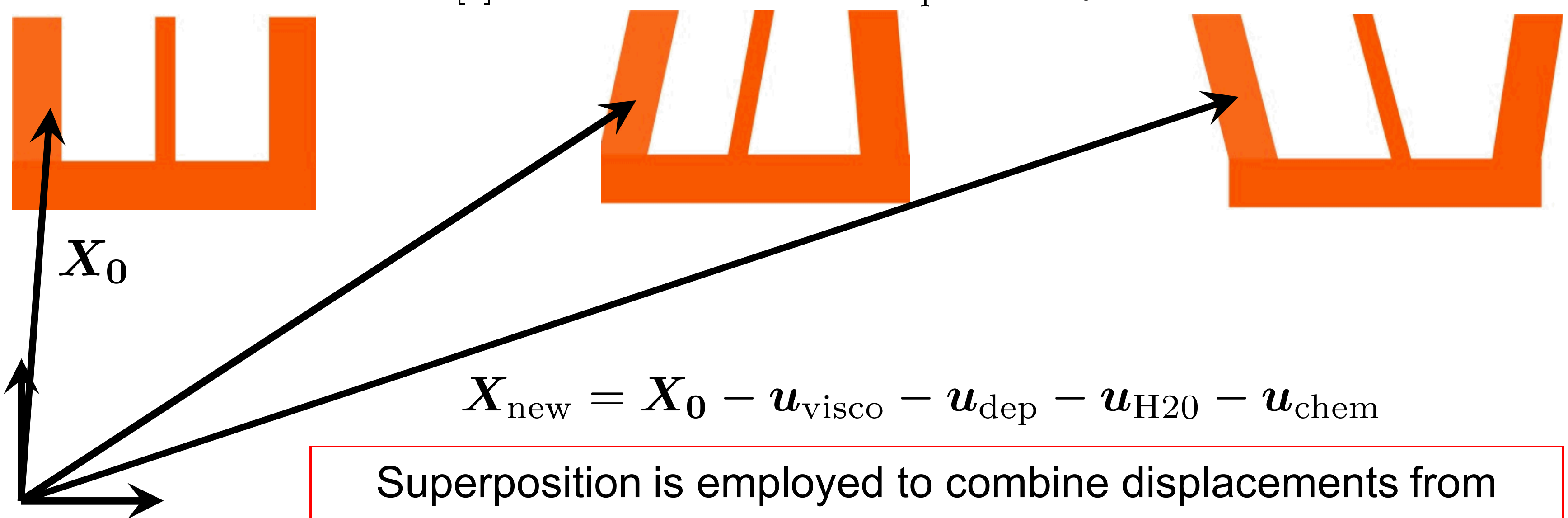
Inputs

Manufacturing Conditions

Initial Mold Design

→ Cradle-to-Grave Simulation → **Output** Final Mold Shape

$$\boldsymbol{X}[t] = \boldsymbol{X_0} + \boldsymbol{u}_{\text{visco}} + \boldsymbol{u}_{\text{dep}} + \boldsymbol{u}_{\text{H20}} + \boldsymbol{u}_{\text{chem}}$$

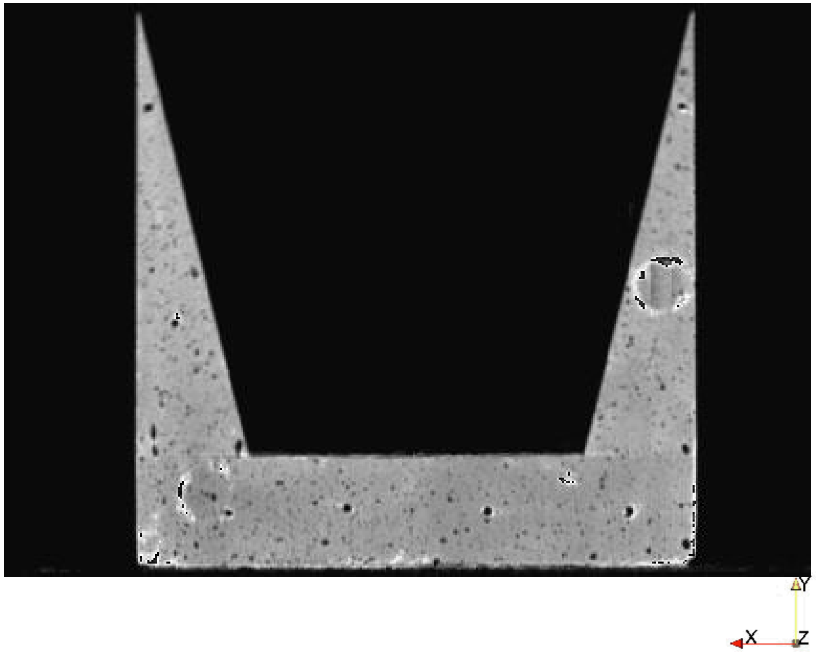


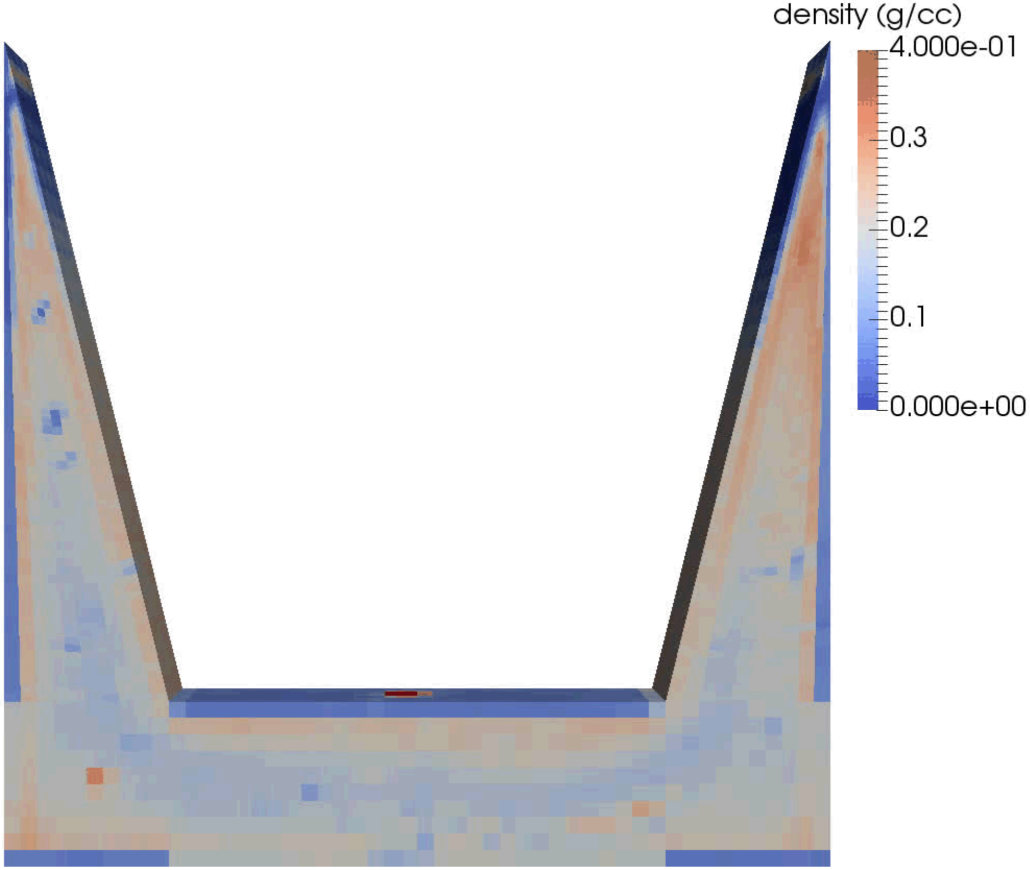
$$\boldsymbol{X}_{\text{new}} = \boldsymbol{X_0} - \boldsymbol{u}_{\text{visco}} - \boldsymbol{u}_{\text{dep}} - \boldsymbol{u}_{\text{H20}} - \boldsymbol{u}_{\text{chem}}$$

Superposition is employed to combine displacements from different mechanisms and then to “inverse warp” the initial mold design

Initial Calculations of the U-staple

- Uniform Gauge Pressure (12 psig), Density from the X-ray CT
- **1000 X Displacement for Visualization**





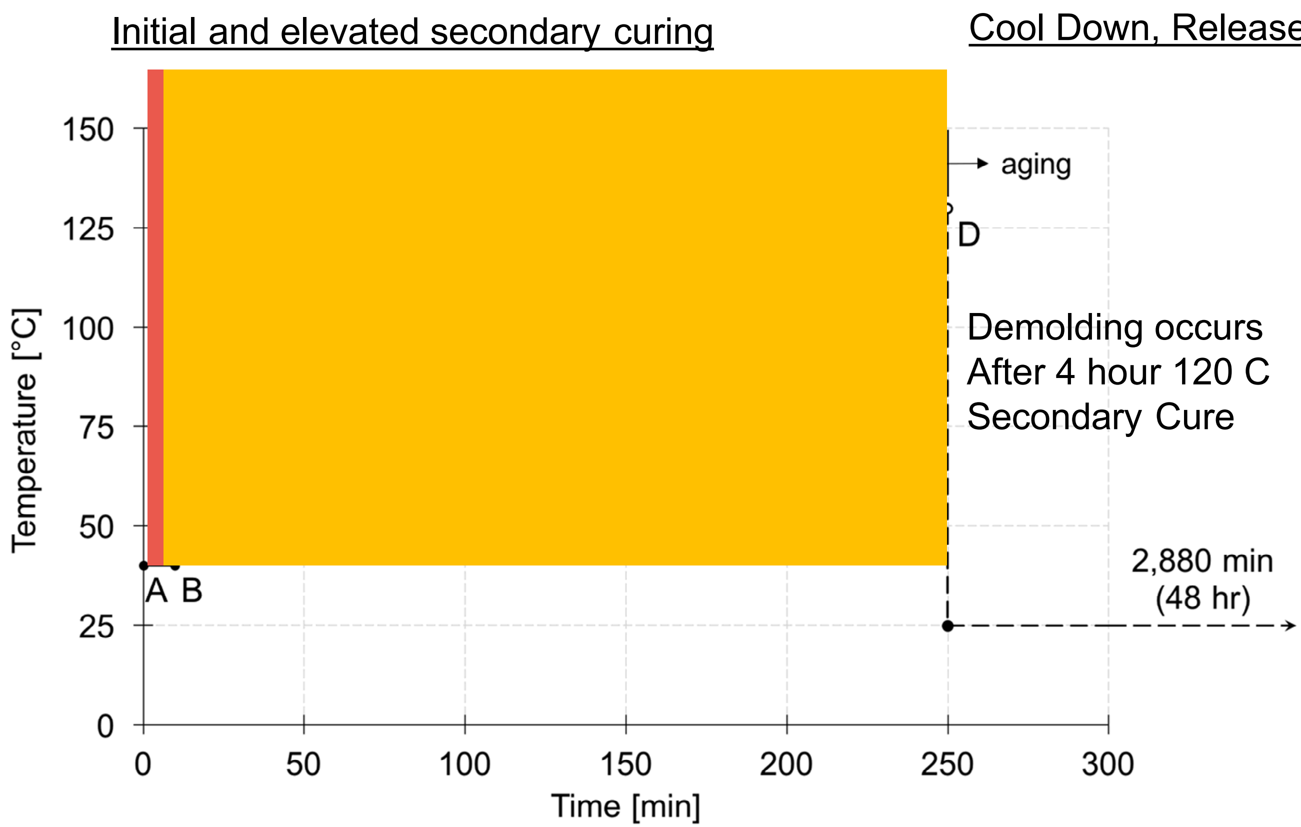
Depressurization consistently produces 1/10 or less the deformation compared with viscoelastic residual stress relaxation

The role of residual stress and non-linear viscoelasticity in part warpage

RESIDUAL STRESS RELAXATION MANUFACTURING SENSITIVITY STUDY

The Sandia / AWE Staple Simulations

A benchmark problem to experimentally and computational investigate warpage quantitatively



Boundary Conditions

Thermal:

1. Essential BCs until The end of the 4 hour 120 C secondary cure
2. Convective cooling to room temperature thereafter

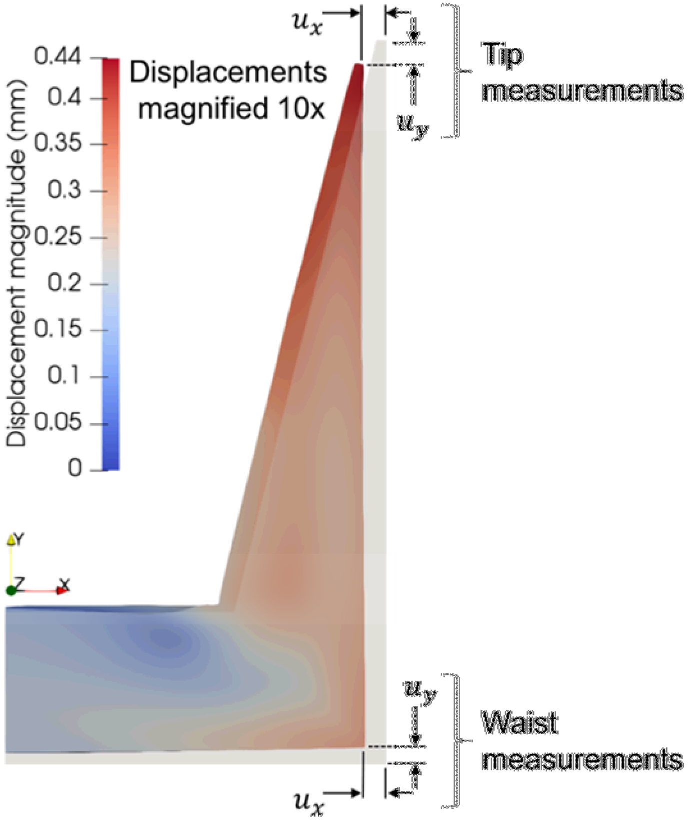
Mechanical:

1. Essential (zero displacement) until demolding
2. Traction free post demolding

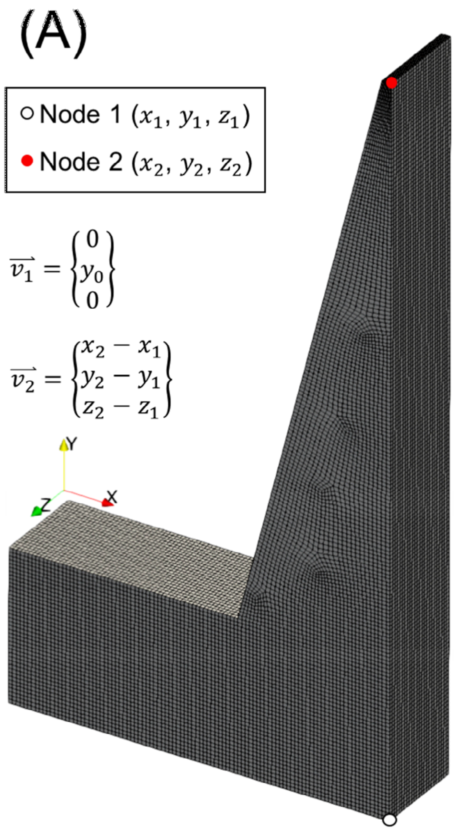
A KCNSC Cure Schedule for the PMDI10S Foam. Parametric Study Parameters During Cooldown

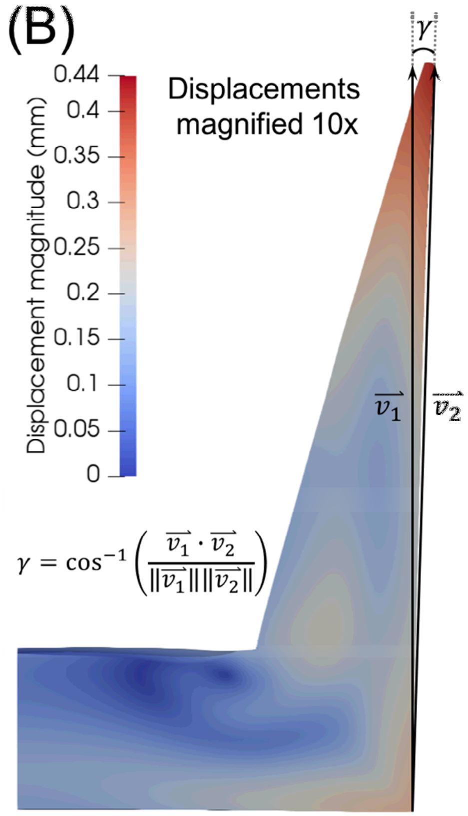
Sandia Staple Displacement Definitions

Displacements

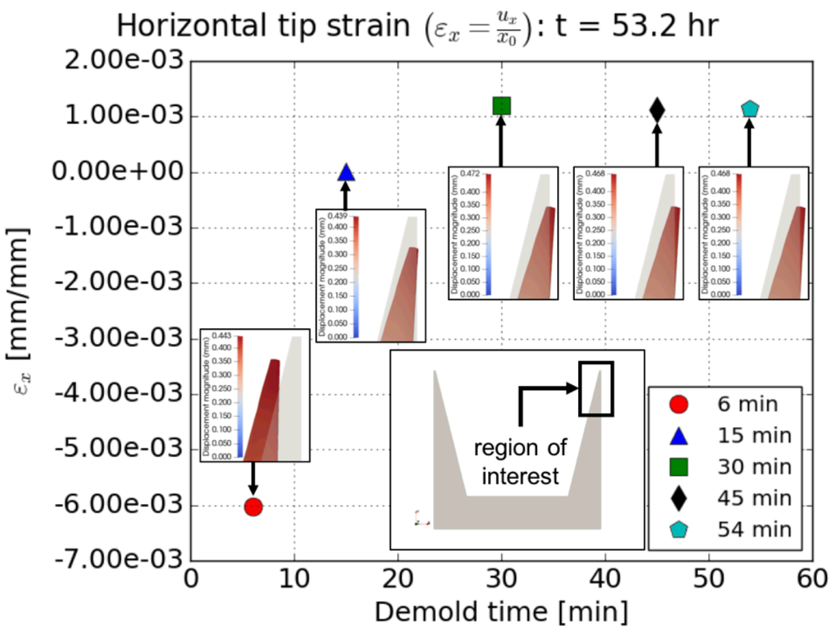


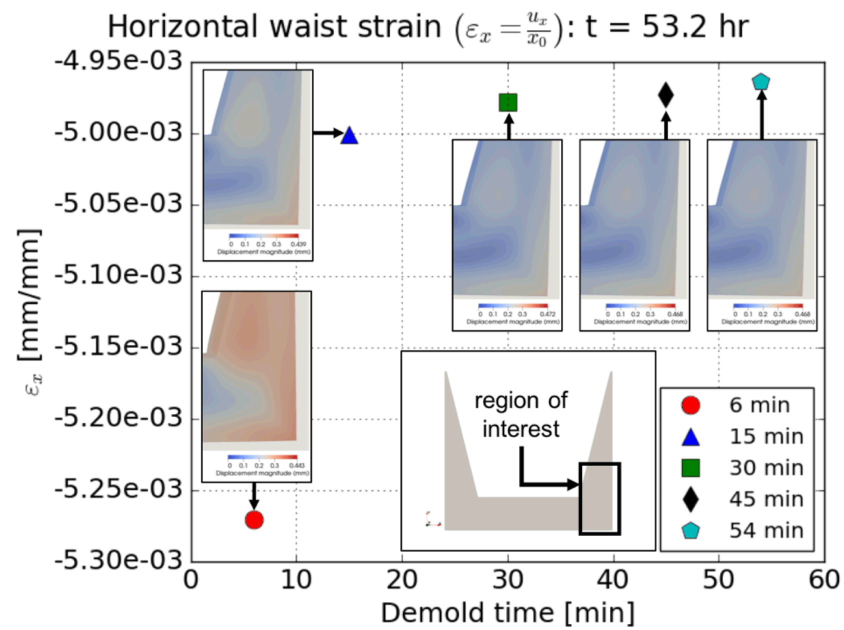
Arm Angle

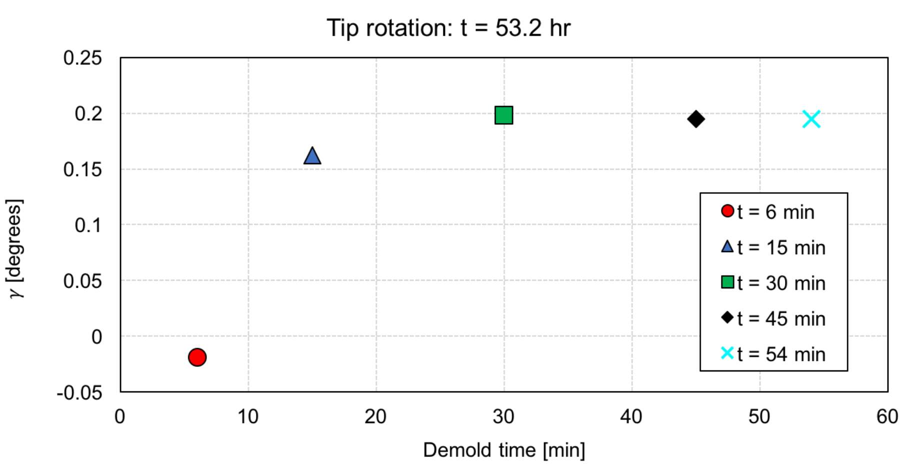




Demolding Sensitivity Study

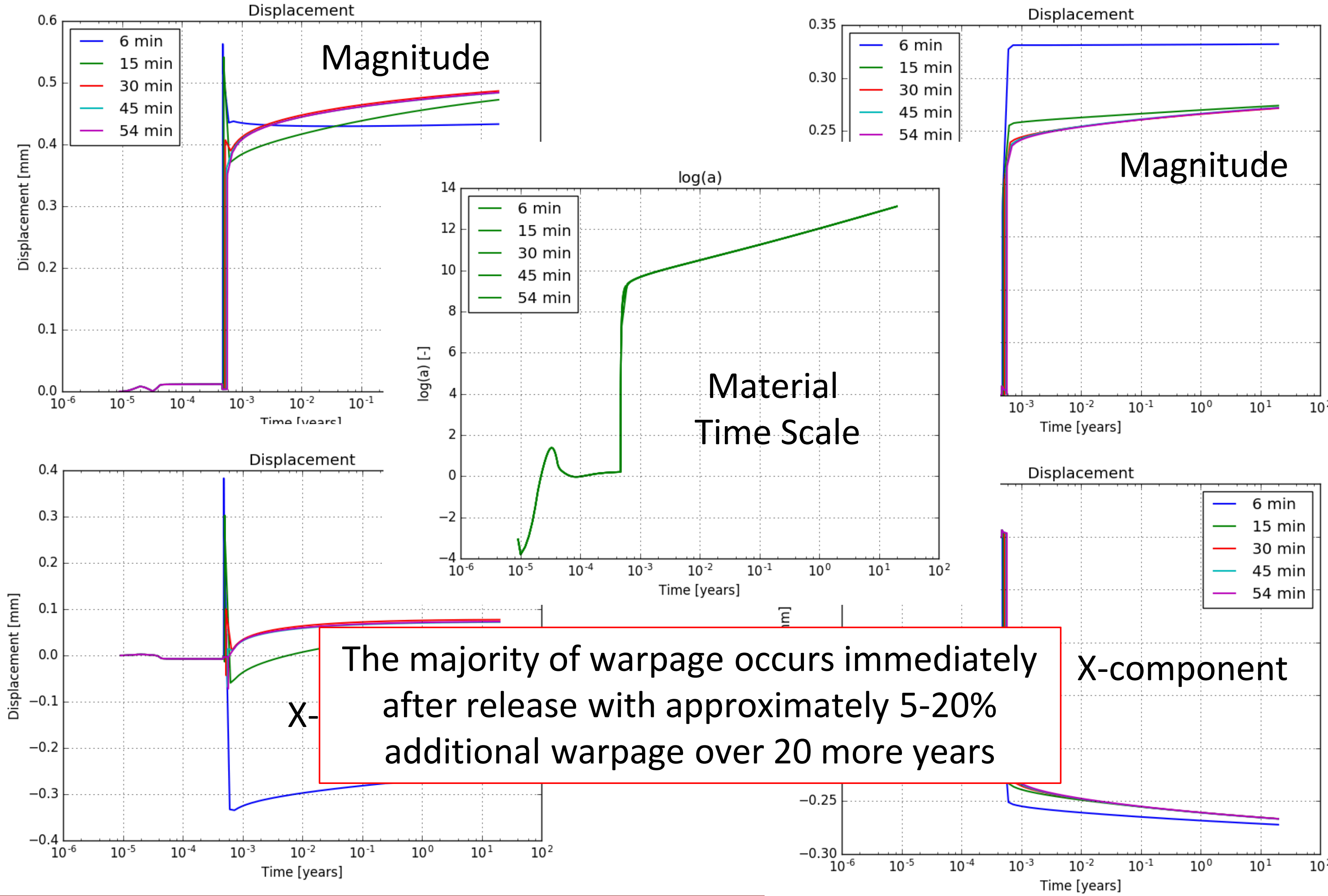






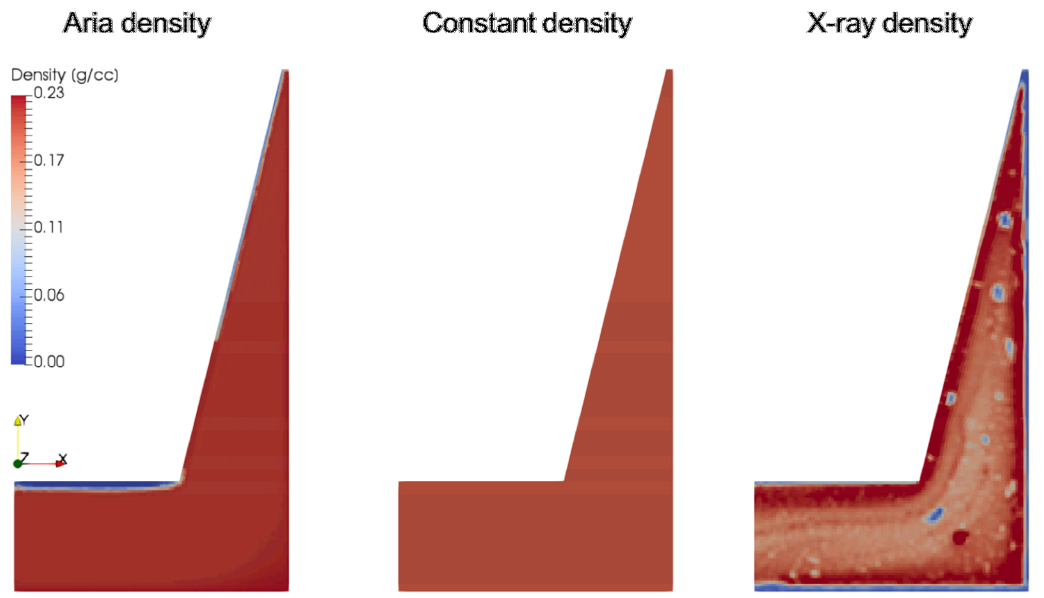
Demolding too hot (close to the glass transition) significantly changes the Warpage response

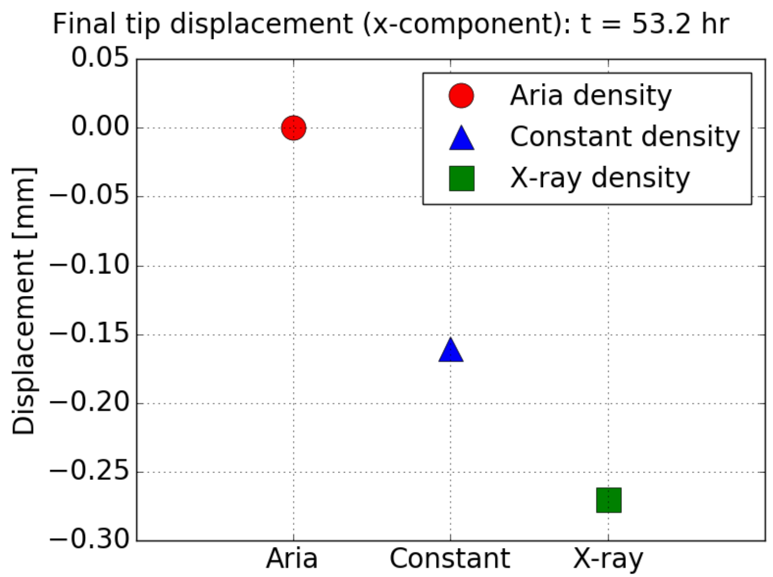
Demolding Sensitivity Study: 20 Years of Traction Free / RT Physical Aging

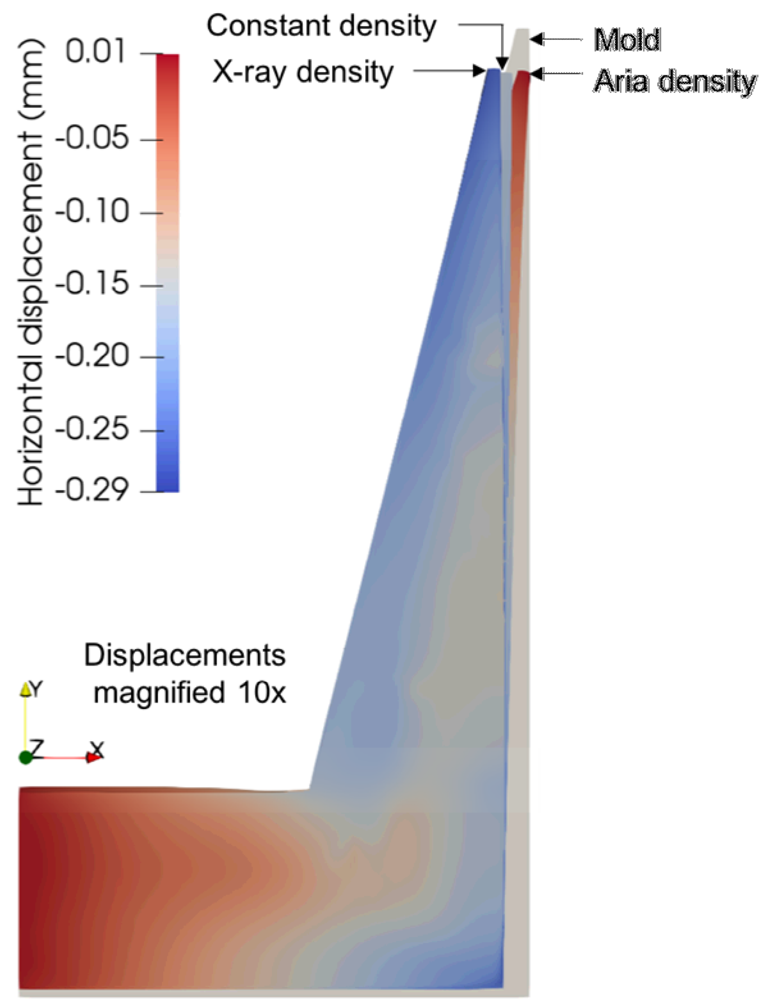


The majority of warpage occurs immediately after release with approximately 5-20% additional warpage over 20 more years

Density Sensitivity Study



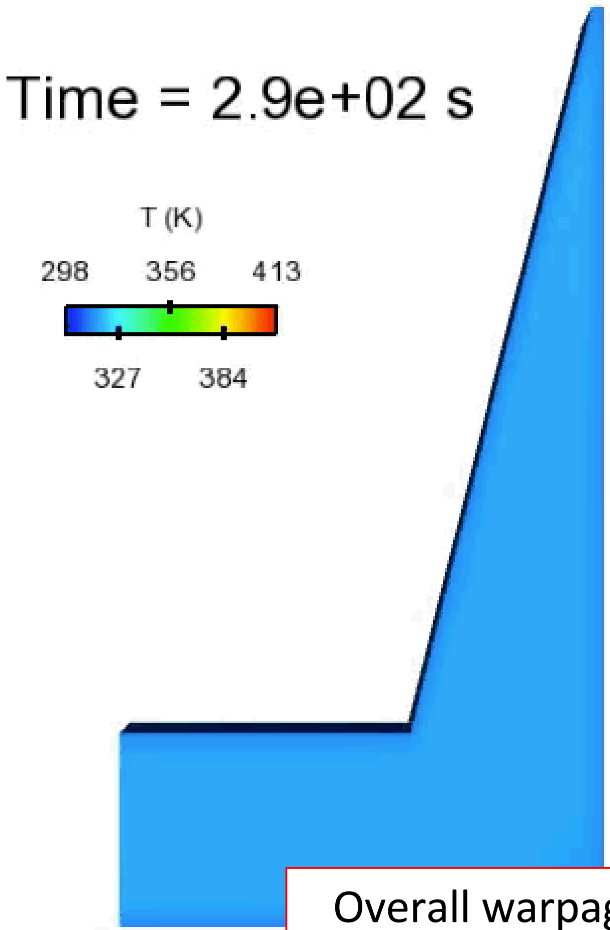




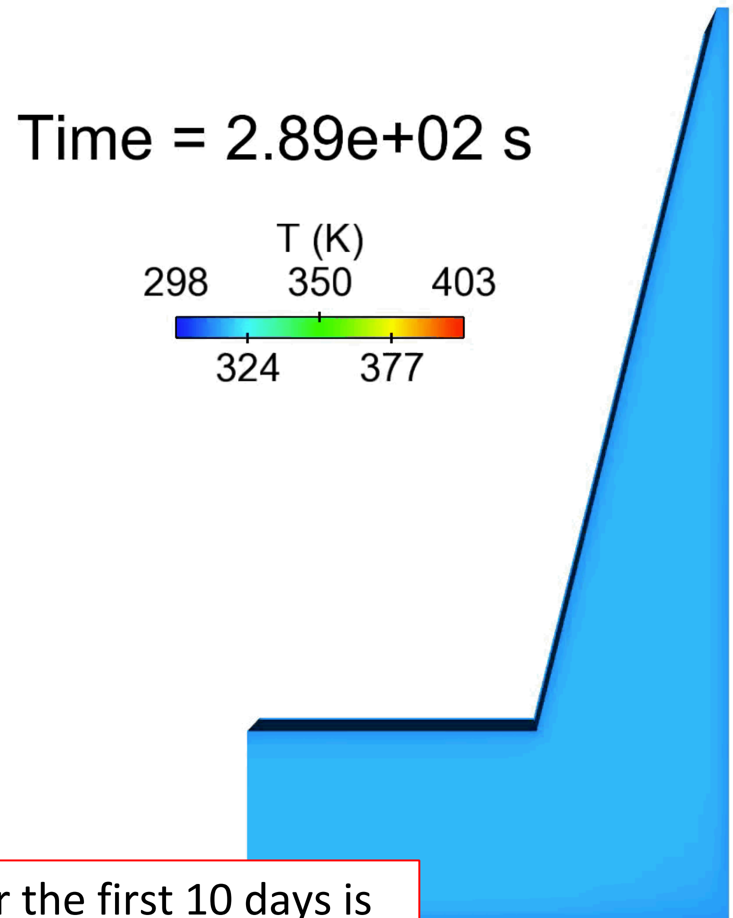
Density variations lead to fundamentally different warped shapes at the staple arms

Density Variation Time Histories

Constant Density

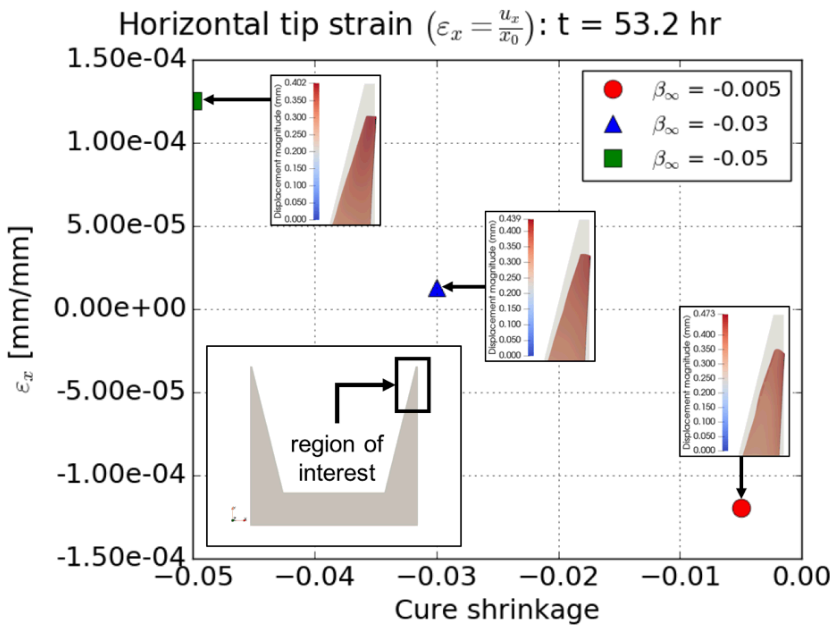


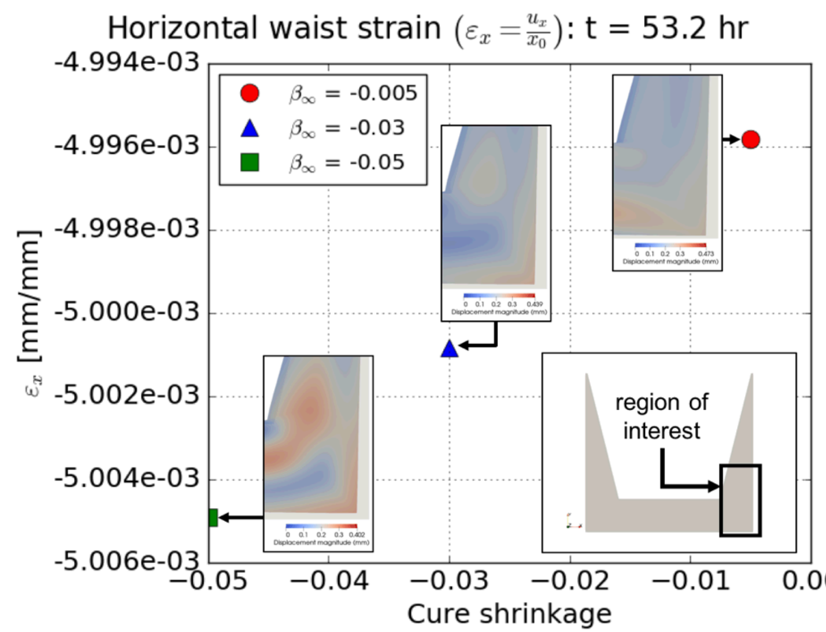
X-Ray CT Density

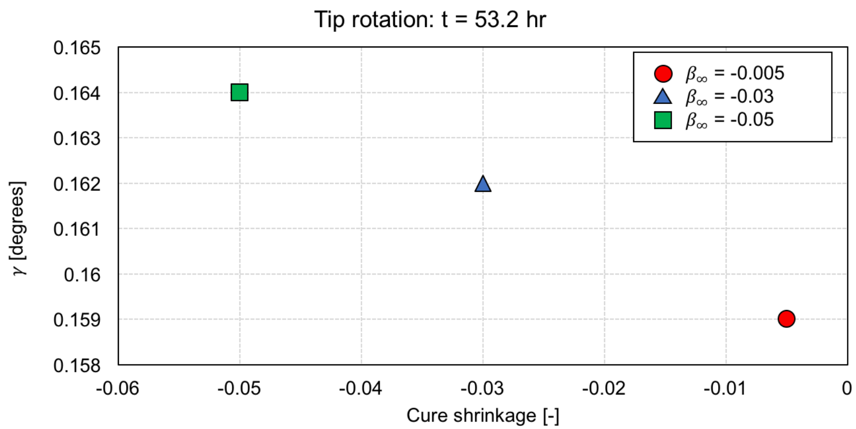


Overall warpage behavior over the first 10 days is qualitatively similar between different densities

Cure Shrinkage Sensitivity Study







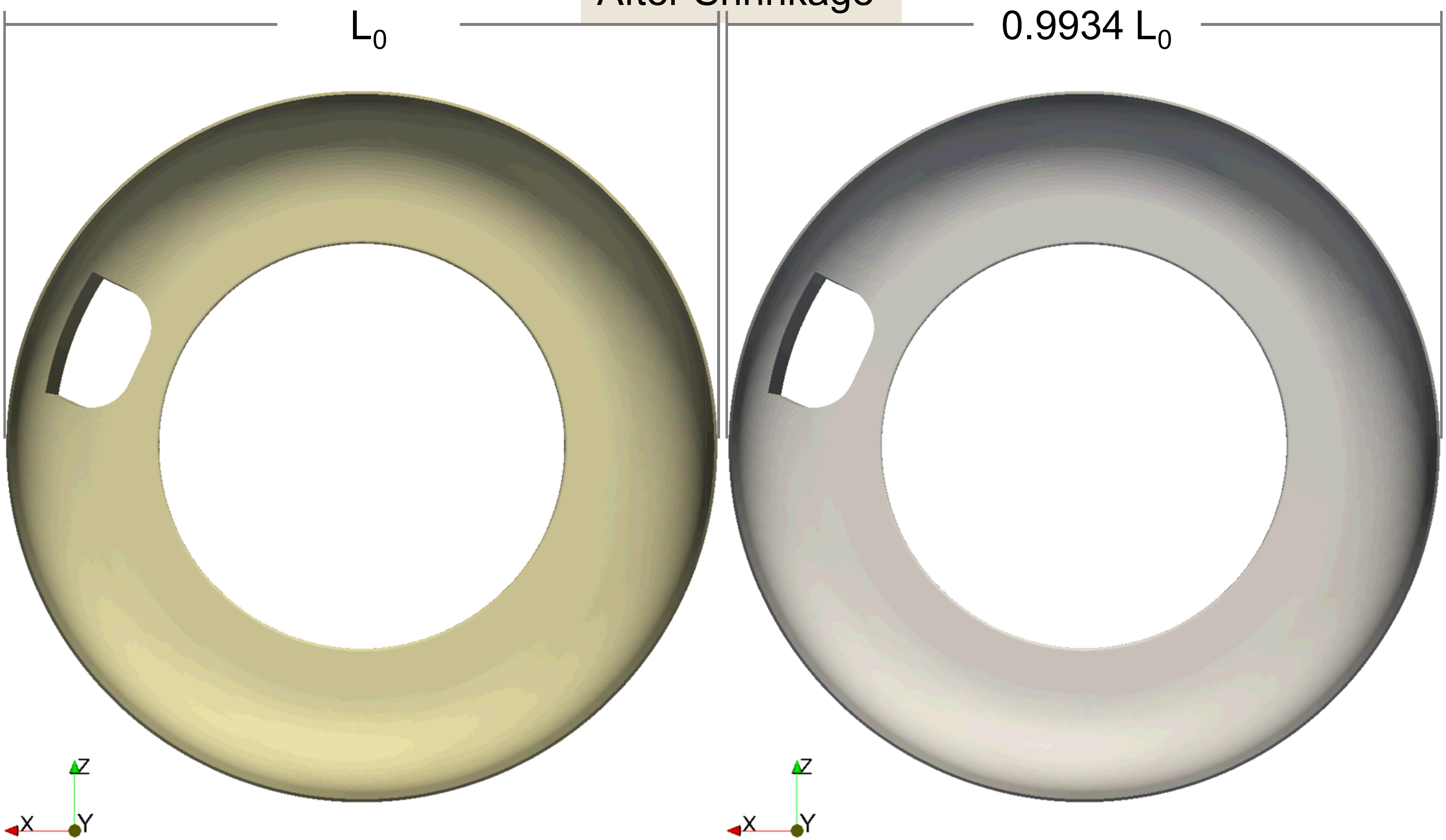
The effects of the cure volume change parameter on staple warpage are small.
→We don't need to accurately determine This parameter in the model

WARPAGE PREDICTIONS IN 10 PCF PMDI STRUCTURAL COMPONENTS 48 HOURS AFTER RESIN POOR

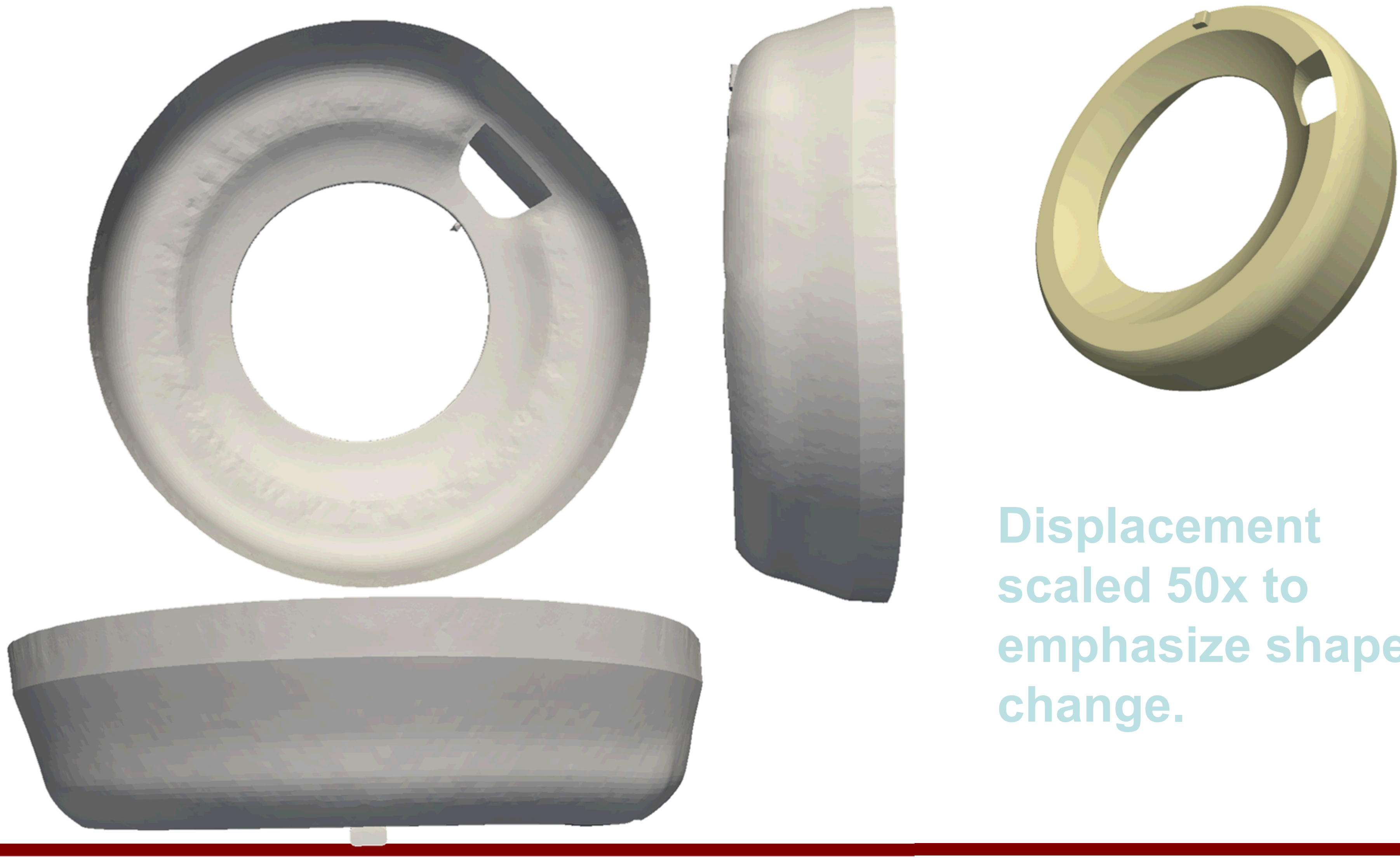
Exemplar Part With Featured Regions

As-Molded

After Shrinkage

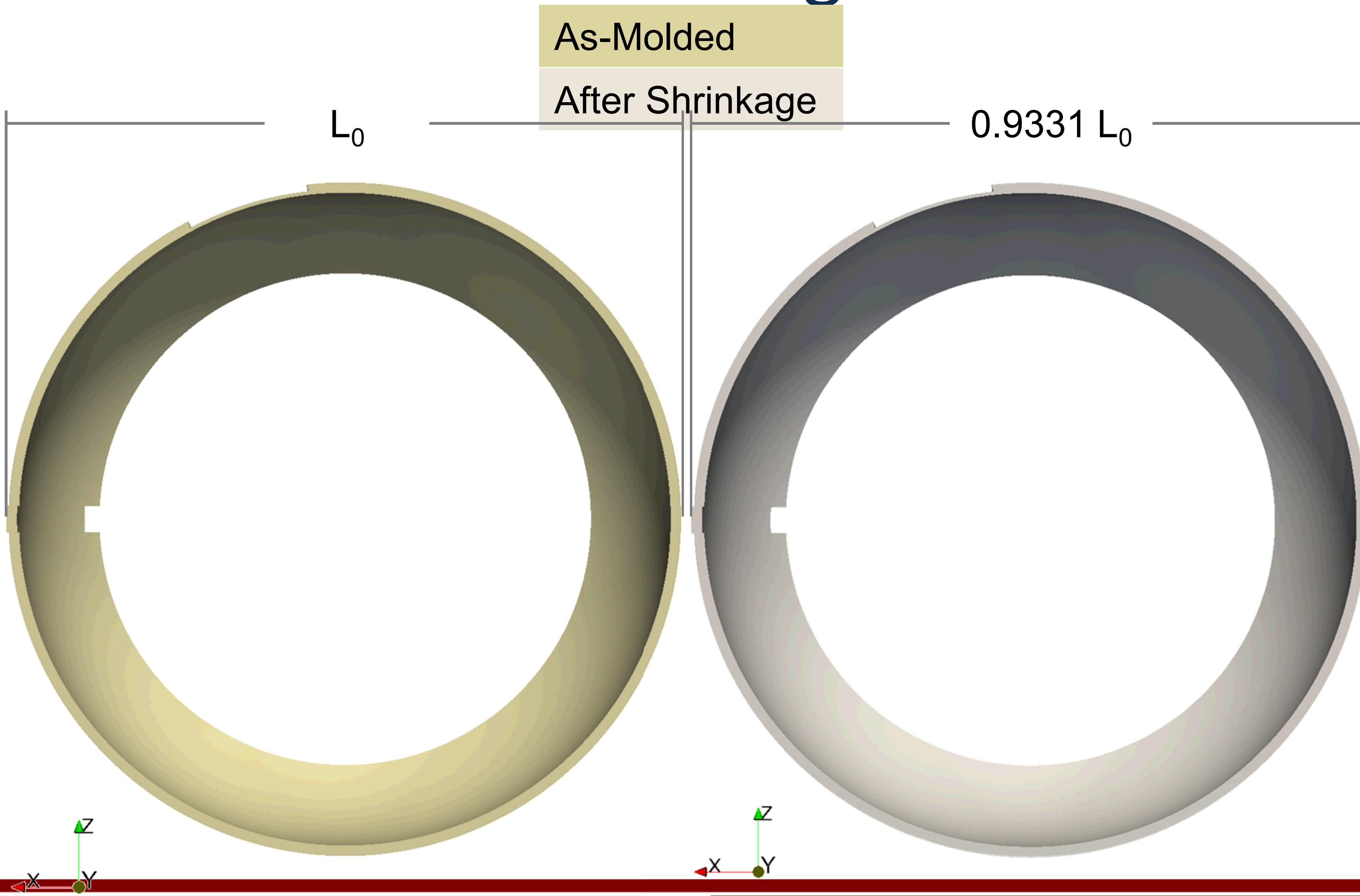


Warpage accentuated near holes and slender regions

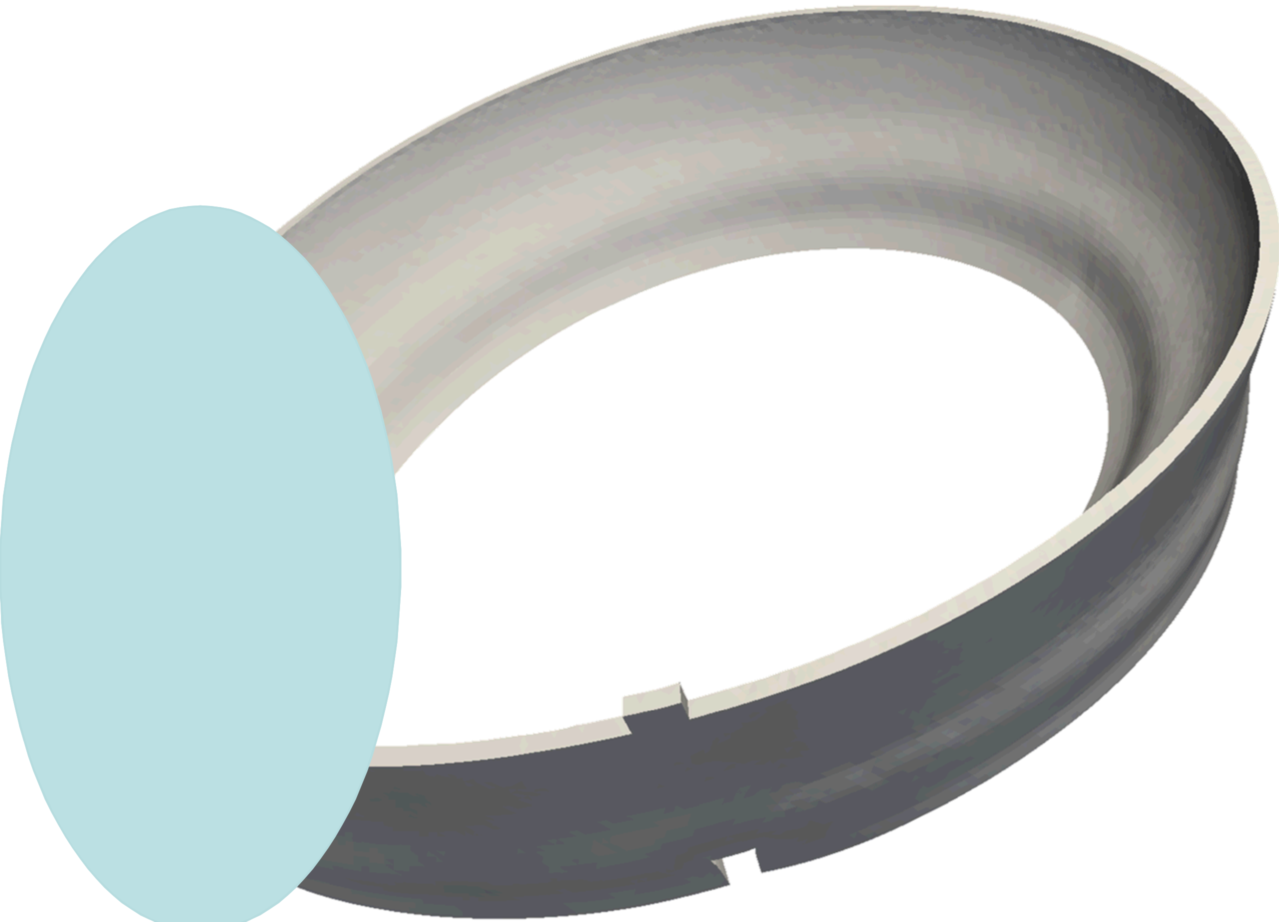


Displacement scaled 50x to emphasize shape change.

Exemplar Part With Notched Features and Thin and Thick Region Transitions



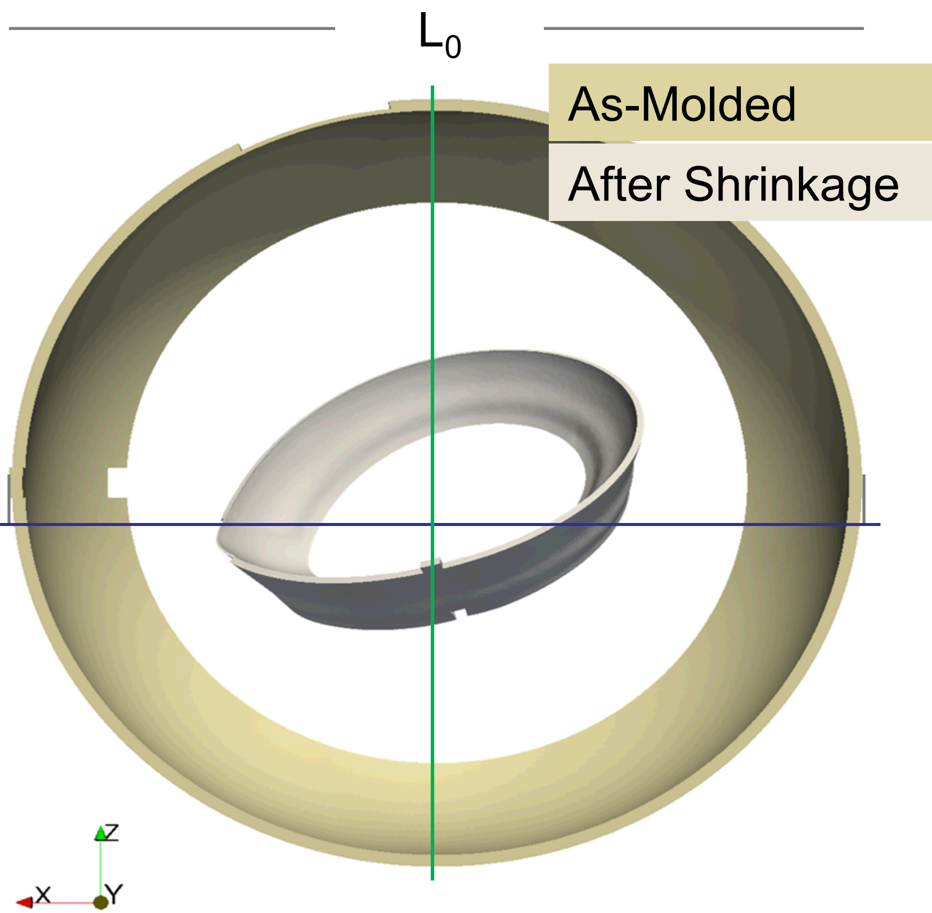
Shrinkage Accentuated Near Thin-Thick Region Transition

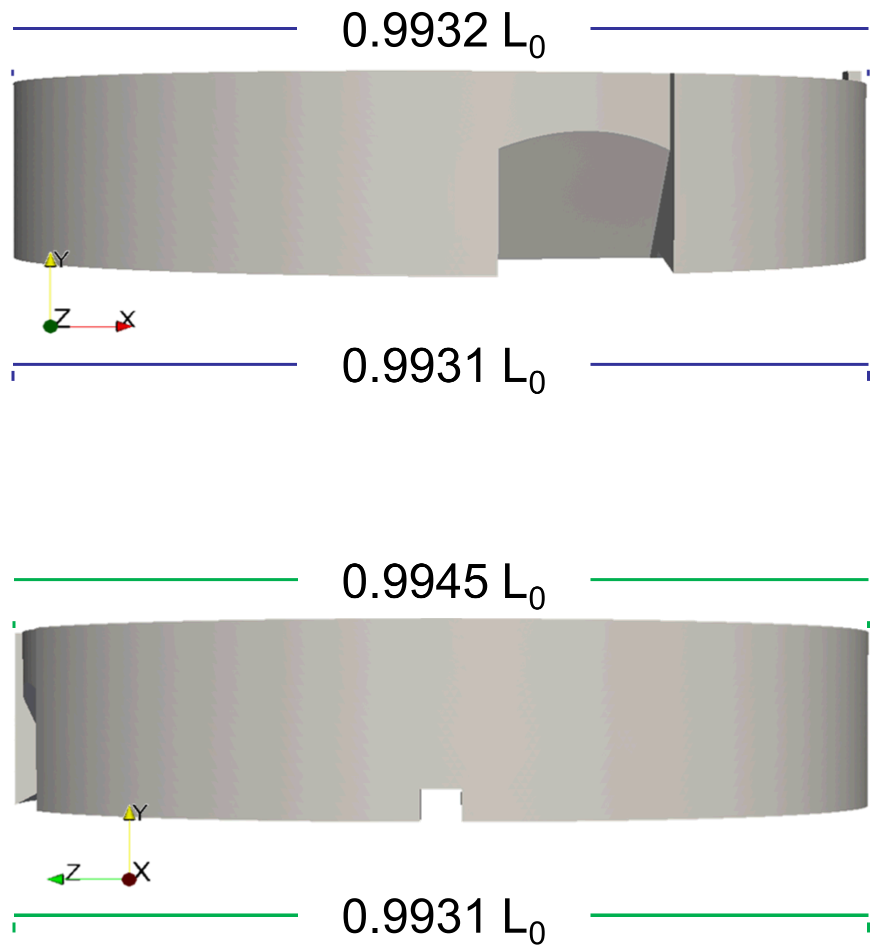


Displacement scaled 50x to emphasize shape change.

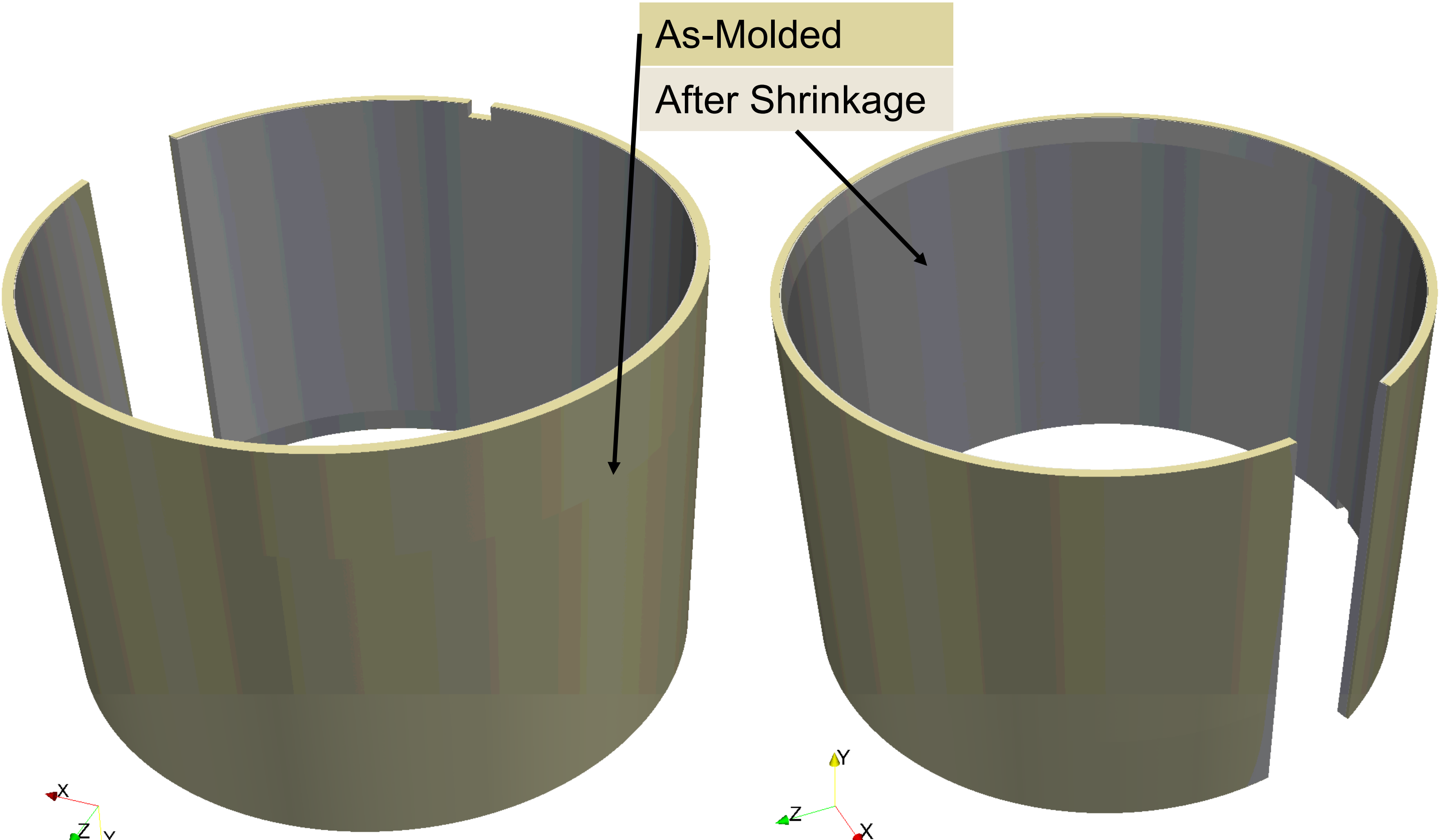
Notch Remains Largely Unwarped

Top and Bottom Shrink Differently

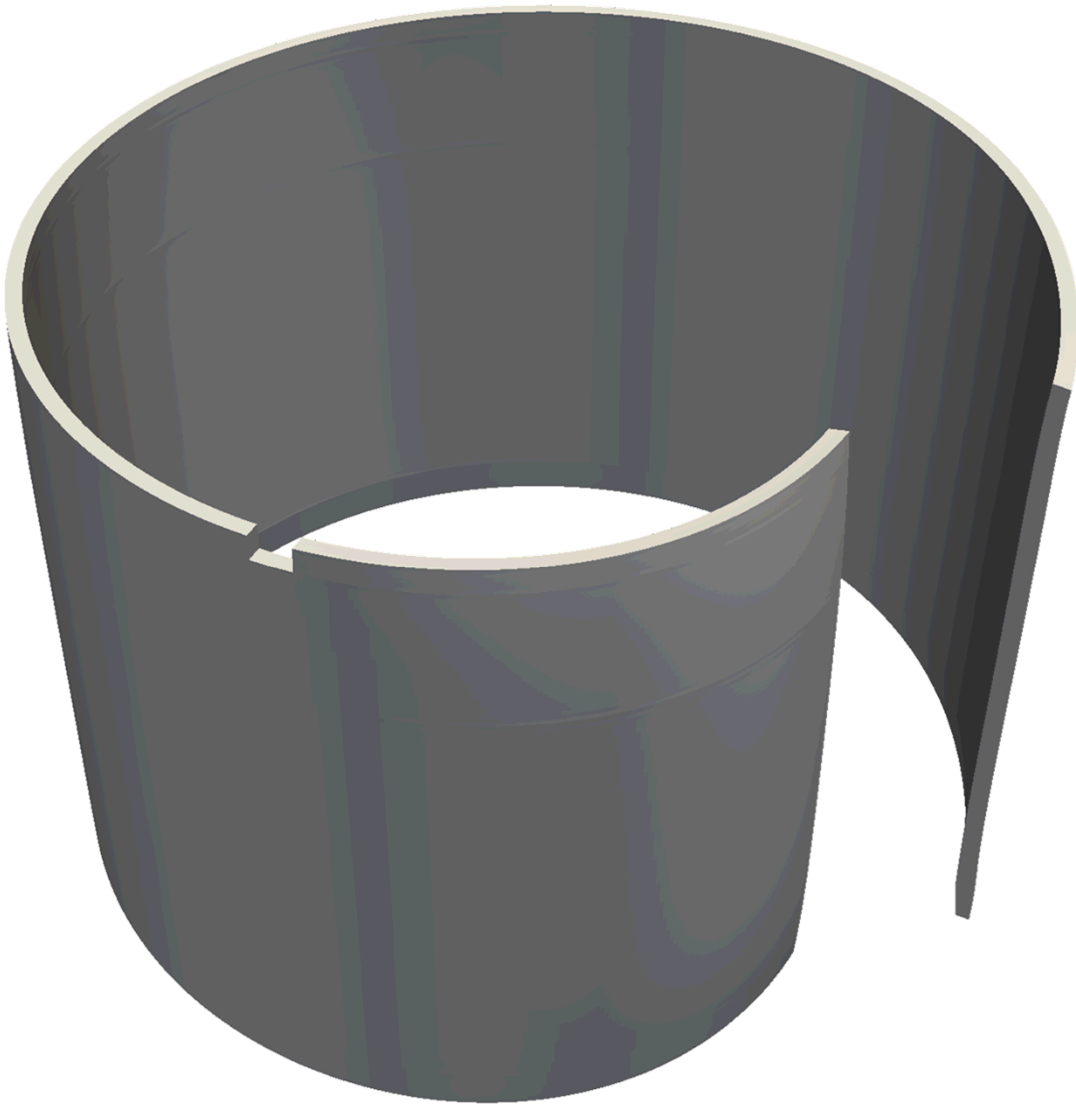


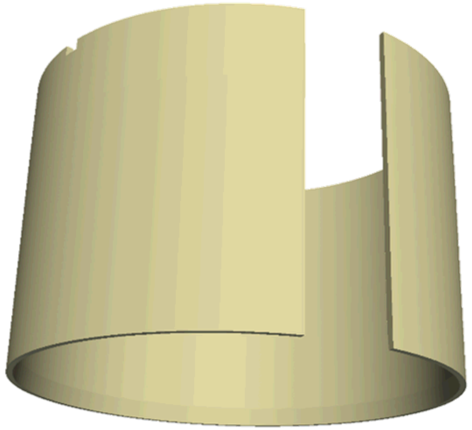


Different Top/Bottom Warpage Suggests The Component Will Not Simply Shrinking in Volume Uniformly



As-Molded Exterior vs. After-Shrinkage Interior





This design is particularly susceptible to bending given the integrated error around the specimen circumference

Displacement scaled 20x to emphasize shape change.

Key Findings and Conclusions

Current inverse mold design simulations were successfully developed and deployed on a number of support components

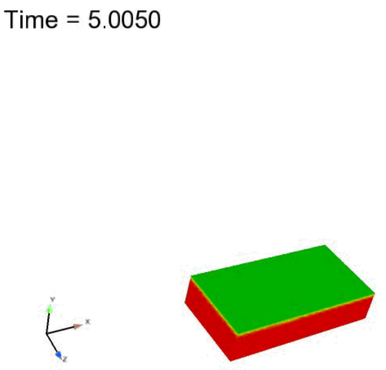
- Demolding hot results in more warpage in the present study compared with cooling further into the glass
- Density variation strongly influences shape change in slender regions and should be reduced
- Warpage predictions were in reasonably good agreement with KCNSC CMM measurements experiments (not shown here)

Kevin Long, knlong@sandia.gov

QUESTIONS?

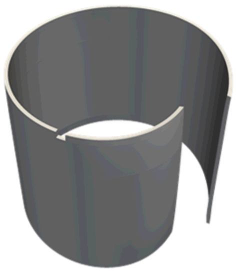
Improving Component Manufacturing Yields and In-Service Reliability:

1. Filling support to reliably fill complex molds
   - Reduce defects and density variation



2. Post-manufacturing support to improve product acceptance yields
   - Change manufacturing conditions AND inverse mold design to reduce out-of-tolerance component warpage

3. Long-term assessment of dimensional stability of foamed components to support surveillance efforts



Objective

Simulate the manufacturing process, develop the residual stress state, and predict component warpage over time (aging)

Non-Linear Curing Viscoelastic Solid Modeling

Balance Laws and Solution Fields:

- Mass + Momentum (*Displacements*) ← Lagrangian FEM
- Species Balance (*Chemical Reaction Extent*) ← ALE FEM
- Energy (*Temperature*) ← ALE FEM

Solid State Non-Linear Viscoelastic (NLVE) Model Initial Conditions

- Initialize *temperature, foam density, and reaction extent* from simulation stage 1
- Directly initialize the stress-free reaction and temperature (expansion free)
- Assume the NLVE viscous stresses are initially zero

Stress prediction based on the universal curing model developed at SNL

DB Adolf and RS Chambers, "A thermodynamically consistent, nonlinear viscoelastic approach for modelling thermosets during cure," J. Rheology, 2007.

Cauchy Stress: SNL Non-linear Viscoelastic Curing Model (Adolf & Chambers 2007)

$$\underline{\underline{\sigma}} = \underline{\underline{\sigma}}\left[\log \underline{\underline{U}},\ T,\ x,\ \text{histories}\right]$$

Logarithmic Strain — Temperature — Extent of matrix cure

Material and Laboratory Time Relation

$$dt^* = \frac{dt}{a[t]} \qquad \log \mathrm{a} = -\hat{C}_1\left(\frac{N}{\hat{C}_2 + N}\right)$$

Density Scaling

$$\psi[\rho_0] = \left(\frac{\rho_0}{\rho_{ref\,0}}\right)^p \psi[\rho_{ref\,0}] \quad \text{Free Energy}$$

$$\underline{\underline{\sigma}}[\rho_0] = \left(\frac{\rho_0}{\rho_{ref\,0}}\right)^p \underline{\underline{\sigma}}[\rho_{ref\,0}] \quad \text{Cauchy Stress}$$

Curing NLVE Model Continued

Relaxation behavior and mechanical properties depend on the *temperature, extent of cure, and histories of deformation*

Material Time Dependencies

Thermal

Pressure

$$N=\left\{\left[T(t)-T_{ref}\right]-\int_0^t ds\ f_1\left(t^*-s^*\right)\frac{dT}{ds}(s)\right\}+C_3\left\{I_1(t)_{ref}-\int_0^t ds\ f_1\left(t^*-s^*\right)\frac{dI_1}{ds}(s)\right\}$$

$$+C_4\left\{\int_0^t\int_0^t ds\,du\,f(t^*-s^*,t^*-u^*)\frac{d\underline{\underline{\varepsilon}}_{dev}(s)}{ds}:\frac{d\underline{\underline{\varepsilon}}_{dev}(u)}{du}\right\}+C_5\left(x(t)\right)\left\{\left[x(t)-x_{ref}\right]-\int_0^t ds\ f_1\left(t^*-s^*\right)\frac{dx}{ds}(s)\right\}$$

Shear Deformation

Matrix Cure

Glass Transition Evolution

$$T_{ref}(x)=T_{ref}-\frac{\left[C_3\beta_\infty+C_5\left(x(t)\right)\right]\left(x(t)-x_{ref}\right)}{(1+C_3\alpha_\infty)}$$

$$C_5\left(x(t)\right)\equiv C_{5a}+C_{5b}\,x$$

Shear Modulus

$$G_g(T)=G_{gref}+\frac{\partial G_g}{\partial T}(T-T_{ref})+\frac{\partial G_g}{\partial x}(x-x_{ref})$$

$$G_\infty(T)=\left\{G_{\infty ref}+\frac{\partial G_\infty}{\partial T}(T-T_{ref})\right\}\left[\frac{x^m-x_g^m}{x_{ref}^m-x_g^m}\right]^n$$

Simple Macroscale Depressurization Model

Macroscale Volumetric Kinematic Split:
Mechanical, Thermal, Depressurization

$$\mathbf{F}^{\mathbf{vol}} = \lambda^v \mathbf{1} = \mathbf{F}_{\mathbf{M}}^{\mathbf{vol}} \mathbf{F}_\theta \mathbf{F}_{\mathbf{d}} = \lambda_M^v \lambda_\theta \lambda_d \mathbf{1}$$

Total Rate of Volume Deformation

$$\mathbf{D}^{vol} = \frac{\dot{\lambda}^v}{\lambda^v}\mathbf{1} = \left(\frac{\dot{\lambda}_M^v}{\lambda_M^v} + \frac{\dot{\lambda}_\theta}{\lambda_\theta} + \frac{\dot{\lambda}_d}{\lambda_d} \right)\mathbf{1} = \mathbf{D}_M^{vol} + \mathbf{D}_\theta + \mathbf{D}_d$$

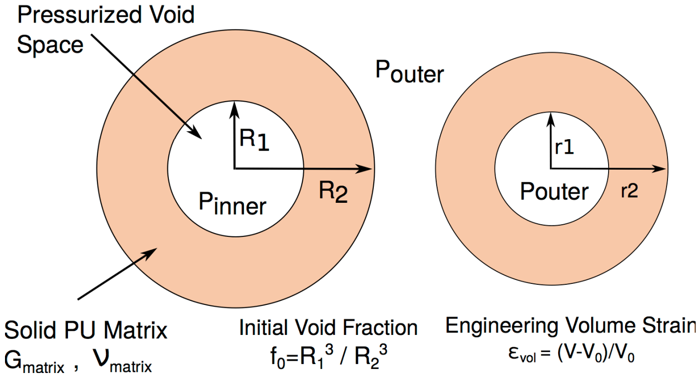
Rate of Isotropic Thermal Deformation

$$\mathbf{D}^\theta = \alpha_L \dot{T} \mathbf{1}$$

Hypoelastic Constitutive Law on the Mechanical Component Component of the Deformation Gradient

$$\dot{\sigma} = \frac{K \mathrm{tr} \dot{\epsilon}_M}{3} \mathbf{1} + 2G \mathrm{dev} \dot{\epsilon}_M$$

Pressurized Configuration   Depressurized Configuration



Outer Boundary Radial Displacement Normalized by its Reference Radius

$$\frac{U_2}{R_2} = \frac{(G(P_1 f_0 - P_2)/3 + K f_0 (P1 - P2)/4)}{(GK(1 - f_0))}$$

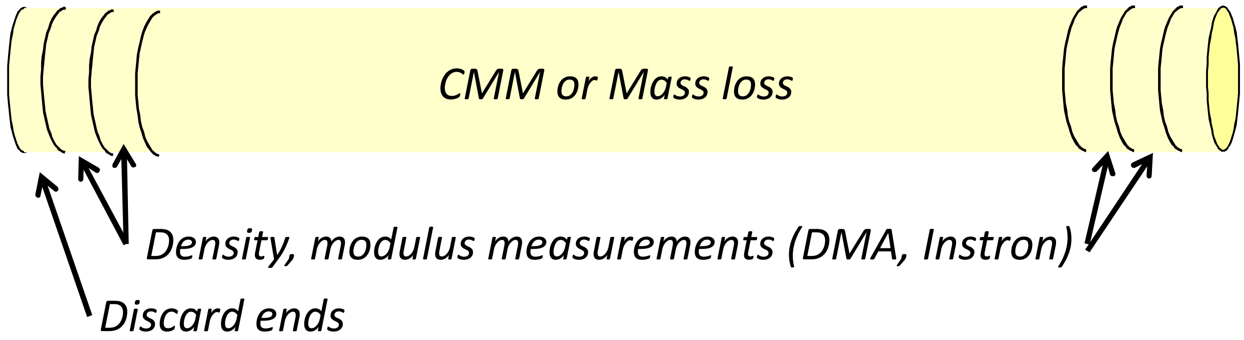
$$\frac{\dot{U}_2}{R_2} = \frac{f_0(4/3G + K)}{(4GK(1 - f_0)} \frac{d}{dt}(P_1 - P_2)$$

Rate of the Depressurization Volume Deformation at the Macroscale

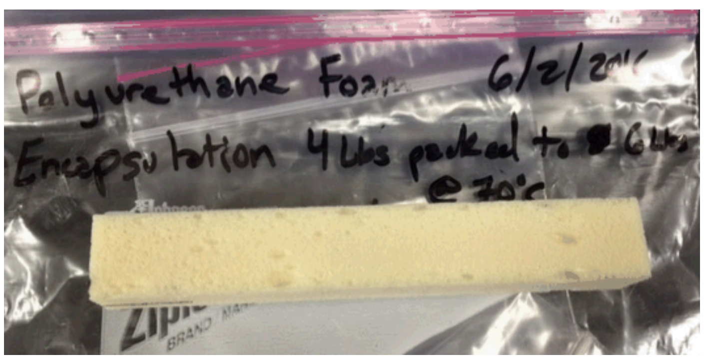
$$\mathbf{D}_d = \frac{\dot{U}_2}{R_2 + U_2}\mathbf{1} = \frac{\dot{U}_2/R_2}{1 + U_2/R_2}\mathbf{1}$$

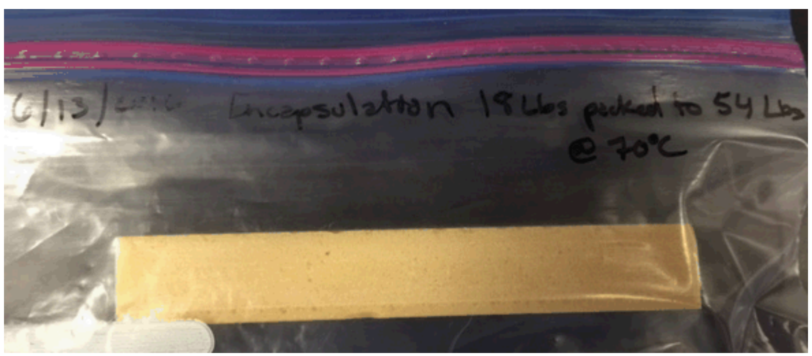
See Sokolnikoff, Timoshenko for the elasticity solution

Shrinkage and Mass Loss in Foam Cylinders



- ¾"X8" and 1"X8" cylinders (with skin) and machined to square cross-sections (without skins)
- Density from 6 to 54 pcf at different over packings





Shrinkage and Mass Loss in Foam Cylind

CMM measures dimensional changes

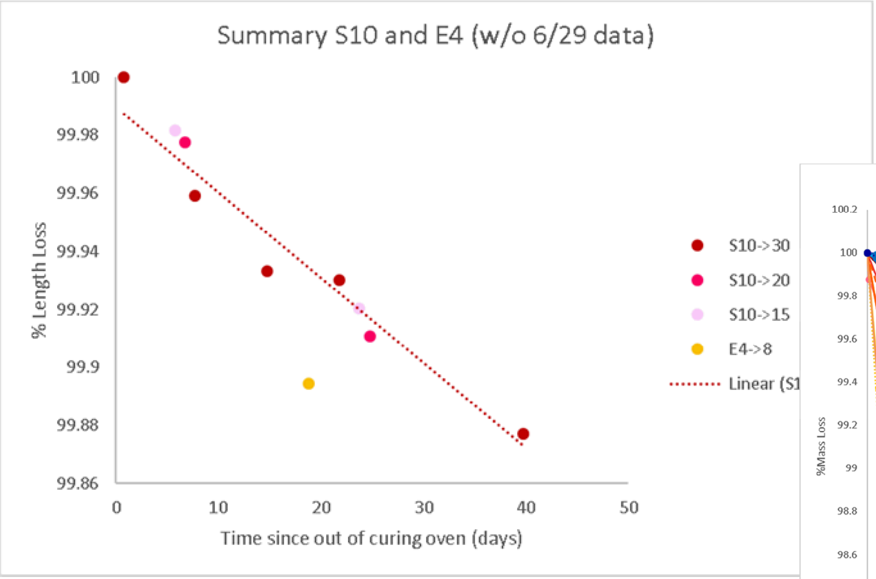
Manufacturing Process

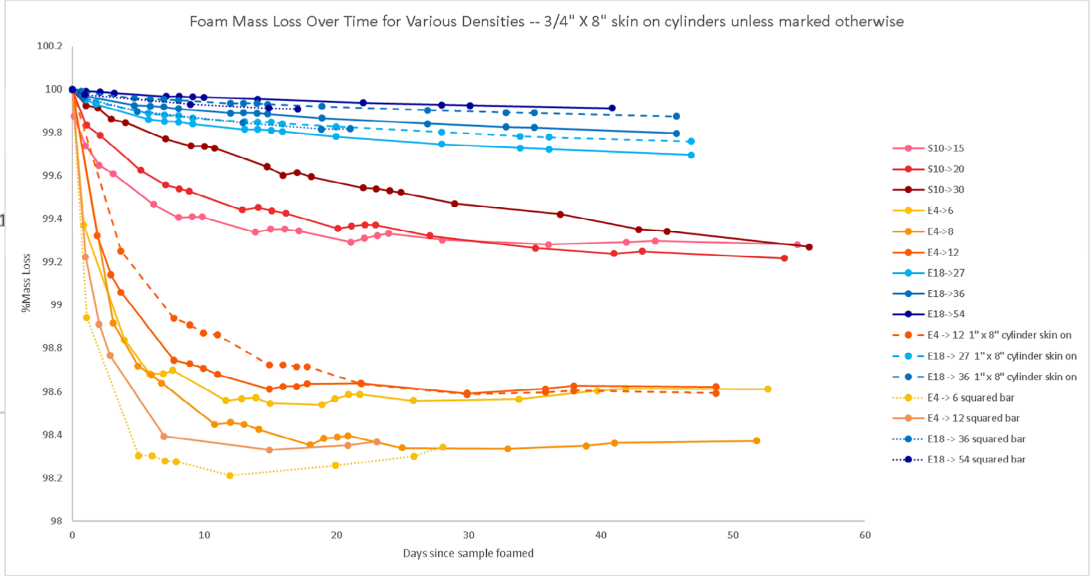
- PMDI foam injected at 40 °C, overpacked to various densities
- After 15 mins, cured in oven at 120 °C for 4 hrs

Dimensional Change via a Xyce Coordinate Measurement Machine (CMM)

Mass Changes Measured on a Milligram Scale at Room Temperature

Linear shrinkage seems less sensitive to density than mass loss in our limited data to date

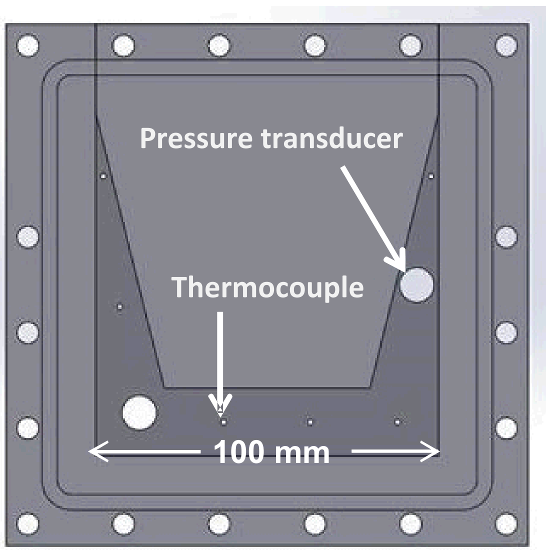




Shrinkage in a Relevant Geometry

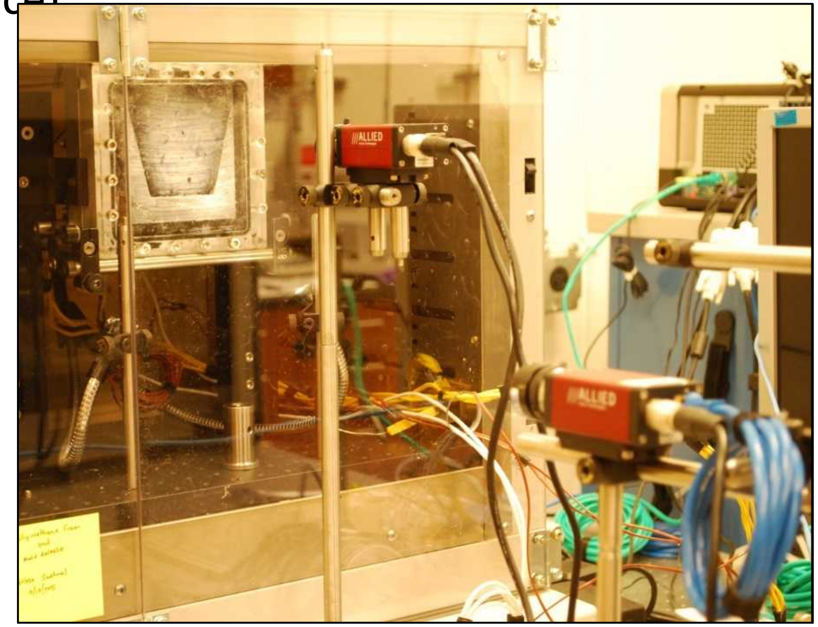
Goal: Quantify warpage over months to provide model validation data and physical insight

- Geometry involves both thin and bulky regions
- Initially, filling conditions approximate in-house cure schedule
  - **PMDI S10** foam injected at **40 ºC**, overpacked to **12.5 lb/ft^3**
  - After 15 mins, cured in oven at **121 ºC for 4 hrs**
  - Two separate filling orientations “C” and “U”
- Coordinate Measurement Machine (CMM by Xzyce)



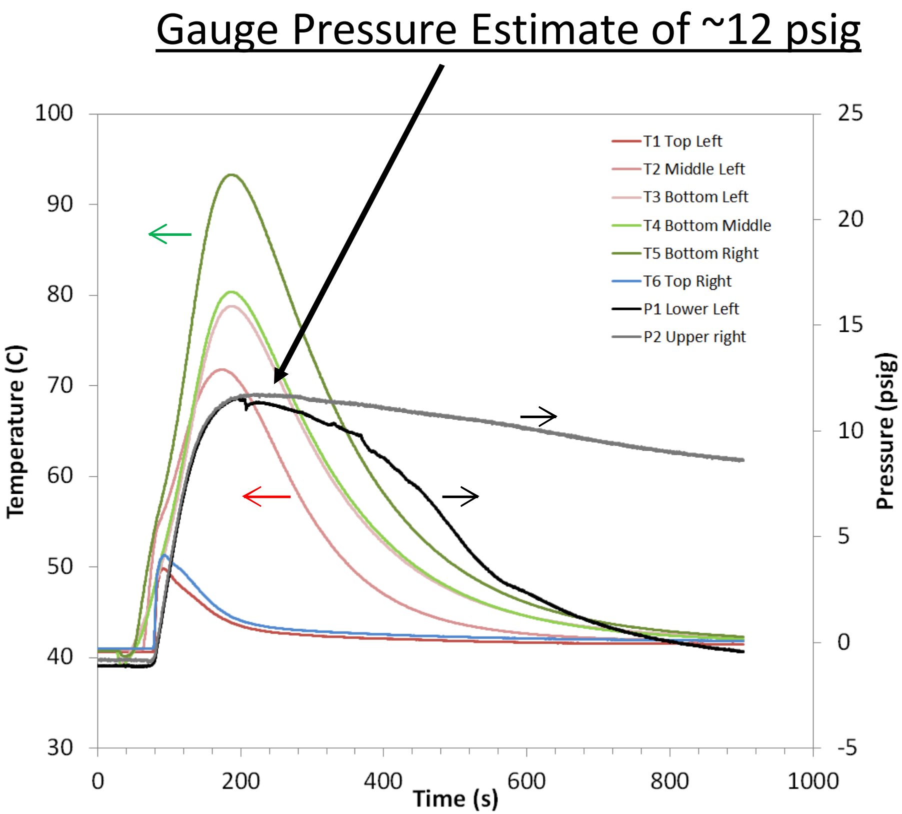
Ports for thermocouples and pressure transducers to record parameters during foaming.

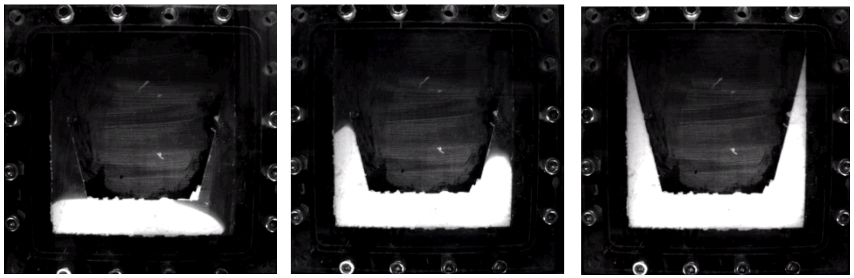
Fill filmed using cameras, transparent oven door



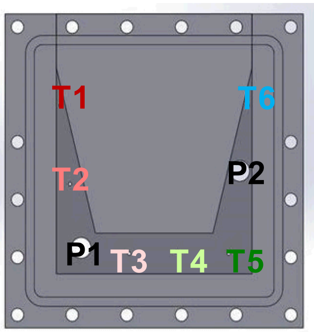
Foaming U-shaped staple mold

- Over many repeats, temperature, pressure, and flow profile are remarkably repeatable
- Imperfectly symmetric fill common
- Pressure rises as foam expands, relaxes at lower corner and stays positive at P2





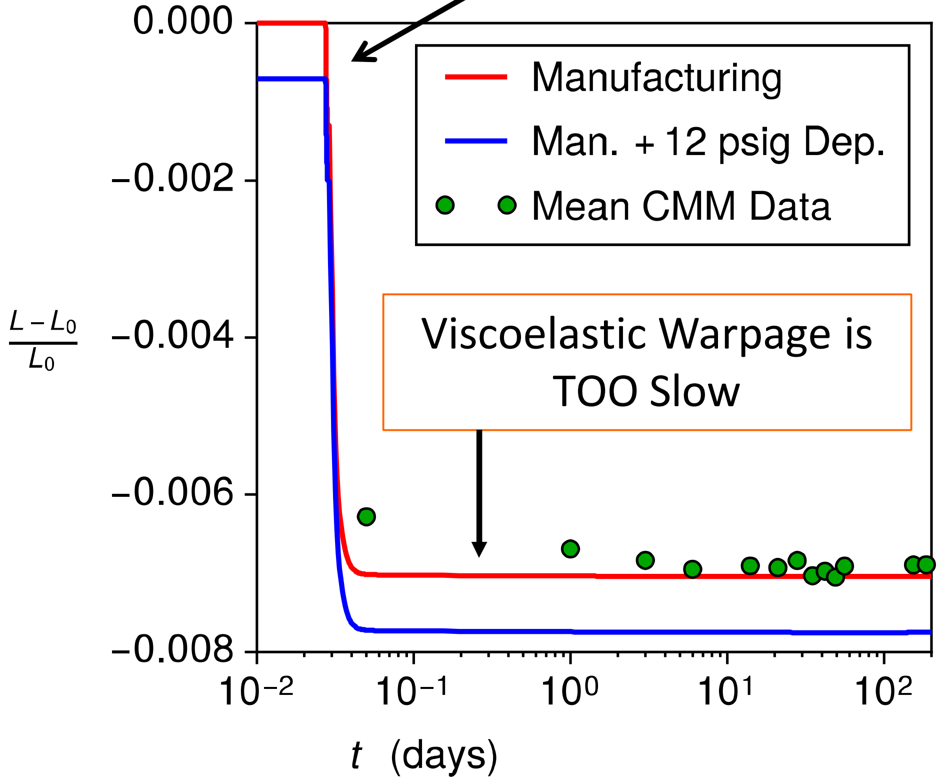
Some slight asymmetry due to bias of initial injection



Our First Hypothesis: Viscoelastic Relaxation of Residual Stress

Manufacturing → Cure Shrinkage + Boundary Conditions → Residual Stress Generation

Elastic Unload + Thermal-Contraction



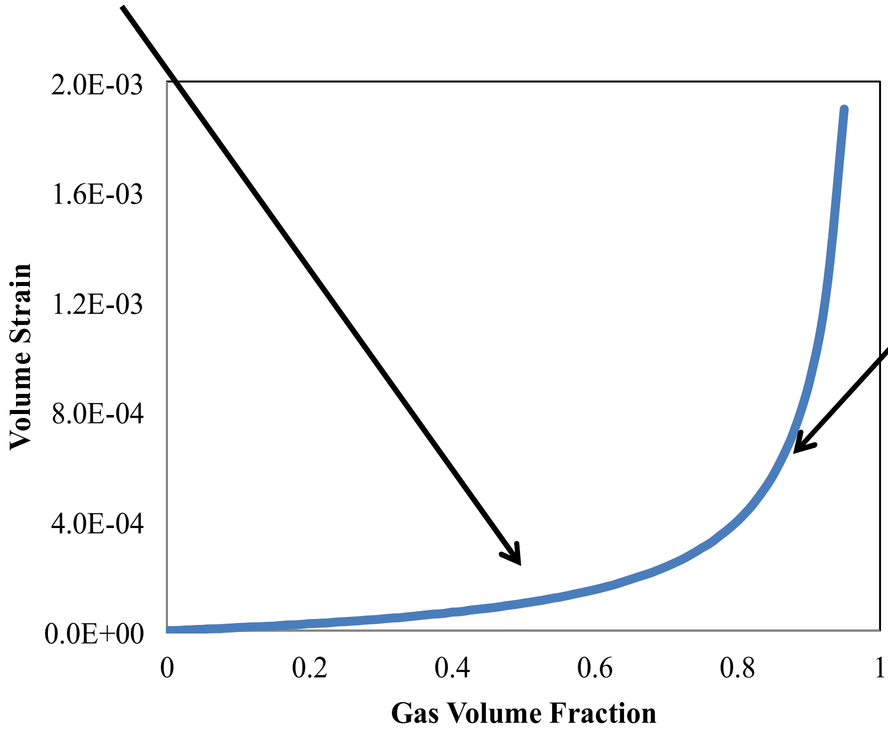
Model captures the elastic unload and cool-down reasonably well, but it misses the long term aging response

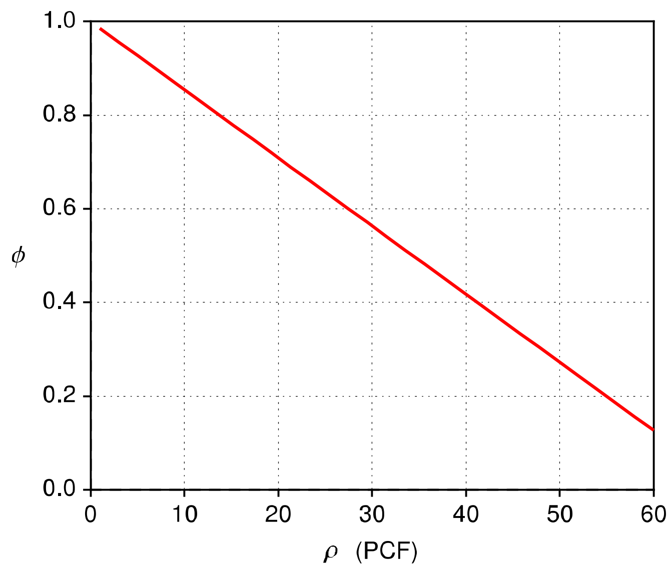
The Viscoelastic Time Scale is TOO Long (by a few orders of magnitude)

What about Bubble Depressurization?

Originally, we focussed on higher density foams: 40, 50, 55 PCF
→ Depressurization was insignificant

Below 20 PCF, it matters!





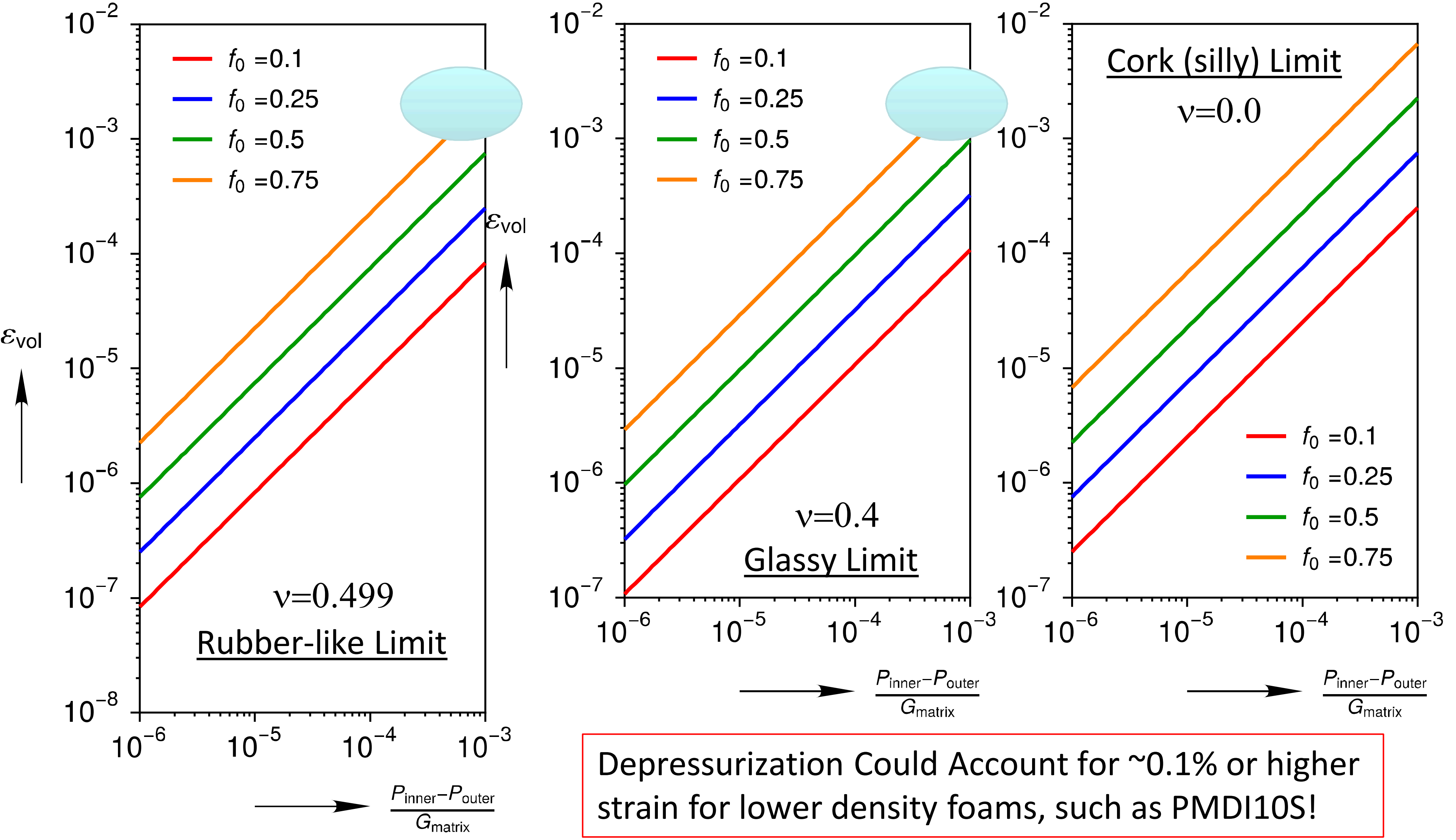
Bubble depressurization matters especially for smaller density (assuming a fixed gauge pressure…)

Consider Simple (Analytic) Depressurization Strains

- Imagine:
  - The foam is of uniform density (no voids, no skin)
  - The foam is initially in a state of uniform gauge pressure

- Ignoring the dynamics associated with CO_2 leaving the component, we can estimate the (isotropic) shrinkage strain a foamed component would experience as a function of:
  - Gauge pressure normalized by the matrix shear modulus (glassy shear modulus of the foam)
  - Poisson Ratio of the Matrix Phase
  - Porosity (Void Volume Fraction)

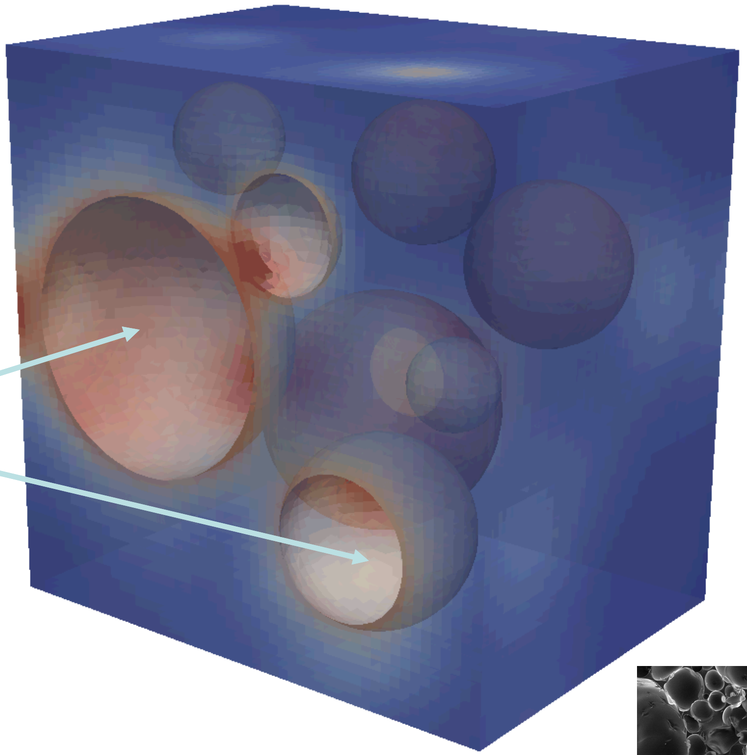
Consider Simple (Analytic) Depressurization Strains

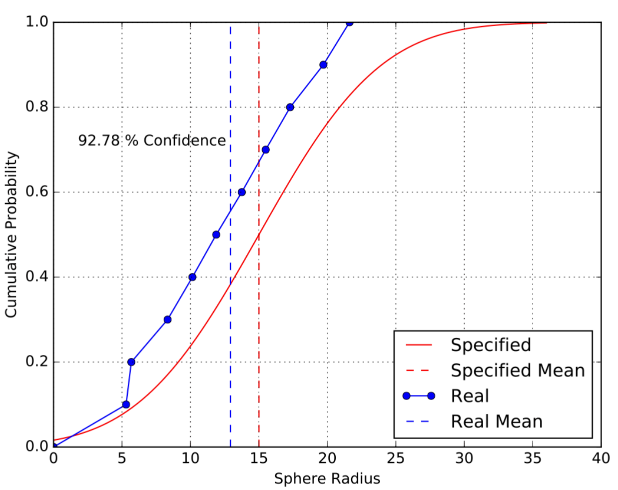


Depressurization Could Account for ~0.1% or higher strain for lower density foams, such as PMDI10S!

Micromechanics Validation of the Analytic Model

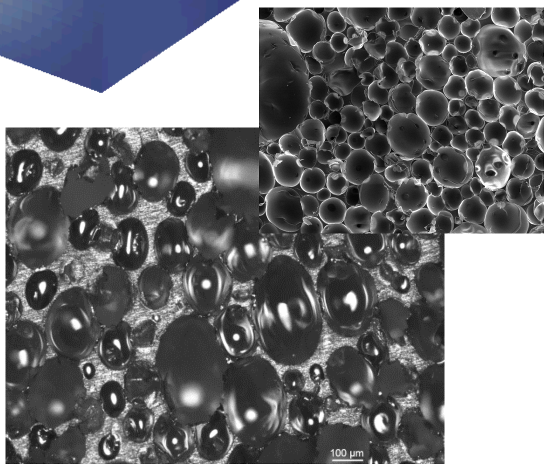
- Prescribed porosity
- Depressurization from 20 psig applied to pores



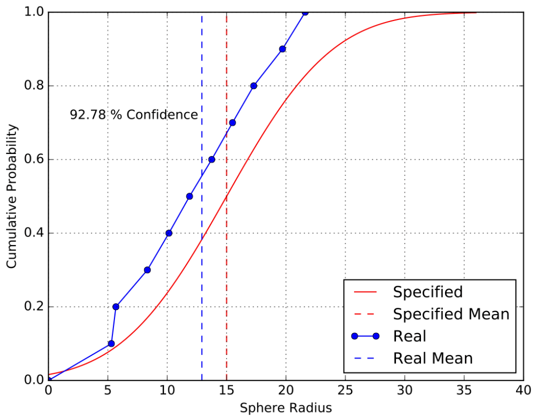


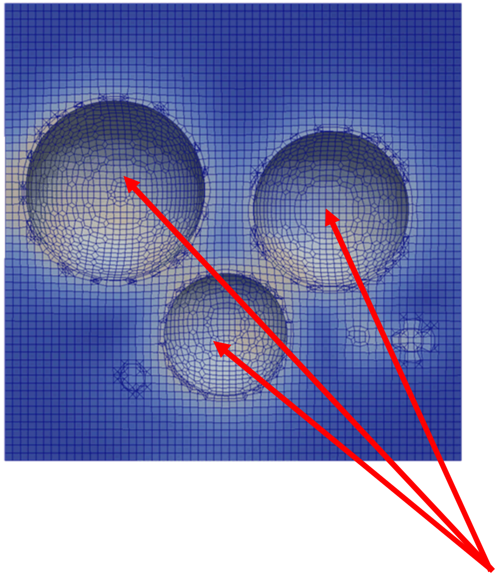
Different size distributions

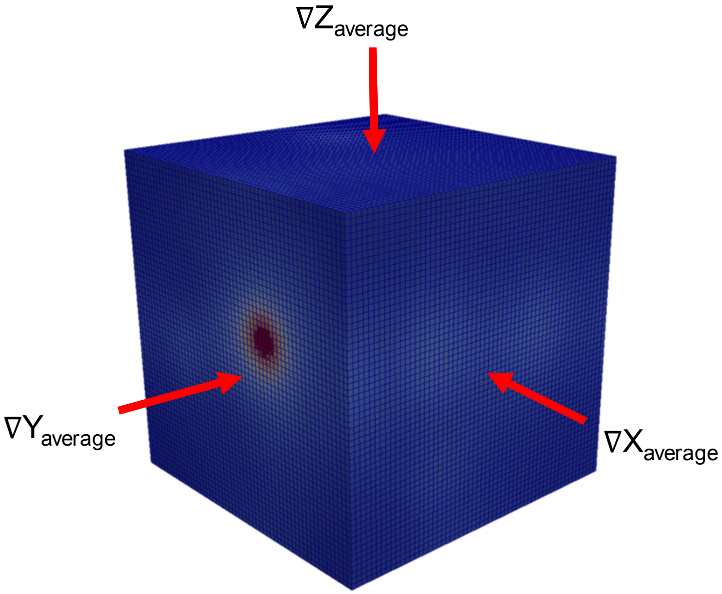
- Gaussian, Uniform



Micromechanics Validation of the Analytic Model







Pore geometries generated for multiple porosities (Gaussian distribution)

→

Porous cubes created and meshed

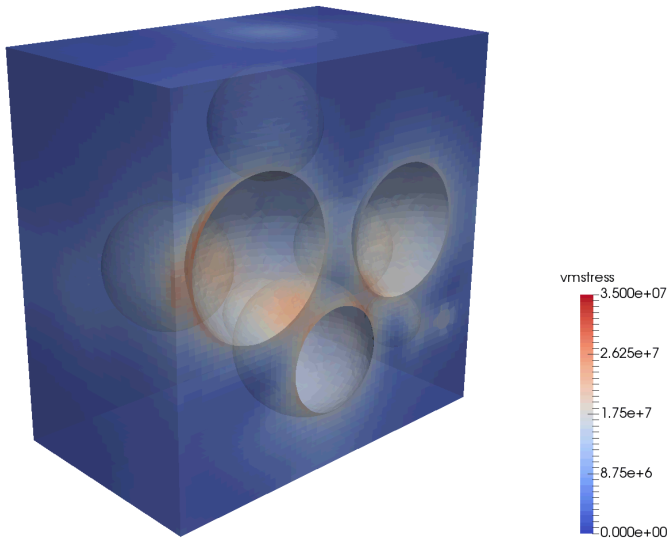
→

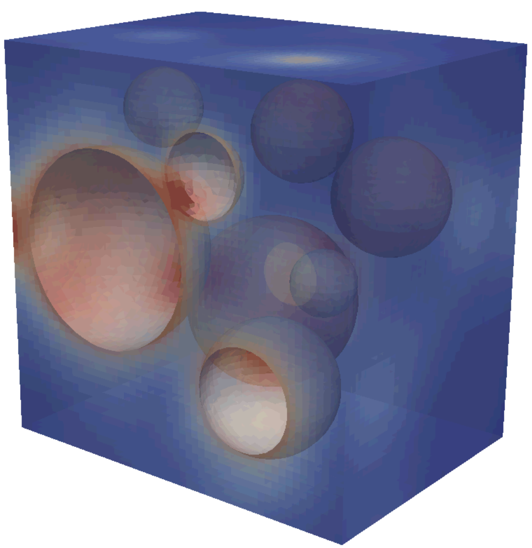
Decreasing gauge pressure applied to pore surfaces

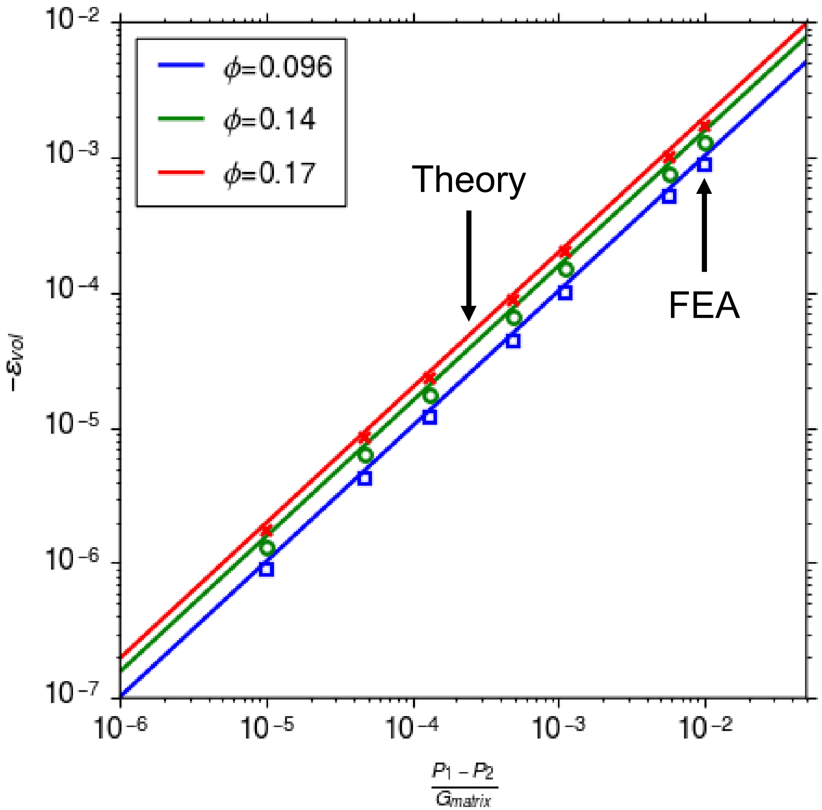
→

Volume strains calculated

Micromechanics Validation of the Analytic Model

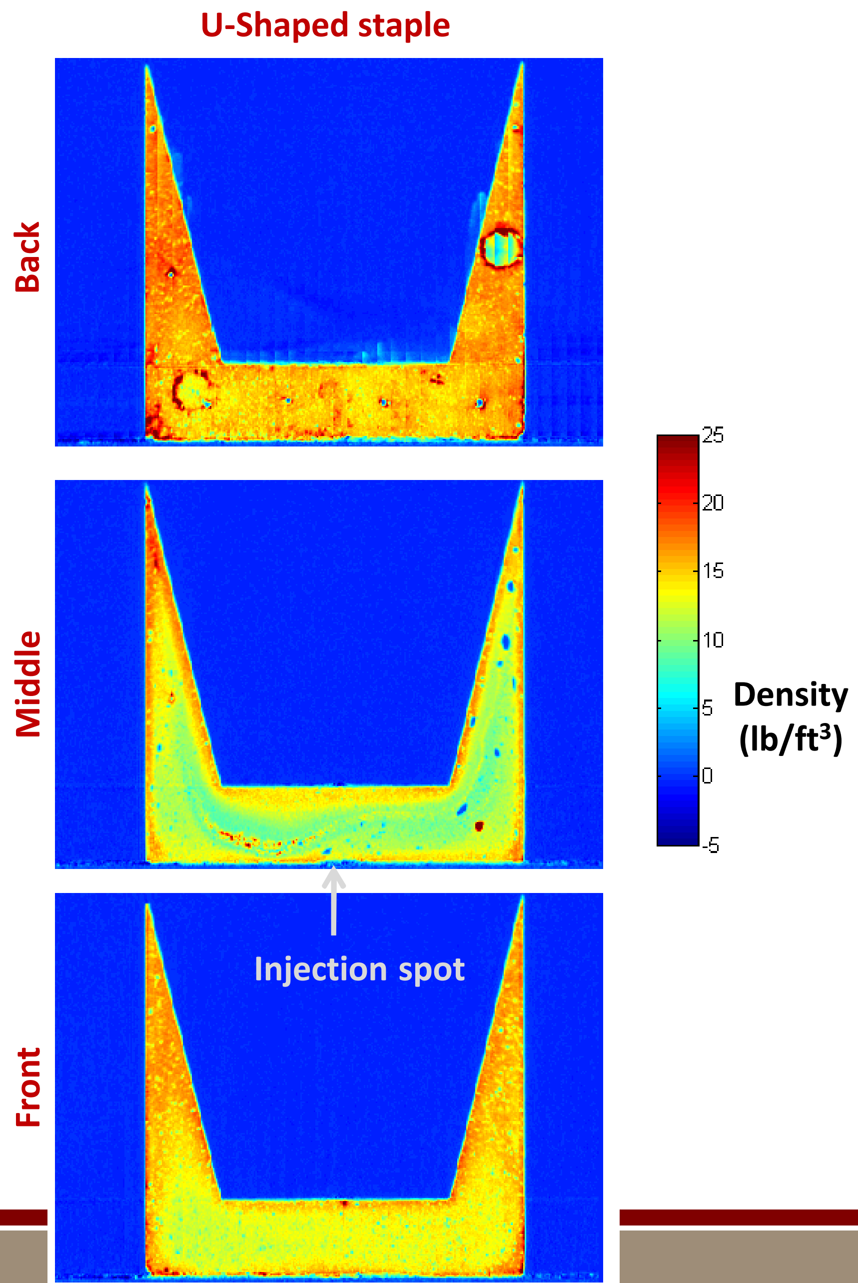






At low porosities, where the analytic model is less likely to perform well, we have good agreement between the micromechanics FEA and Analytic Shell Model
→ *The Analytic Model Reasonable Well Represents Deformation Due to Depressurization for Isotropic Foams*

Density is important! Let's measure it with X-ray CT



A skin is apparent (25 lb/ft³), whereas the interior density is as low as 7 lb/ft³

Large voids-- primarily in the arms of the staple.

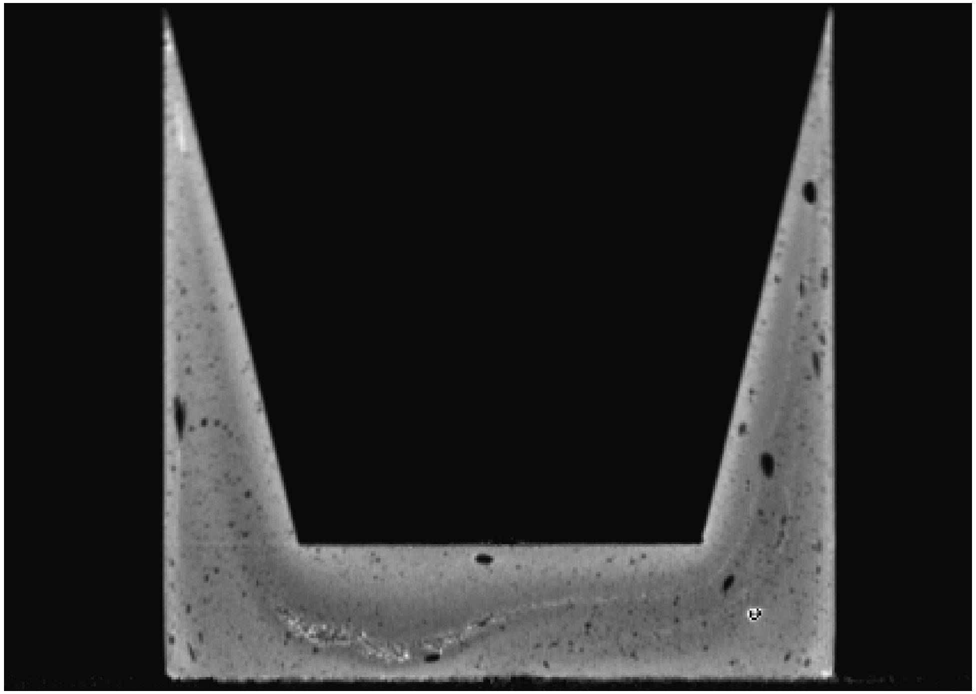
- Coalescence seen in other thin PMDI samples
- Larger numbers of voids in C-shaped staple (more shear overall)

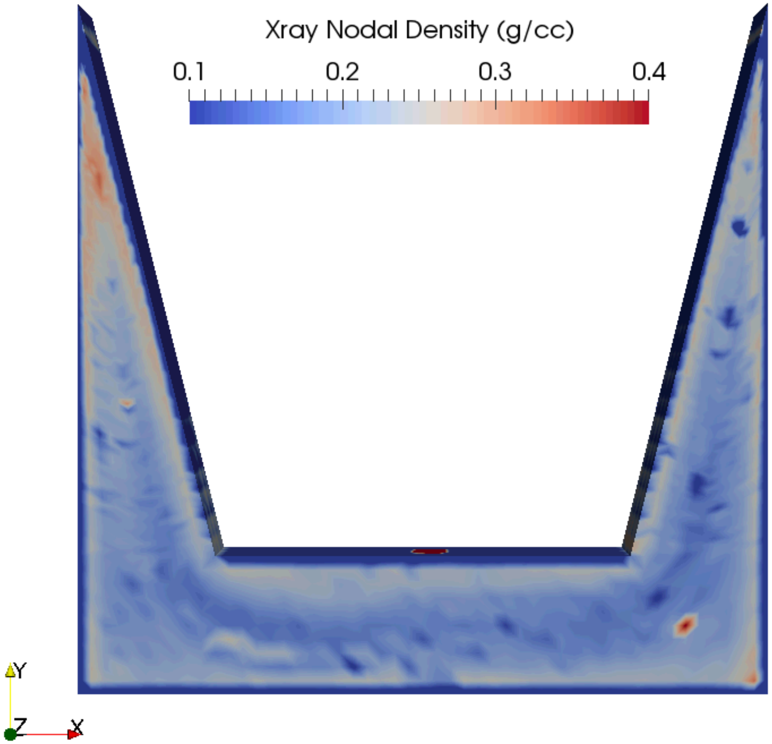
Large bubbles could be source of pressure decay not predicted by model

Focus on bottom portion for shrinkage measurements

Initial Calculations of the U-staple

- Non-Uniform Density from X-ray CT
- Uniform Depressurization (12 PSIG)





Mid-plane Cross-section showing the raw data (X-ray CT) and the Interpolated Nodal Data (Field Input to the Simulation)

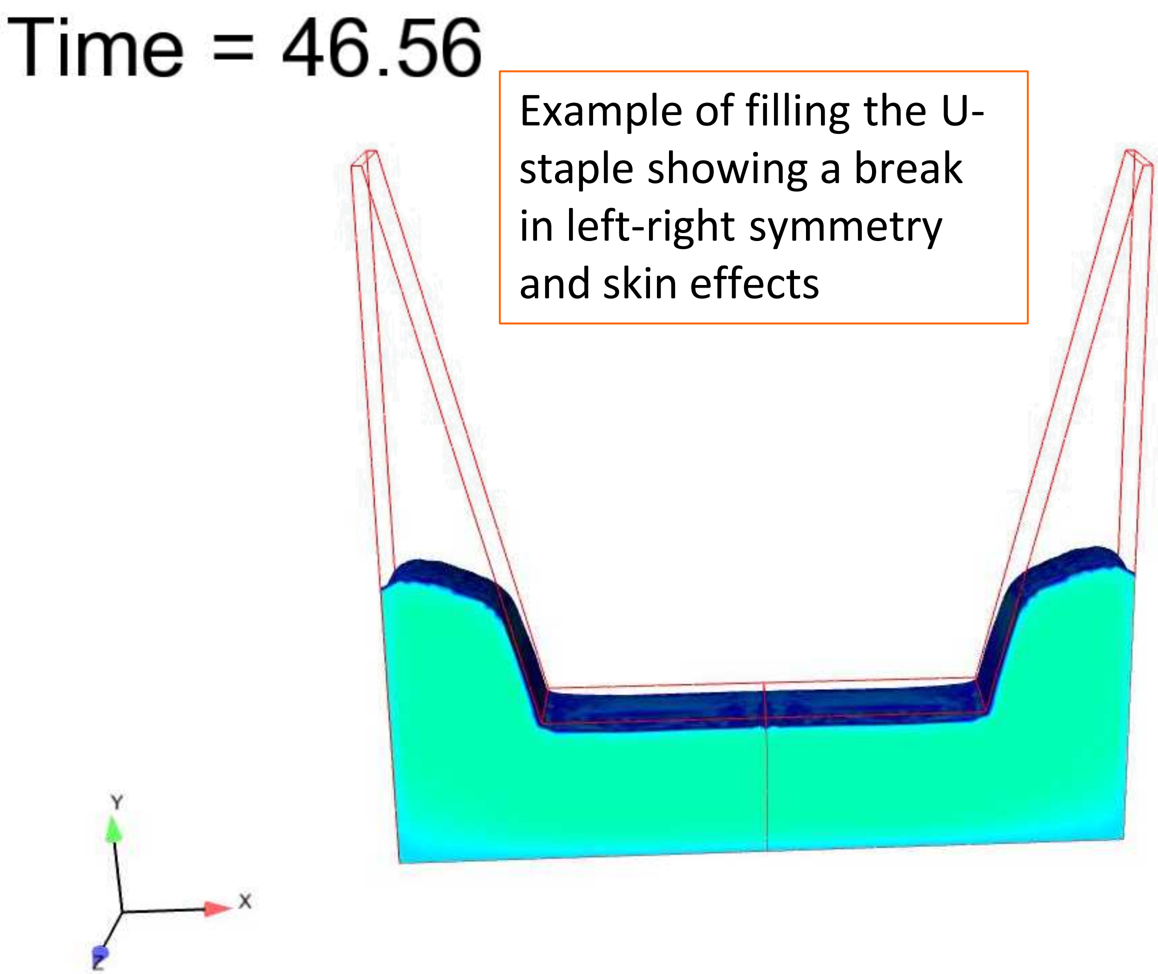
Conclusions

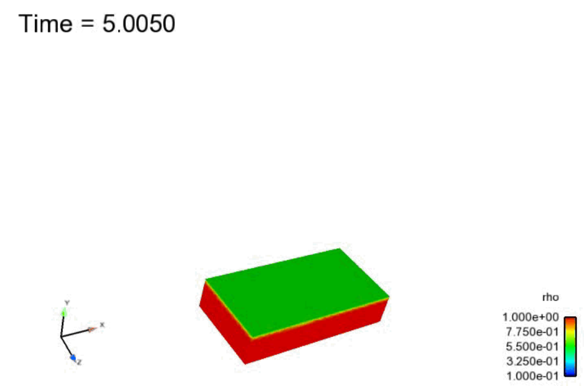
- Viscoelasticity and Residual Stress relaxation properly account for the majority of the warpage due to manufacturing
  - The Time Scale for Continued warpage is too slow from this mechanism compared with our experimental data
- Bubble depressurization results in warpage over the right time scale (according to the literature), but the magnitude of warpage is a strong function of the bubble gauge pressure
  - How do we measure this?
  - Are the moduli of the PU matrix phase a function of the CO2 concentration?
- Is the CMM machine the most robust method for monitoring warpage in soft materials?

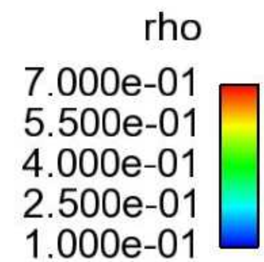
Future Efforts: Mold Filling Simulations That Better Predict Density and Gauge Pressure

Example of filling the U-staple showing a break in left-right symmetry and skin effects

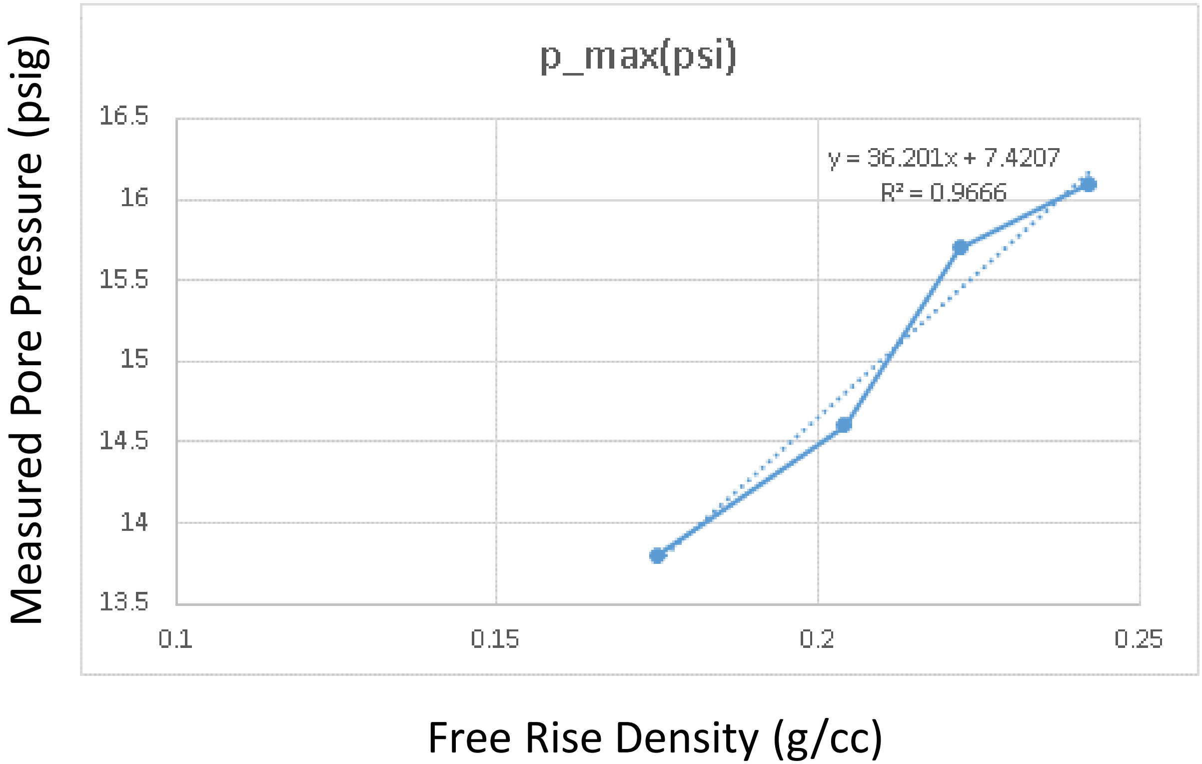
Quarter Symmetry Filling Example







Determine How Gauge Pressure Depends on the Free Rise Density and Overpacking



How Much Displacement Does the CMM Probe Cause During Contact?

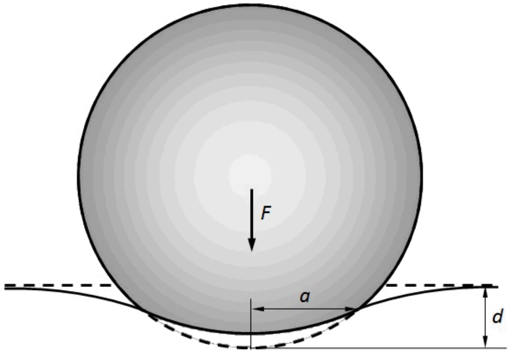
- 100 mN Force Probe Force
- ASSUME the metallic sphere is <u>much</u> stiffer than the foam
- Foam Young's Modulus of Approximately 300 Mpa for glassy 10 PCF PMDI10S Foam

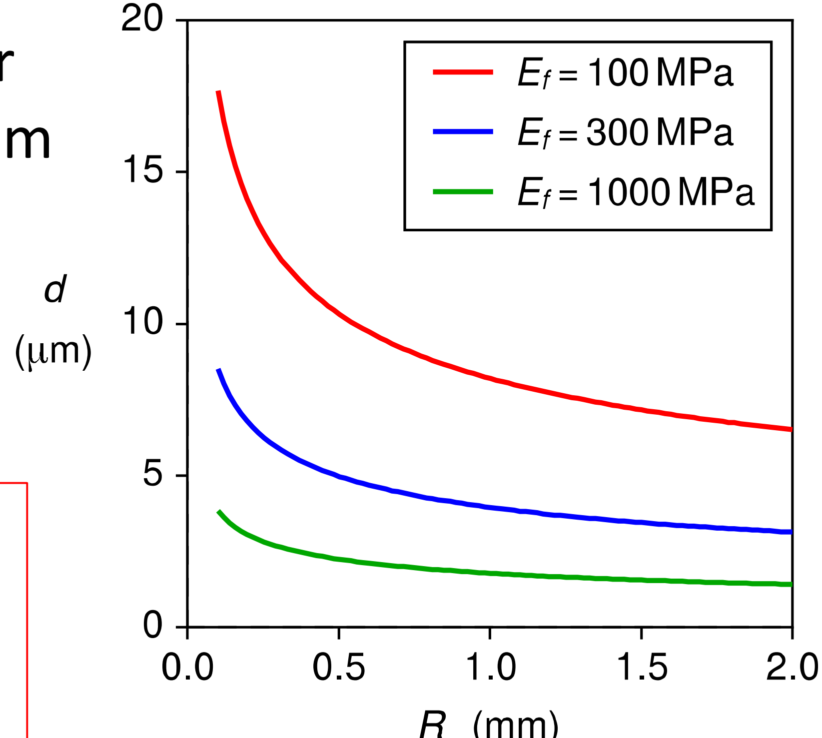
$$d = \left(\frac{9F^2}{16E_*^2R}\right)^{1/3}$$

$$\frac{1}{E_*} = \frac{1-\nu_1^2}{E_1} + \frac{1-\nu_2^2}{E_2} \approx \frac{1-\nu_2^2}{E_2}$$

Depending on the foam density (Young's Modulus), the apparent "strain" for the Staple 10 cm span due to probe indentation ranges from 4E-5 to 1.6E-4…These Are HUGE

Hertz Contact Solution[1]



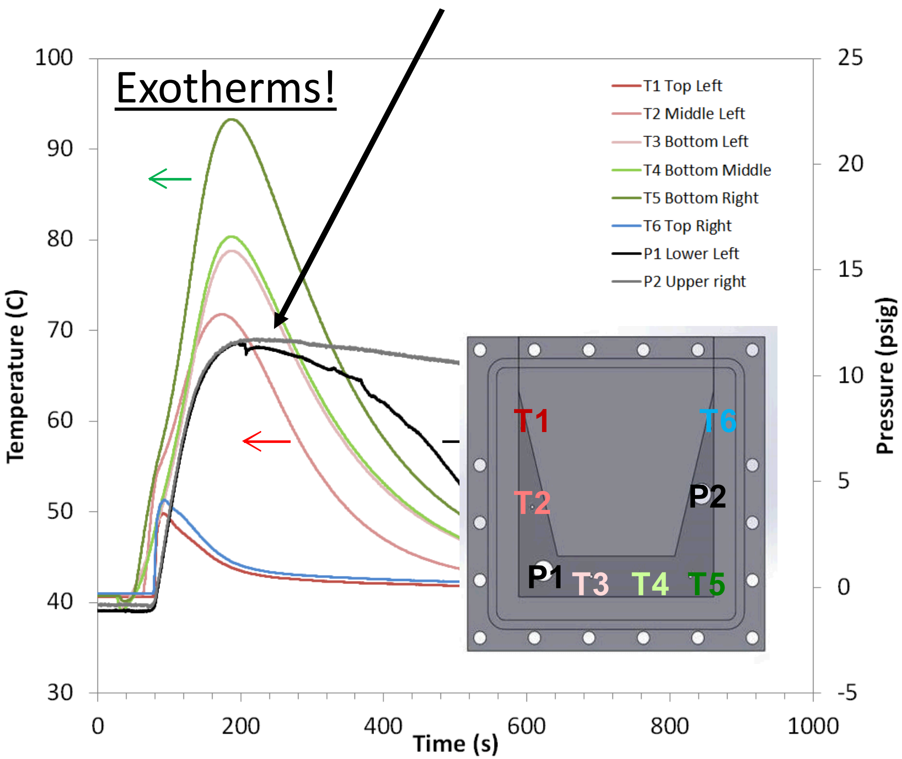


[1]Wikipedia: Contact Mechanics

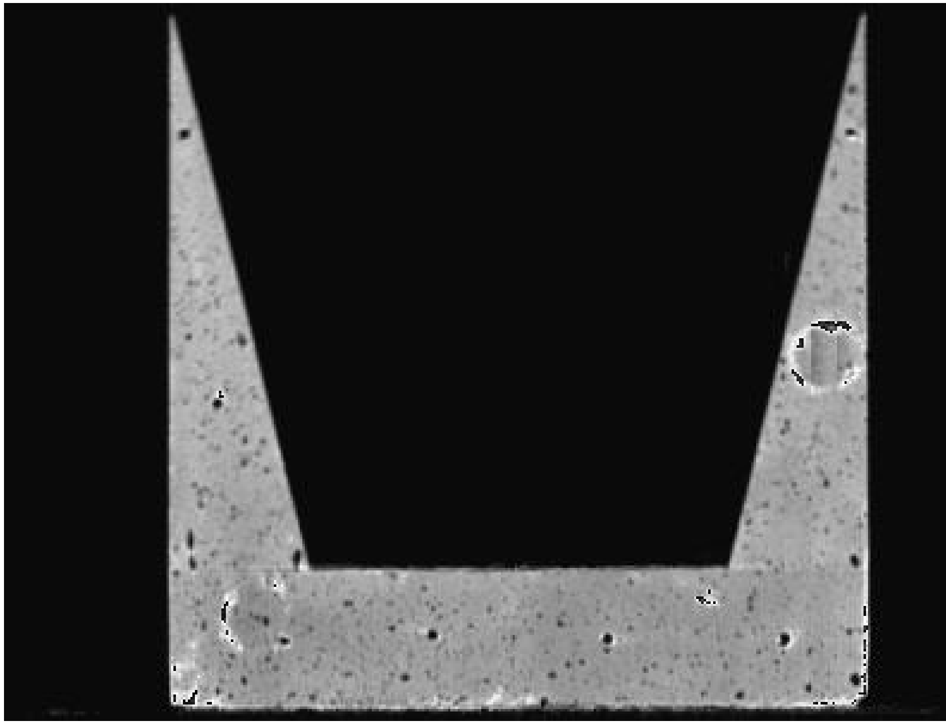
Foaming U-shaped staple mold

- Over many repeats, temperature, pressure, and flow profile are remarkably repeatable
- Imperfectly symmetric fill common
- Pressure rises as foam expands, relaxes at lower corner and stays positive at P2

Gauge Pressure Estimate of ~12 psig



Significant Density Variation Exists from Near Free-Rise Conditions AND Injection Process



Chemical and Physical Processes from Manufacture to Component Aging

Sandia National Laboratories

Stage I

Fluid

Pre-Gel Foam Filling
(0-10^3 seconds)

Chemistry:
-gas production (foaming)
-matrix polymerization (curing)

Foaming liquid expands to fill the mold until polymer matrix gelation

Gelation

Stage II

Soft-Solid

Post-Gel Curing
(10^3– 10^4 seconds)

Temperature and flow variation cause variations in density and extent of cure

Solid polymer matrix locks in density gradients

Further gas production pressurizes pores with minimal volume increase

Vitrification

Stage III

Solid

Cooling and Demolding
(10^4-10^5 seconds)

Continued cure attenuates as the foam vitrifies

Boundary conditions strongly influence residual stresses

Stage IV

Solid

Long-Term Aging
(10^5 + seconds)

Material warps post-manufacturing from:

Moisture uptake, swelling, and continued chemistry

Reactive Fluid State
See Rekha Rao's Talk

Solid State Curing and Vitrification:
Residual Stress Development and Initial Acceptance Testing

Physical Aging
Depressurization
Chemical Aging