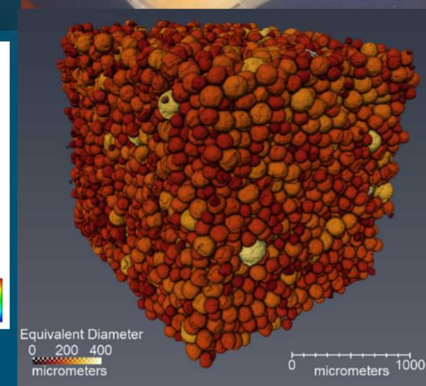
SAND2019-14212PE

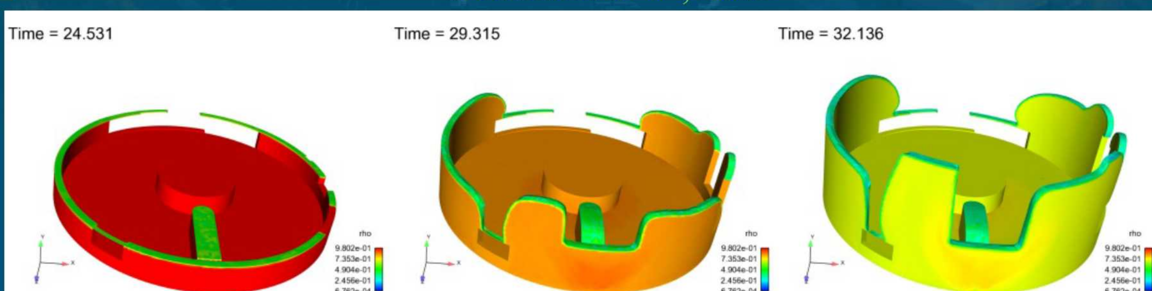
Foam process models for polyurethane, including blowing and curing kinetics



Evonik Meet Science, North America 2019

Philadelphia, Pennsylvania

December 5-6th, 2019



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SAND2019-????

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Polyurethane foams are widely used in manufacturing due to ease of use and useful material properties

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Horia Varlan (CC-BY-2.0)

We are developing models that can predict foam mold filling, void location, and final properties including density and modulus for structural foams and thermal conductivity for insulating material.

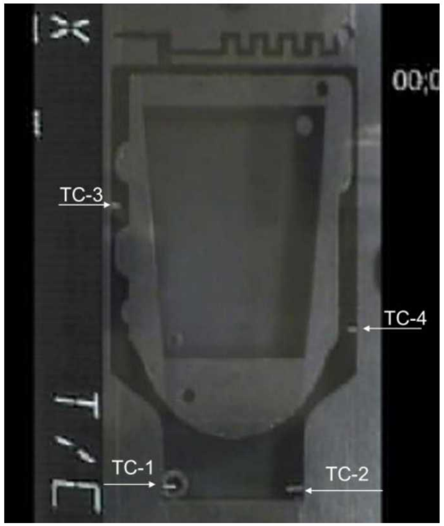
Introduction

Overarching Goal: **Cradle-to-grave model for foaming, vitrification, cure, aging**

Focus on moderate density PMDI foams

Injection, foaming and initial curing at lower T

Oven time at higher T to make sure it is fully cured



Remove from mold – predict cure and thermal stresses

Predict shape and size over years

Introduction

Stage I
Fluid

Pre-Gel
($0\text{-}10^3$ seconds)

Chemistry results in both gas production (foaming) and matrix polymerization (curing)

Foaming liquid rises to fill the mold until polymer matrix gelation

Heat, pressure generated

Gelation

Stage II
Soft-Solid

Post-Gel Cure
(10^3– 10^4 seconds)

Variations in temperature cause variations in density and extent of cure

Solid polymer matrix locks in density gradients

Further gas production causes bubble pressurization with minimal volume increase

Vitrification

Stage III
Solid

Vitrified and Released
(10^4 + seconds)

Residual stresses, density, and properties vary spatially

Both long and short term shape change is possible as different parts of the foam relax at different rates

Boundary conditions strongly influence residual stresses

- Processing parameters at earlier stages will affect quality of part at later stages

Foam Filling is Complex

Foam front moving past camera, with bubble sizes at transparent wall determined with image processing.

3 views of foam filling a mock AFS with several plate spaced unevenly. Vent location is critical to keep from trapping air.

- PMDI is used as an encapsulant for electronic components and lightweight structural parts, to mitigate against shock and vibration.
- **We would like to develop a computational model to help us understand foam expansion for manufacturing applications and how inhomogeneities effect the structural response of the final part, including long term shape stability.**
- Gas generation drives the foam expansion, changing the material from a viscous liquid to a multiphase material.
- Continuous phase is time- and temperature-dependent and eventually vitrifies to a solid.

Polyurethane (PMDI): Model Development

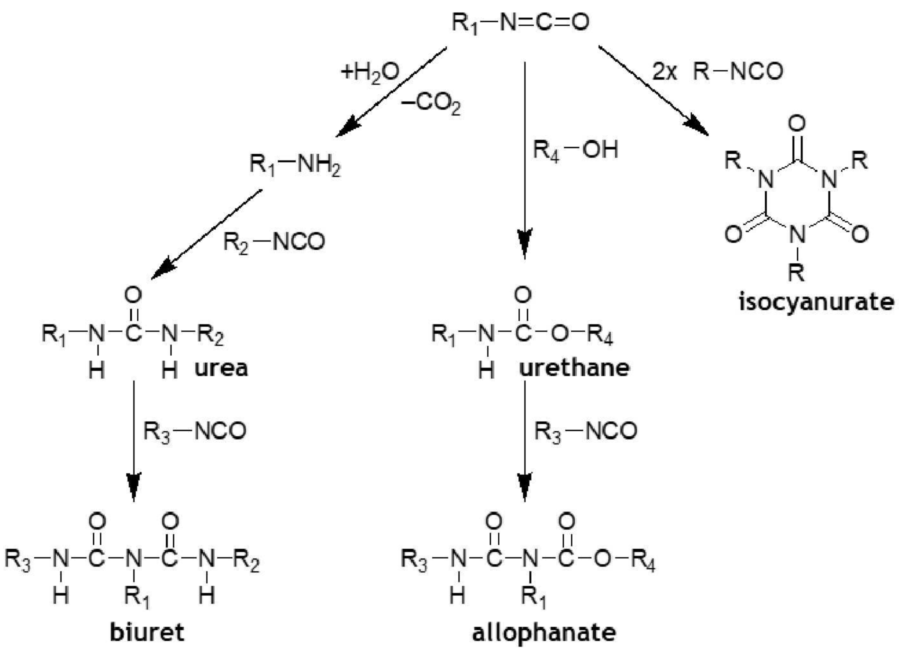
We use a variety of physically and chemically blown foams. PMDI is used as an encapsulant for electronic components, to mitigate against shock and vibration, and to make light-weight structural parts.

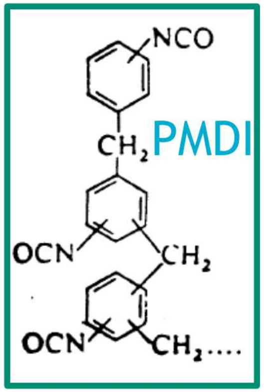
We would like to develop a computational model to help us understand foam expansion for manufacturing applications.

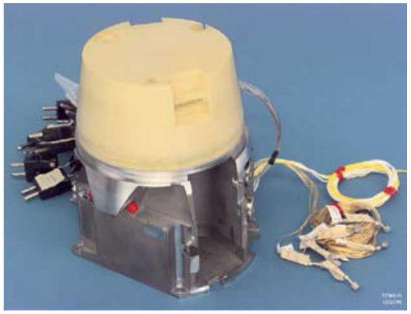
Polyurethane is a chemically blown foam having two primary, competing simultaneous reactions: CO_2 production and polymerization. Separating these reactions can be difficult.

We use IR spectroscopy to track polymerization. IR does not provide a clear signal for the foaming reaction: Tracked with volume generation.

PU has a short pot-life: models can help reduce defects and improve filling process







Mock component encapsulated with PMDI from "KCP Encapsulation Design Guide" (Mike Gerding, UUR)

Kinetic Model Must Include CO_2 Generation and Polymerization Reaction

$$rate_1 = k_1 e^{-\Delta E_1/RT}[isocyanate]^a[polyol]^b$$ **Polymerization**

$$rate_2 = k_2 e^{-\Delta E_2/RT}[isocyanate]^c[H_2O]^d$$ **CO_2 generation**

- Must track five species: water, polyol, polymer, carbon dioxide, and isocyanate , since we have competing primary reaction
- Use experiments to determine Arrhenius rate coefficients

$$\frac{D[CO_2]}{Dt} = +rate_2$$

$$\frac{D[H_2O]}{Dt} = -rate_2$$

$$\frac{D[isocyanate]}{Dt} = -rate_1 - rate_2$$

$$\frac{D[polyol]}{Dt} = -rate_1$$

$$\frac{D[polymer]}{Dt} = +rate_1$$

- Must provide initial conditions for all species
- Integrate rate equations as part of the simulation
- Density predicted from gas generation
- Our kinetics are unique because our formulation is different from literature polyurethanes

$$\rho_{gas} = \frac{PM_{CO_2}}{RT}$$

$$v = \frac{V_{gas}}{V_{liq}} = \frac{M_{CO_2} C_{CO_2}}{\rho_{gas}} \qquad \phi_v = \frac{v}{1+v}$$

$$\rho_{foam} = \rho_{gas}\phi_v + \rho_{liq}(1-\phi_v)$$

Equations of Motion Include Evolving Material Models

Momentum equation and continuity have variable density, shear viscosity, and bulk viscosity

$$\rho \frac{\partial \mathbf{v}}{\partial t} = -\rho \mathbf{v} \bullet \nabla \mathbf{v} - \nabla p + \nabla \bullet (\mu_f (\nabla \mathbf{v} + \nabla \mathbf{v}^t)) - \nabla \bullet \lambda (\nabla \bullet \mathbf{v}) I + \rho \mathbf{g}$$

$$\frac{D\rho_f}{Dt} + \rho_f \nabla \bullet \mathbf{v} = 0$$

Energy equation has variable heat capacity and thermal conductivity including a source term for heat of reaction for foaming and curing reactions

$$\rho C_{pf} \frac{\partial T}{\partial t} + \rho C_{pf} v \bullet \nabla T = \nabla \bullet (k \nabla T) + \rho \varphi_e \Delta H_{rxn} \frac{\partial \xi}{\partial t}$$

Extent of reaction equation for polymerization: condensation chemistry

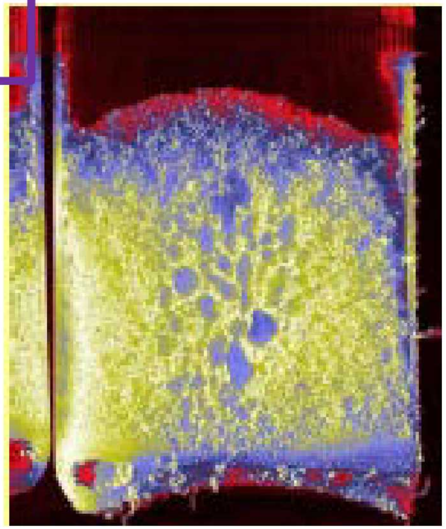
$$\frac{\partial \xi}{\partial t} = \left(\frac{1}{(1 + wa)^{\beta}} \right) \left(k_0 \exp\left(-\frac{E}{RT} \right) \right) (b + \xi^m)(1 - \xi)^n$$

Molar concentration equations for water and carbon dioxide

$$\frac{dC_{H_2O}}{dt} = -k_{H_2O} C_{H_2O}^n \qquad C_{H_2O} = \frac{\rho_{foam} x_{H_2O}}{M_{H_2O}}$$

$$\frac{dC_{CO_2}}{dt} = +k_{H_2O} C_{H_2O}^n \qquad C_{CO_2} = \frac{\rho_{foam} x_{CO_2}}{M_{CO_2}}$$

$$k_{H_2O} = A_{H_2O} \exp(-E_{H_2O} / RT)$$



NMR imaging shows coarse microstructure (Altobelli, 2006)

Complex Material Models Vary with Cure, Temperature, and Gas Fraction

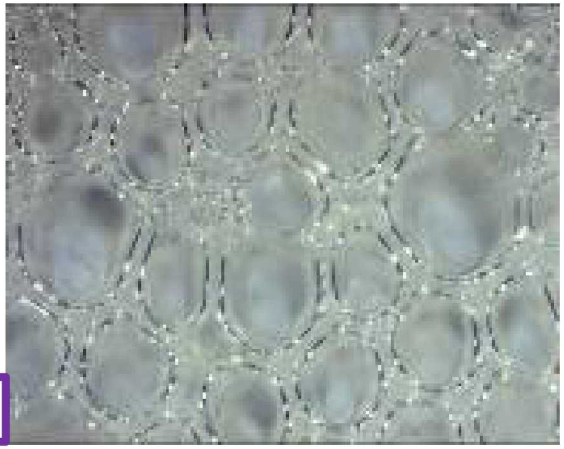
Foaming reaction predicts moles of gas from which we can calculate density

$$\rho_{gas} = \frac{PM_{CO_2}}{RT}$$

$$v = \frac{V_{gas}}{V_{liq}} = \frac{M_{CO_2} C_{CO_2}}{\rho_{gas}} \qquad \phi_v = \frac{v}{1+v}$$

$$\rho_{foam} = \rho_{gas}\phi_v + \rho_{liq}(1-\phi_v)$$

Slight compressibility built into this model via the ideal gas law for gas density



Thermal properties depend on gas volume fraction and polymer properties

$$k = \frac{2}{3}\left(\frac{\rho}{\rho_e}\right)k_e + \left(1-\frac{\rho}{\rho_e}\right)k_v$$

$$C_{pf} = C_{pl}\phi_l + C_{pv}\phi_v + C_{pe}\phi_e$$

Foam is a collection of bubbles in curing polymer

Shear and bulk viscosity depends on gas volume fraction, temperature and degree of cure

$$\mu = \mu_0 \exp\left(\frac{\varphi_v}{1-\varphi_v}\right) \qquad \mu_0 = \mu_0^0 \exp\left(\frac{E_\mu}{RT}\right)\left(\frac{\xi_c^{\,p} - \xi^{p}}{\xi_c^{p}}\right)^{-q}$$

$$\lambda = \frac{4}{3}\mu_0 \frac{(\phi_v - 1)}{\phi_v}$$

- Experiments to determine foaming and curing kinetics as well as parameters for model
- Equations solved with the finite element method using a level set to determine the location of the free surface (Rao et al., IJNMF, 2012)

M. Mooney, *J. Colloid Sci.*, **6**, 162-170 (1951).

Gibson, L. J.; M. F. Ashby. Cambridge University Press, Cambridge, UK, 1990

Extent of Reaction for Polymerization

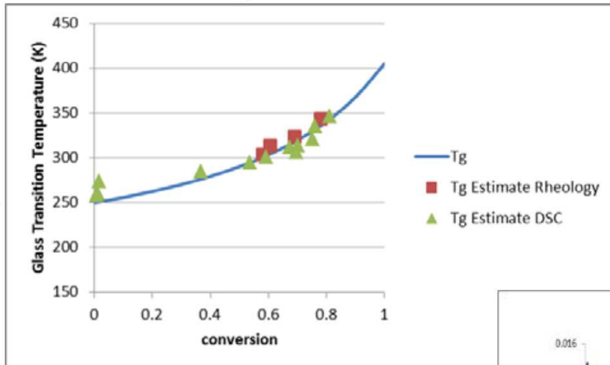
- Fit the rate and the extent of reaction to IR data to a standard equation form
- Fit T_g to both rheology and DSC data: T_g changes as cure progresses making this complex

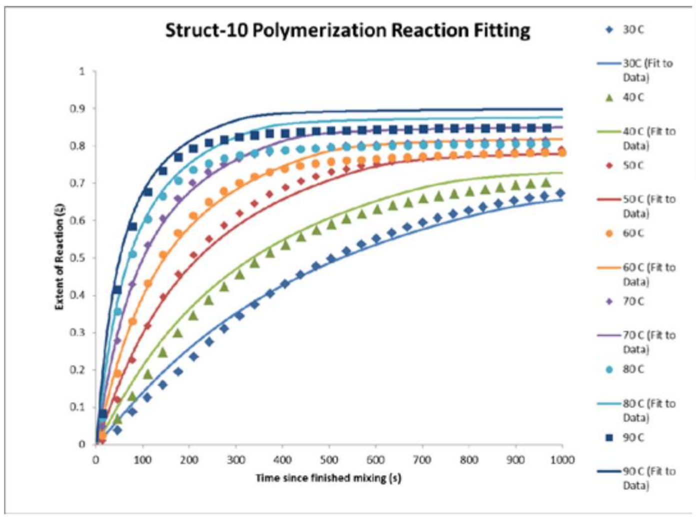
$$\frac{\partial \xi}{\partial t} = \left(\frac{1}{(1+wa)^{\beta}}\right)\left(k_0 \exp\left(-\frac{E}{RT}\right)\right)\left(b+\xi^m\right)(1-\xi)^n$$

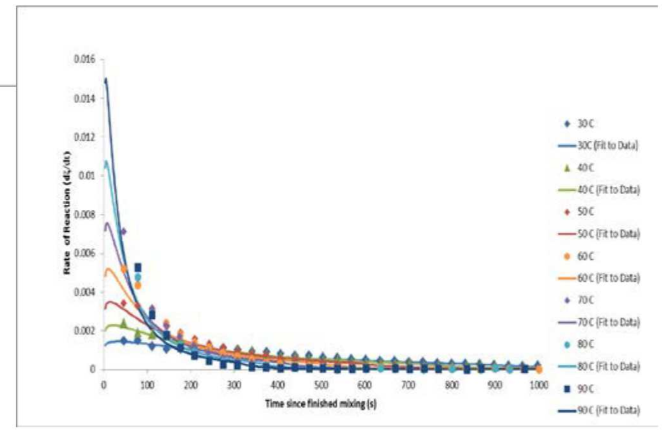
$$\log_{10} a = \frac{-C_1\left(T-T_g\right)}{C_2+T-T_g}$$

$$T_g = \frac{T_{g0}(1-\xi)+A\xi T_{g\infty}}{(1-\xi+A\xi)}$$

- New form captures arrest of reaction below the glass transition temperature (T_g evolves with extent of reaction)







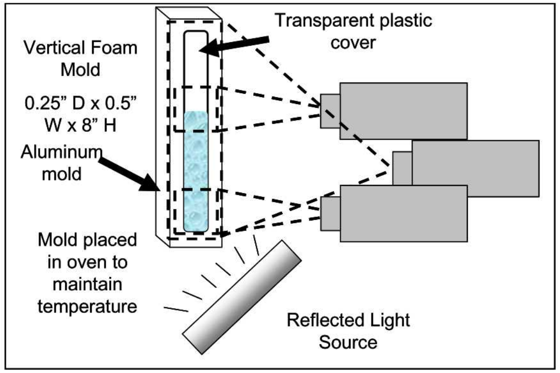
Rate and extent of reaction fit to data, where parameters of the model, including Tg are optimized for lower temperatures expected in the process. The apparent time-to-gel from rheology is correlated with extent to give a Tg with conversion. Similar analysis can be done with DSC and results are consistent.

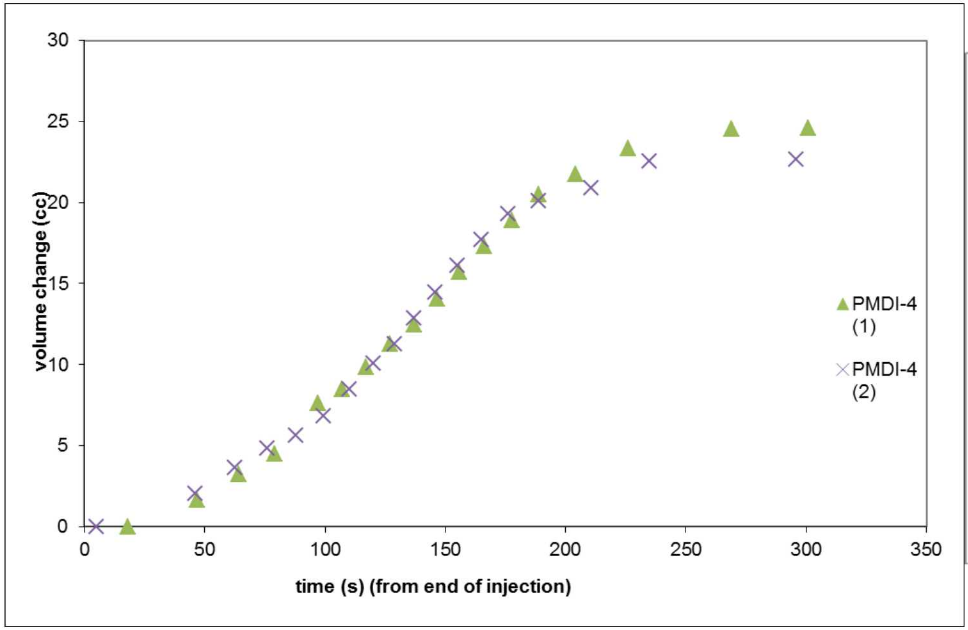
Kamal, M. R., and S. Sourour, *Poly. Eng. Sci* (1973)

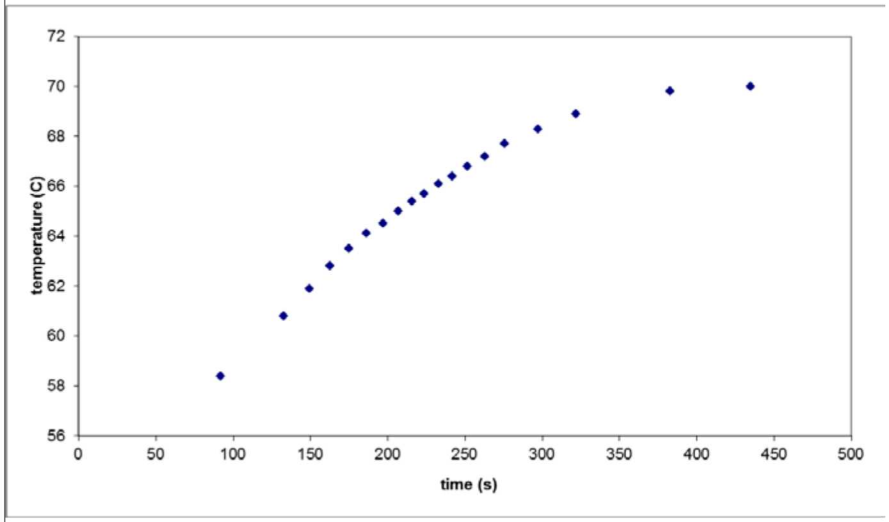
A.T. Di Benedetto, *J. Polymer Sci.*, *Phys.*, **25,** 1949 (1987).

Measure Height Change in Simple Geometry to Quantify Foaming Reaction

- Data have most uncertainty at early times because reaction is occurring during mixing and injections, but bubbles are being destroyed in these processes, too.
- We can only measure height change after these processes.
- CO_2 loss from bubble breakage at top surface? BUT bottom line: engineering model to predict volume change
- The foam cannot be preheated, so during the foam rise the temperature is not steady.

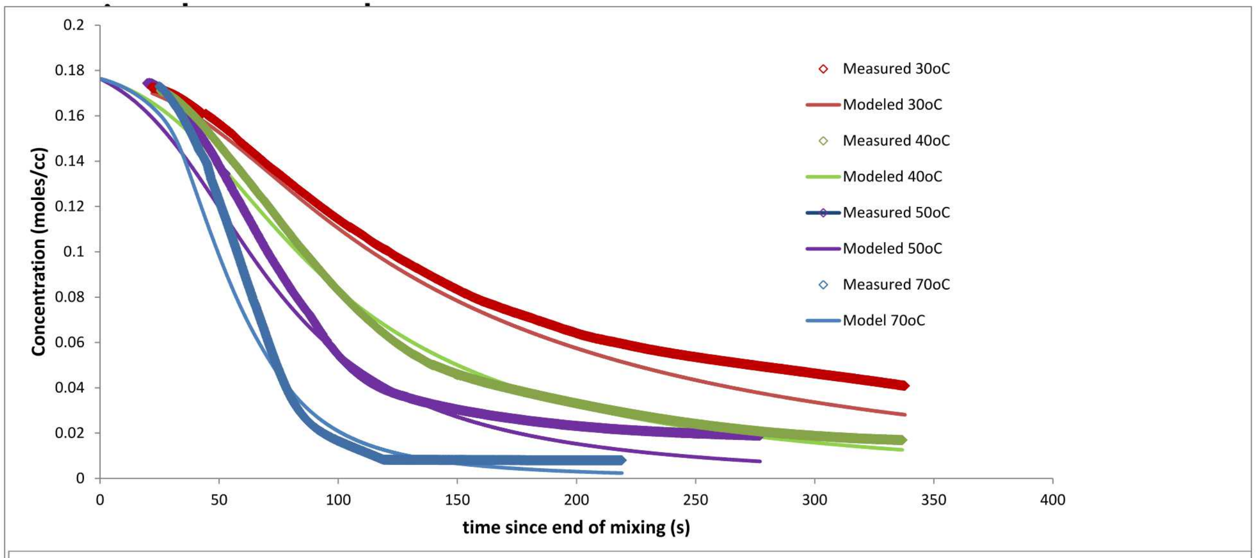


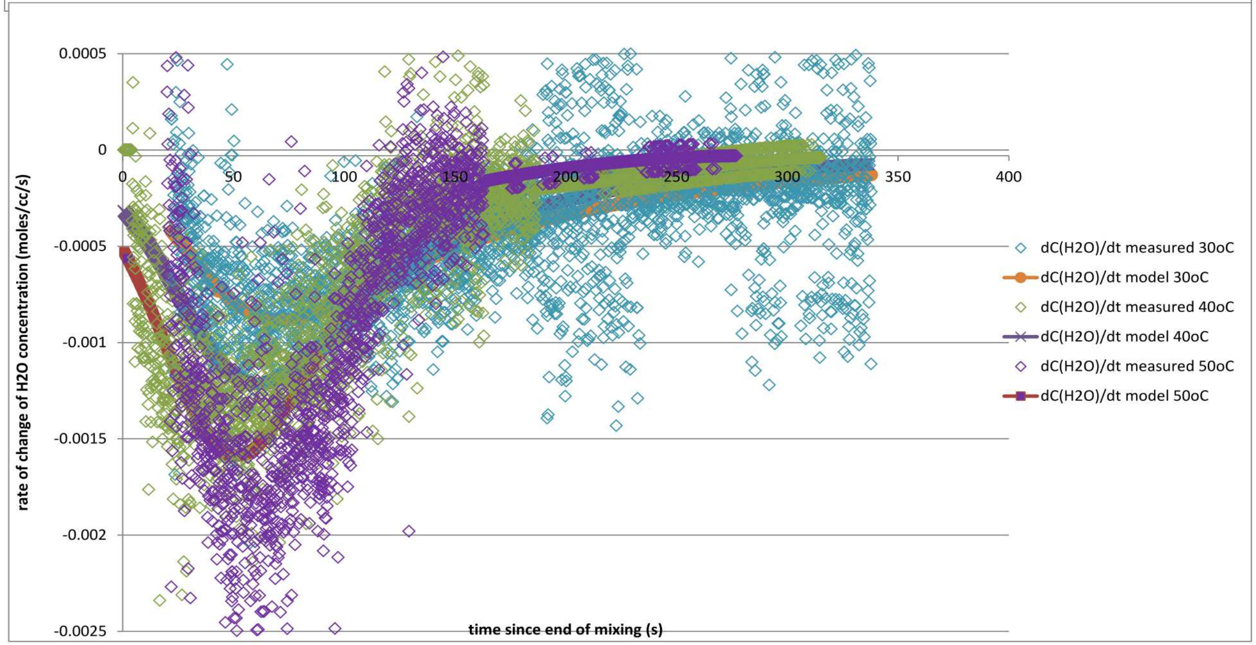




Kinetics of CO_2 Generation

- Fit the concentration of water and its rate of disappearance





$$\frac{dC_{H_2O}}{dt} = -Nk_{H_2O}C_{H_2O}{}^{n}$$

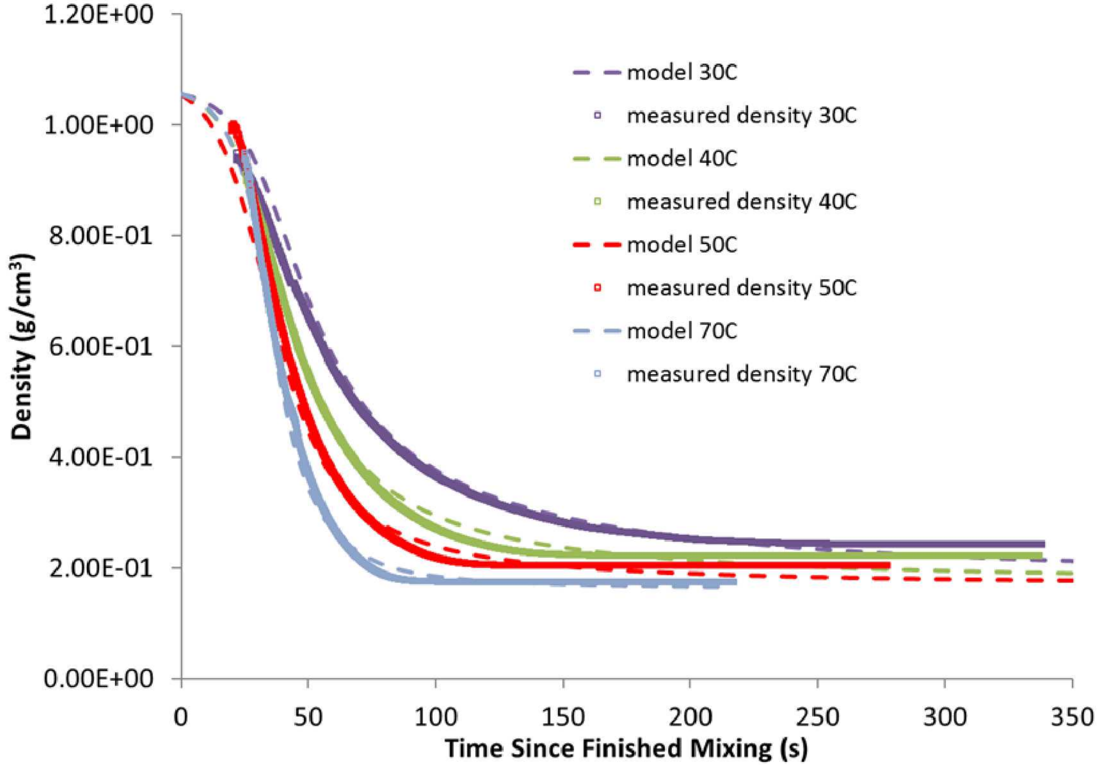
$$\frac{dC_{CO_2}}{dt} = +Nk_{H_2O}C_{H_2O}{}^{n}$$

$$N = 0.5\left\{1 + \tanh\left(\frac{t - t_{nucleation}}{t_{scale}}\right)\right\}$$

- Apparent water concentration shows a change in slope
- Model must capture this
- Physically it relates to the solubility of the carbon dioxide in the polymer
- Must super saturate before nucleation and growth

Kinetics of CO_2 Generation

Predictions of density using a nucleation time of 40s and a time scale of 20s compared to measured density with time in the channel for various temperatures.



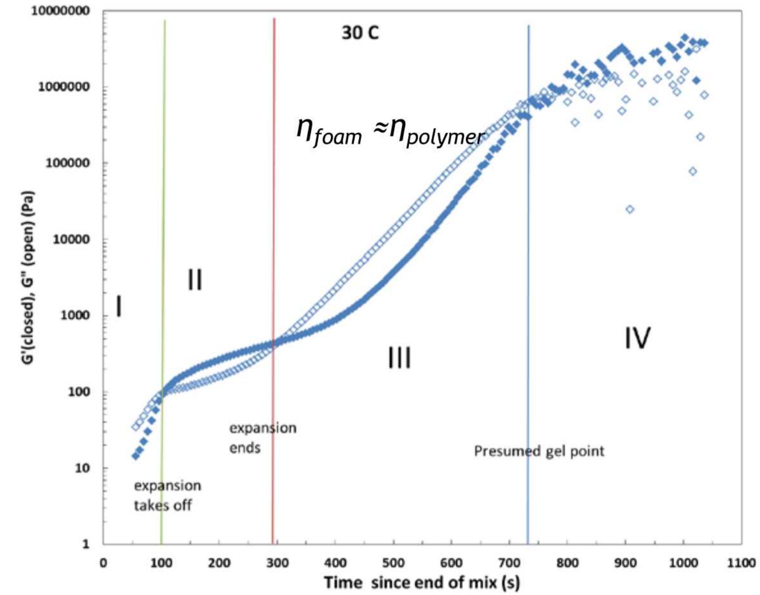
$$\frac{dC_{H_2O}}{dt} = -Nk_{H_2O}C_{H_2O}{}^{n}$$

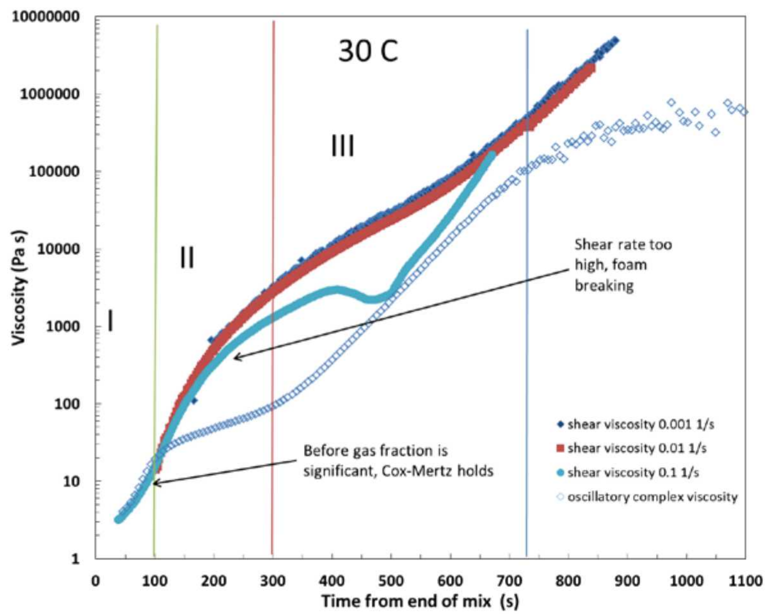
$$\frac{dC_{CO_2}}{dt} = +Nk_{H_2O}C_{H_2O}{}^{n}$$

- Experiments give us average density
- Hard to determine evolving density gradients
- Measure density gradients from post-test experiments

Rao et al., "Polyurethane kinetics, for foaming and polymerization," *AICHE Journal*, 2017

Viscosity of Foam is Complex

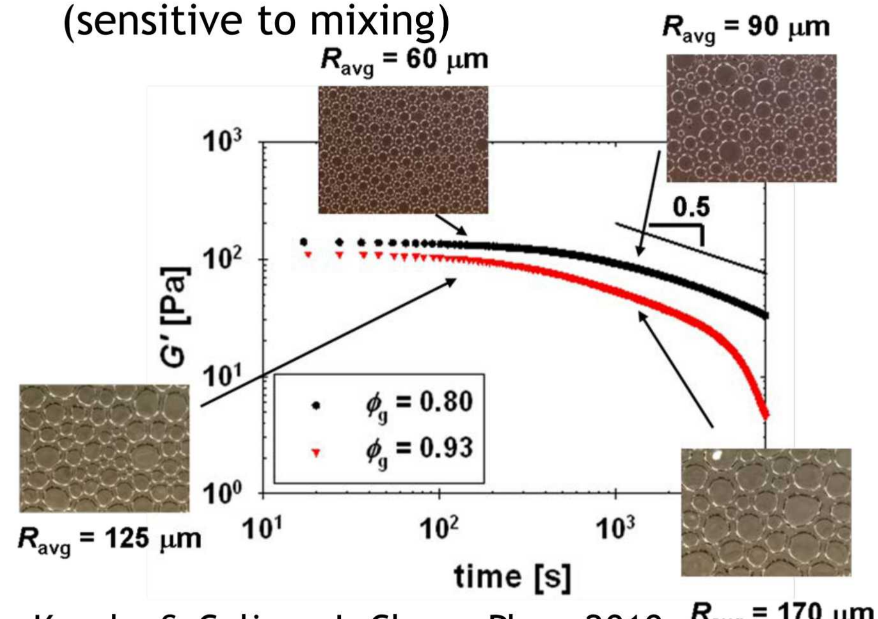




- Foam rheology evolves as gas fraction and polymerization increase

$$\eta_{foam} = \eta_{polymer}\eta_{\phi}$$

- After Bouayad et al. Int J. Mater Form (2009), plot foam rheology as function of distinct phenomenological characteristic times
- Test foam viscosity with steady shear at low shear rates
- Be aware of slip
- Effect of bubble size & coarsening (sensitive to mixing)



Kropka & Celina, J. Chem. Phys. 2010

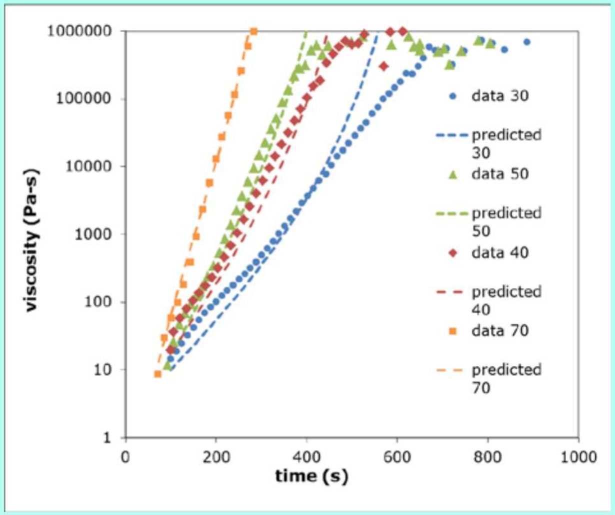
Model Foam Viscosity as f(ξ,ϕ)

Start with continuous phase viscosity only

- IR kinetics + dry formulation rheology (two sets of experiments) give an approximation of the curing continuous phase rheology
- Relate time of gel point to ξ to find ξ_c.

$$\mu_{polymer} = \mu_0^0 \left(\frac{\xi_c - \xi}{\xi_c} \right)^{-6} \qquad \xi_c = 0.86$$

$$\mu_0^0 = 600 e^{-1549/RT} \text{ Pa-s}$$

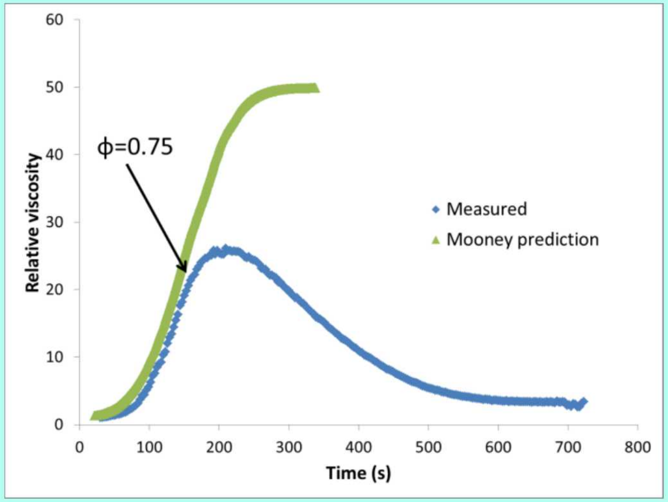


Relate foam viscosity to continuous phase viscosity

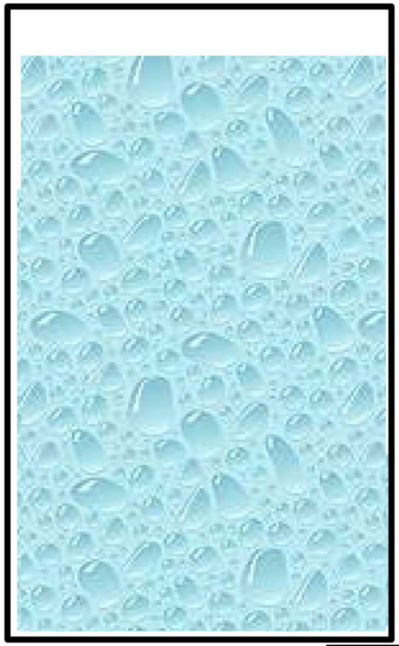
- Foam rise + wet formulation rheology (two sets of experiments) give an approximation of the rheology as a function of gas fraction
- Mooney prediction (for $\varphi_{gas} < 0.5$)

$$\mu_\varphi = \mu_{polymer} \exp\left(\frac{\varphi_g}{1 - \varphi_g} \right)$$

- For $\varphi_{gas} > 0.75$ estimate $\mu_{foam} = \mu_{cure} * f(\xi)$



Coupled Finite Element Method/Level Set to Solve Foam Dynamics



•Given fluid velocity field, u(x,y,z), evolution on a fixed mesh is according to:

$$\frac{\partial \phi}{\partial t} + u \cdot \nabla \phi = 0$$

•Purely hyperbolic equation … fluid particles on $\phi(x,y,z) = 0$ should stay on this contour indefinitely

- Does not preserve $\phi(x,y,z)$ as a distance function
- Introduces renormalization step.

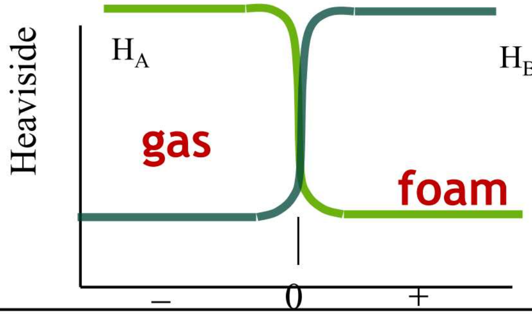
•Equations of motion, kinetics and energy balance averaged based on level set, ϕ

$$H_A \rho_A \frac{Du}{Dt} + H_B \rho_B \frac{Du}{Dt} = -\nabla P + H_A \nabla \cdot (\mu_A \dot{\gamma}) + H_B \nabla \cdot (\mu_B \dot{\gamma}) + (H_A \rho_A + H_B \rho_B) g + I.T.,$$

$$H_A \frac{D\rho_A}{Dt} + H_B \frac{D\rho_B}{Dt} + (H_A \rho_A + H_B \rho_B) \nabla \cdot u = 0$$

$$H_A + H_B = 1$$

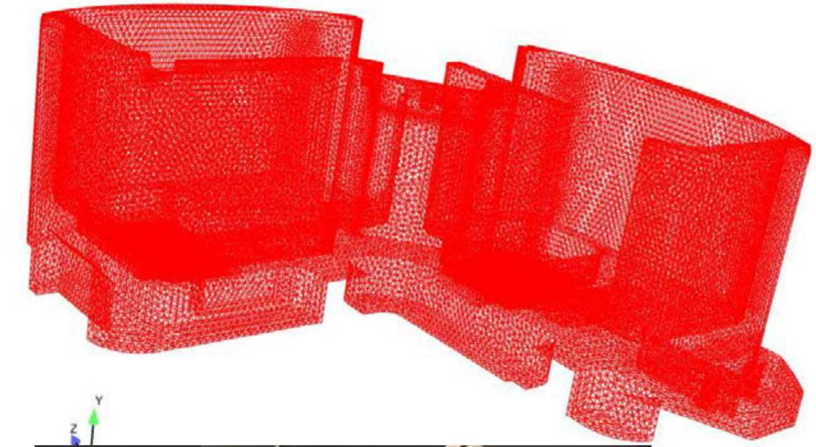
Rao et al, IJNMF, 2012

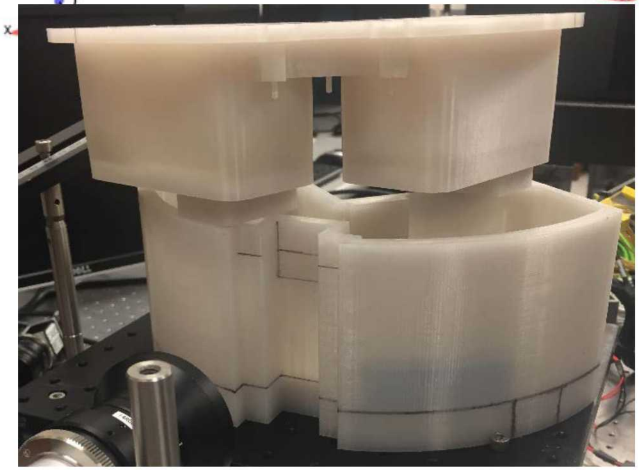


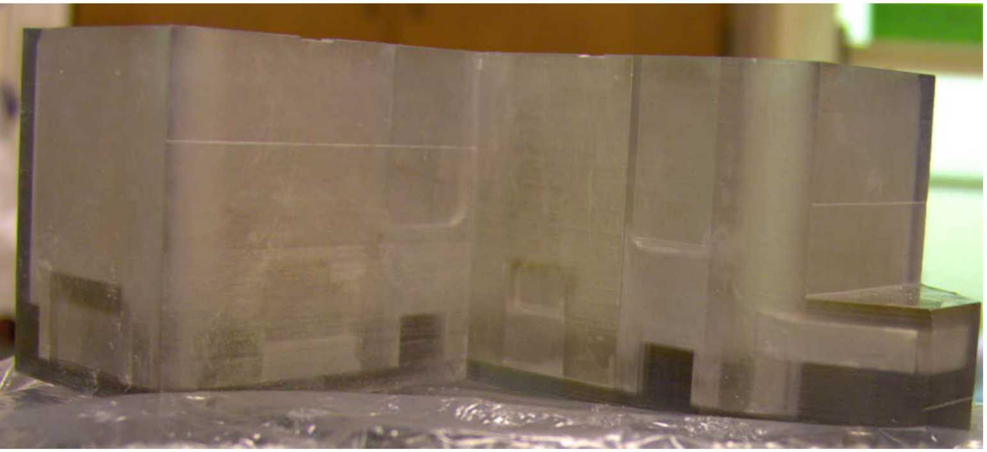
Simulations & Experiments

Simulations
- Flat configuration
- 5º tilt
- 20º tilt
- 20º tilt toward the shelf feature
- Study of vent locations

Experiments
- Flow visualization experiments
- Additive manufacture mold

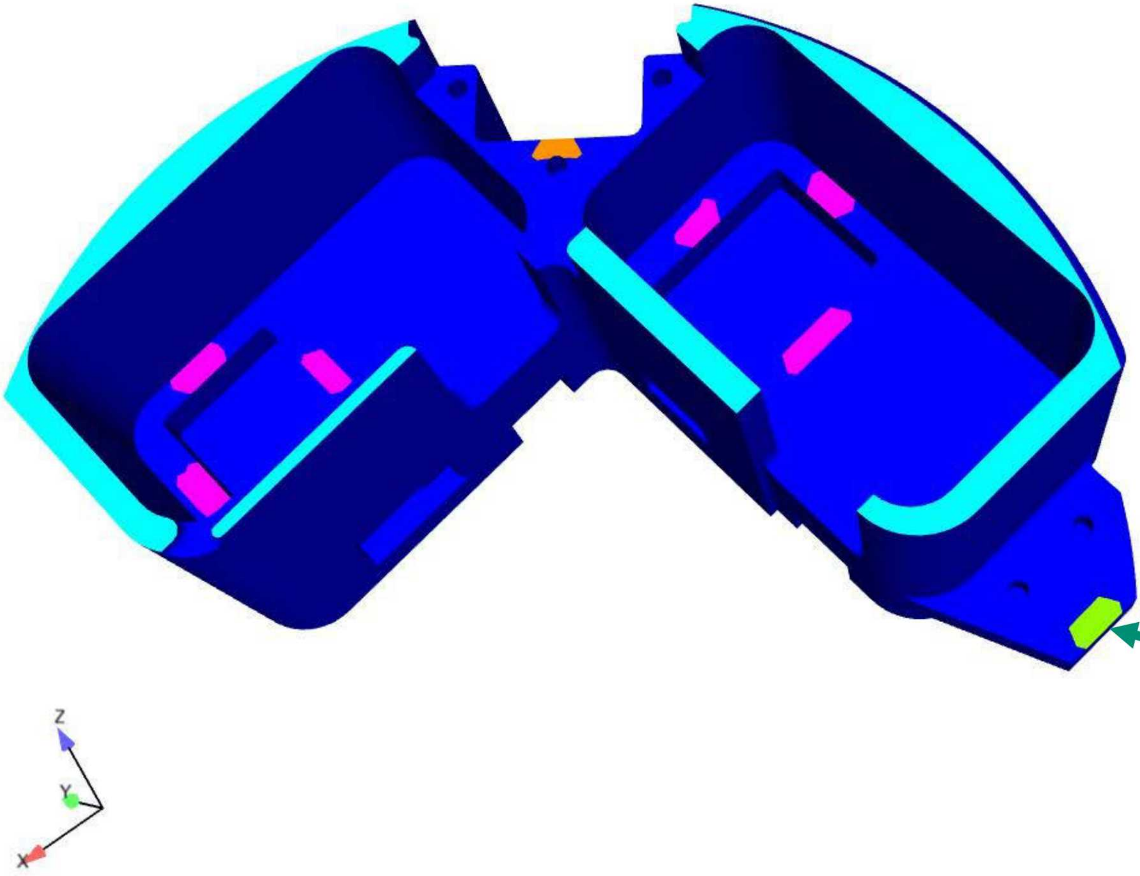






Goal: Use foaming and filling modeling and flow visualization experiments to develop confidence in foam model

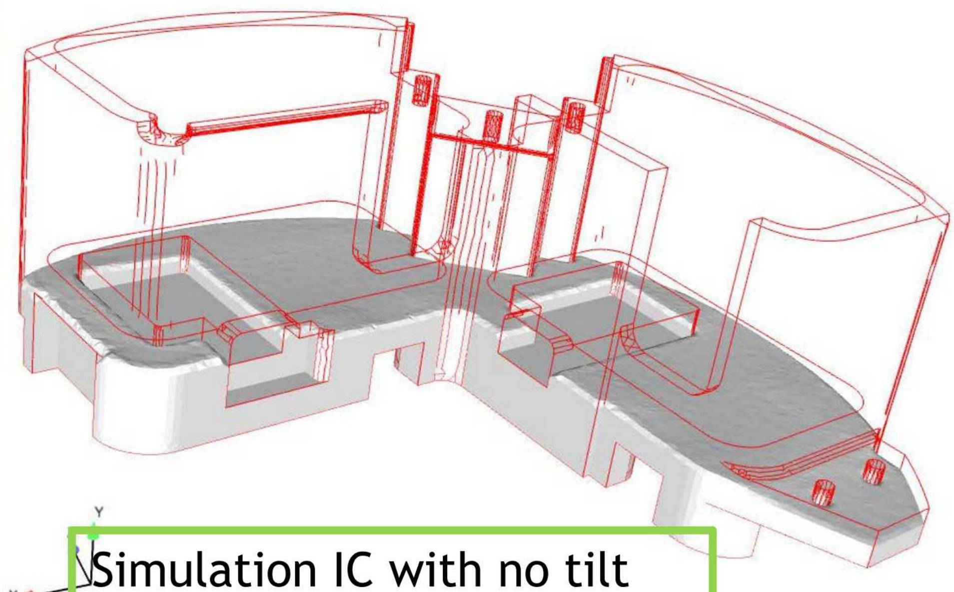
These Vent Locations Seem Representative of a Foaming Process



Simulation tests the idea of adding a vent on the shelf feature

Initial Conditions for Model: Experiments Show Shelf Starts Well-Filled

Flow visualization study using opaque mold to determine filling of shelf supports use of flat initial condition



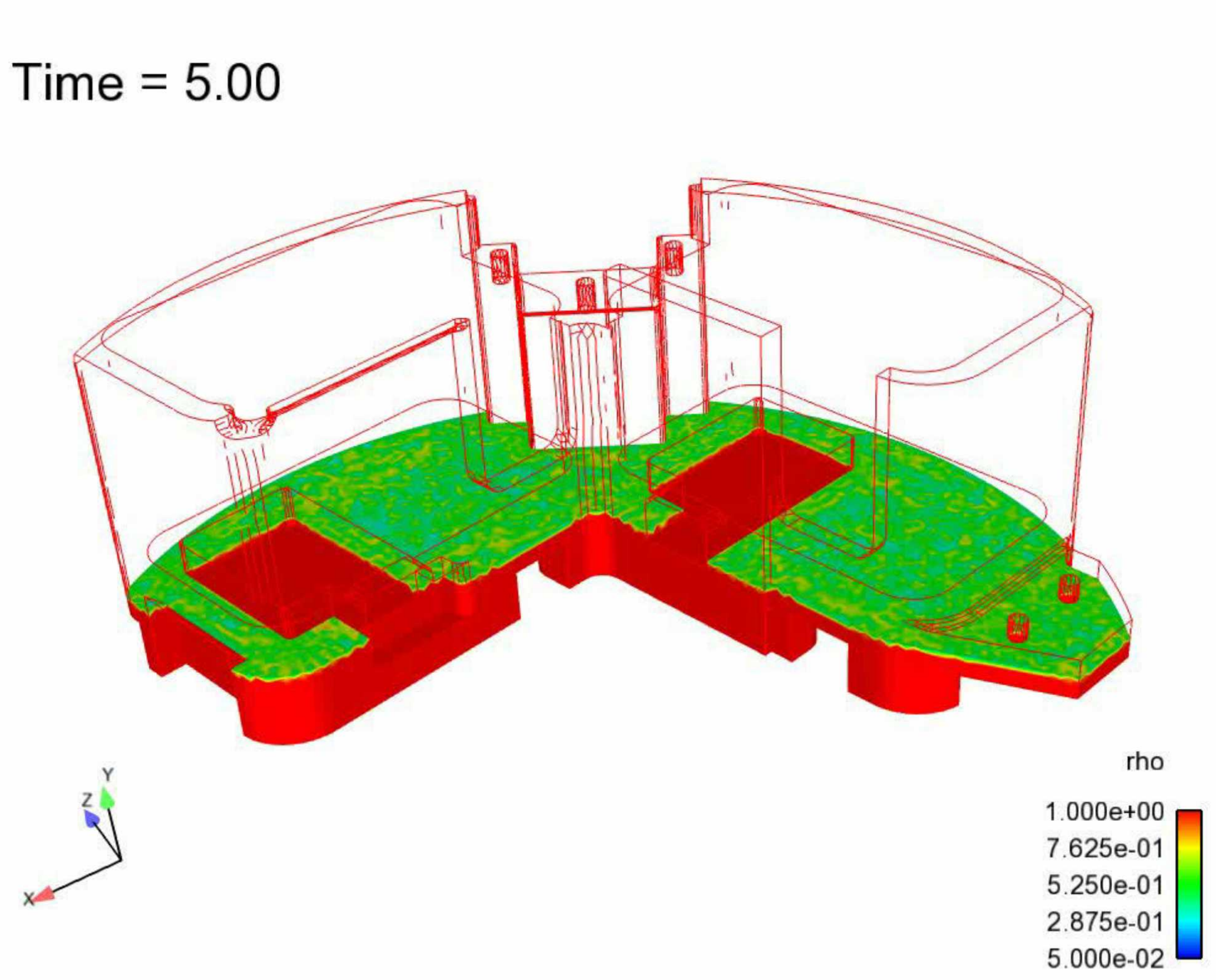
Flow visualization verifies initial condition:

- *Foam levels well and flows to fill she area*
- *Simulation initial condition of a flat interface seems fairly accurate*

Simulation IC with no tilt

- Shelf is half-filled at start of the simulation

Foam Filling and Curing for Flat Configuration

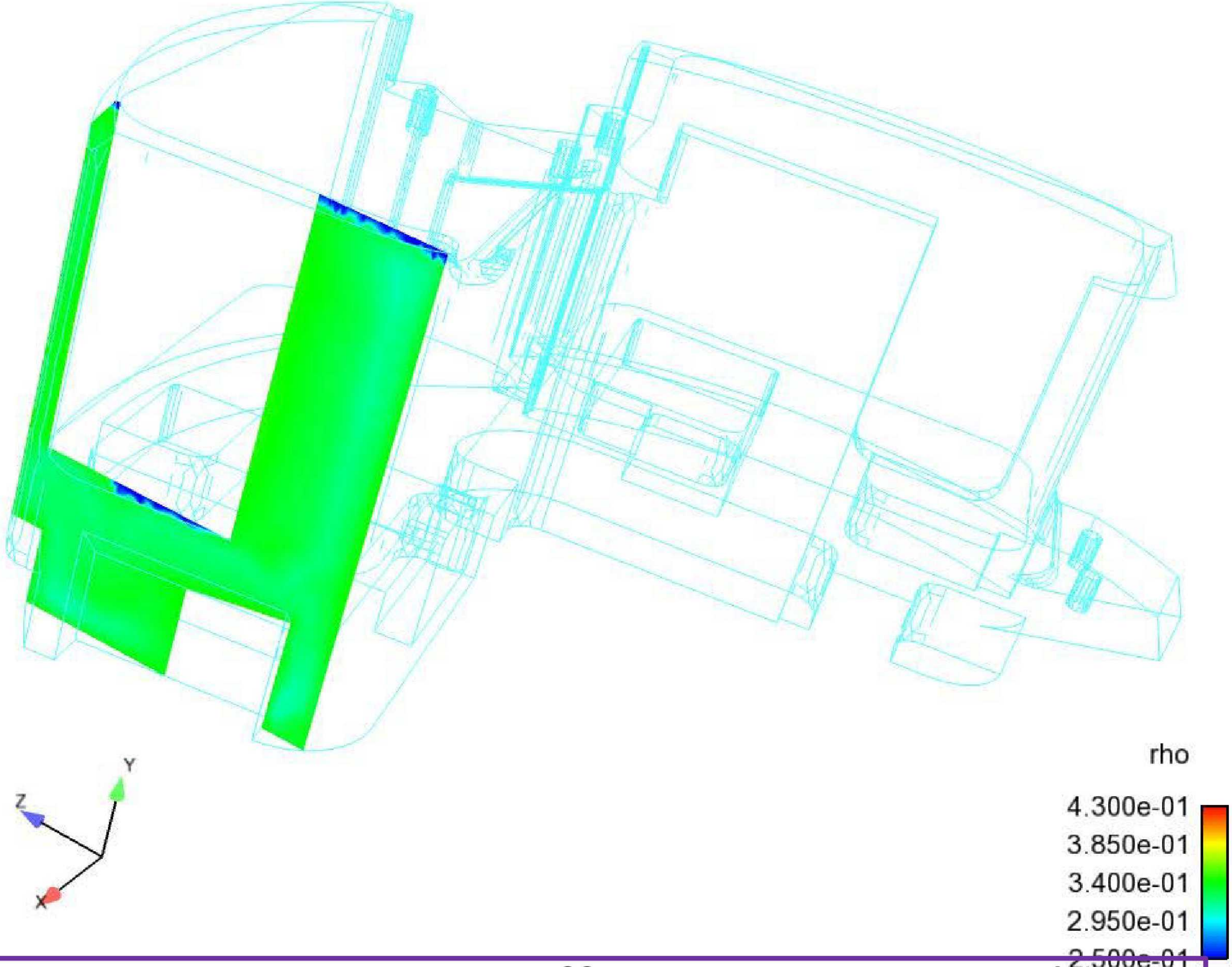


Base Case:

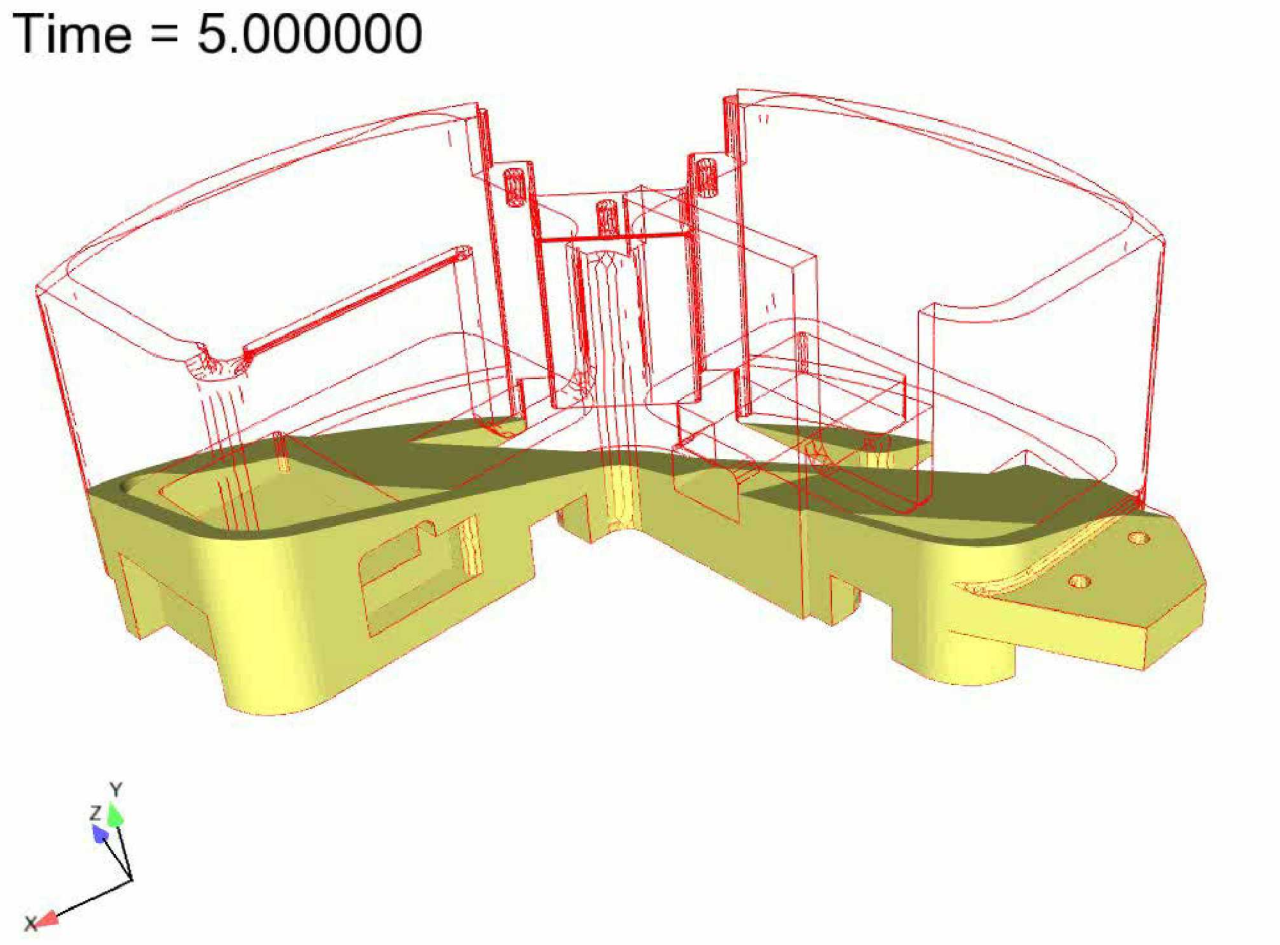
- Look at issues for filling the mold when it is flat on the table
- Model shows density evolution and filling profile over time

Density Variations at Different Locations: Flat Mold with Shelf Vent

time=82.7s
voids = 3.6%



Dynamics of Filling with 20º Tilt Angle

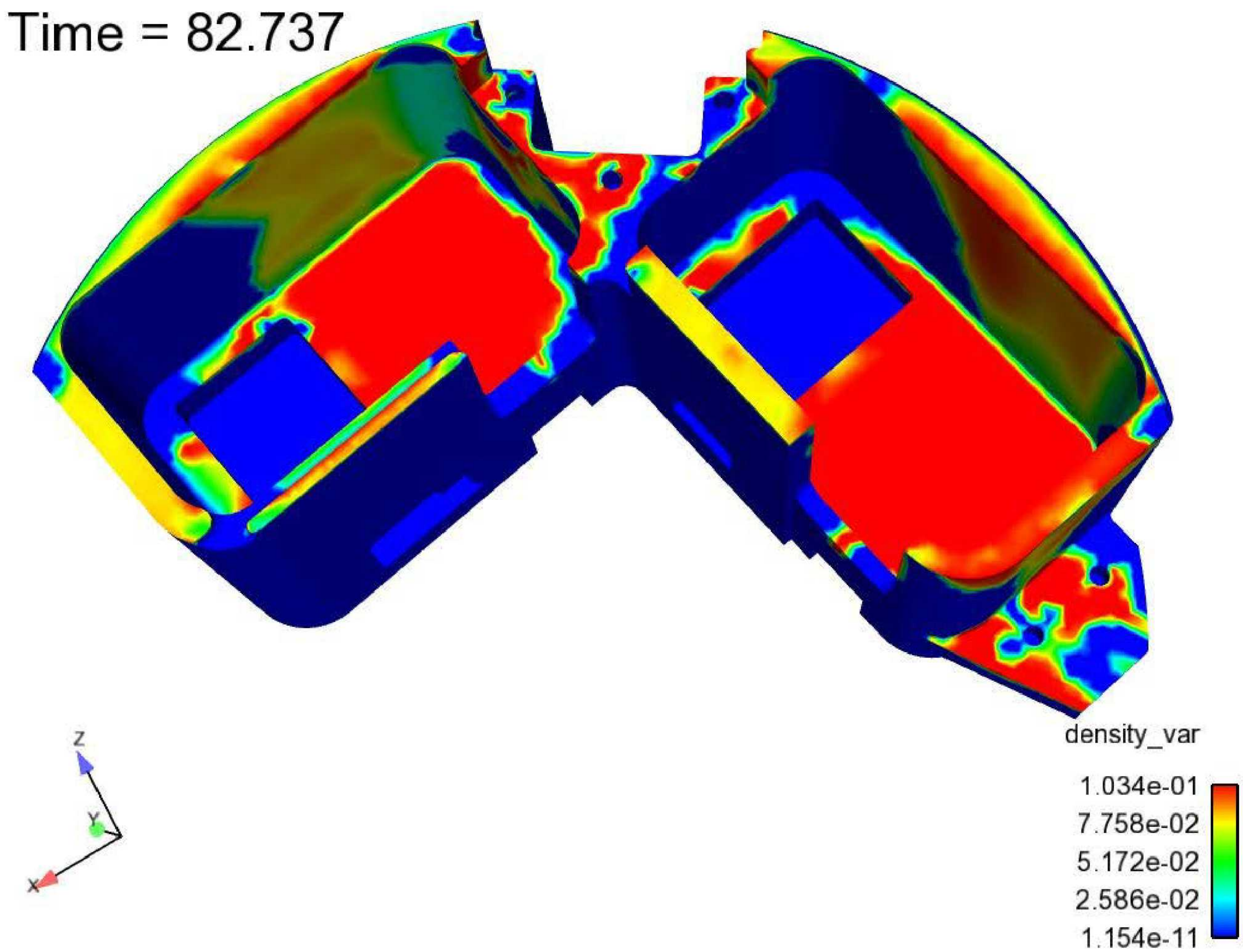


Foam Using a 20º Tilt Angle forward similar to legacy process

- Initial condition has a tilt forward for foam position and a flat interface
- Gravity vector is also tilted

Plot of Density Variation From Nominal

FLAT FILL



Density Variation:

$(\rho_{local} - \rho_{nominal})^2$

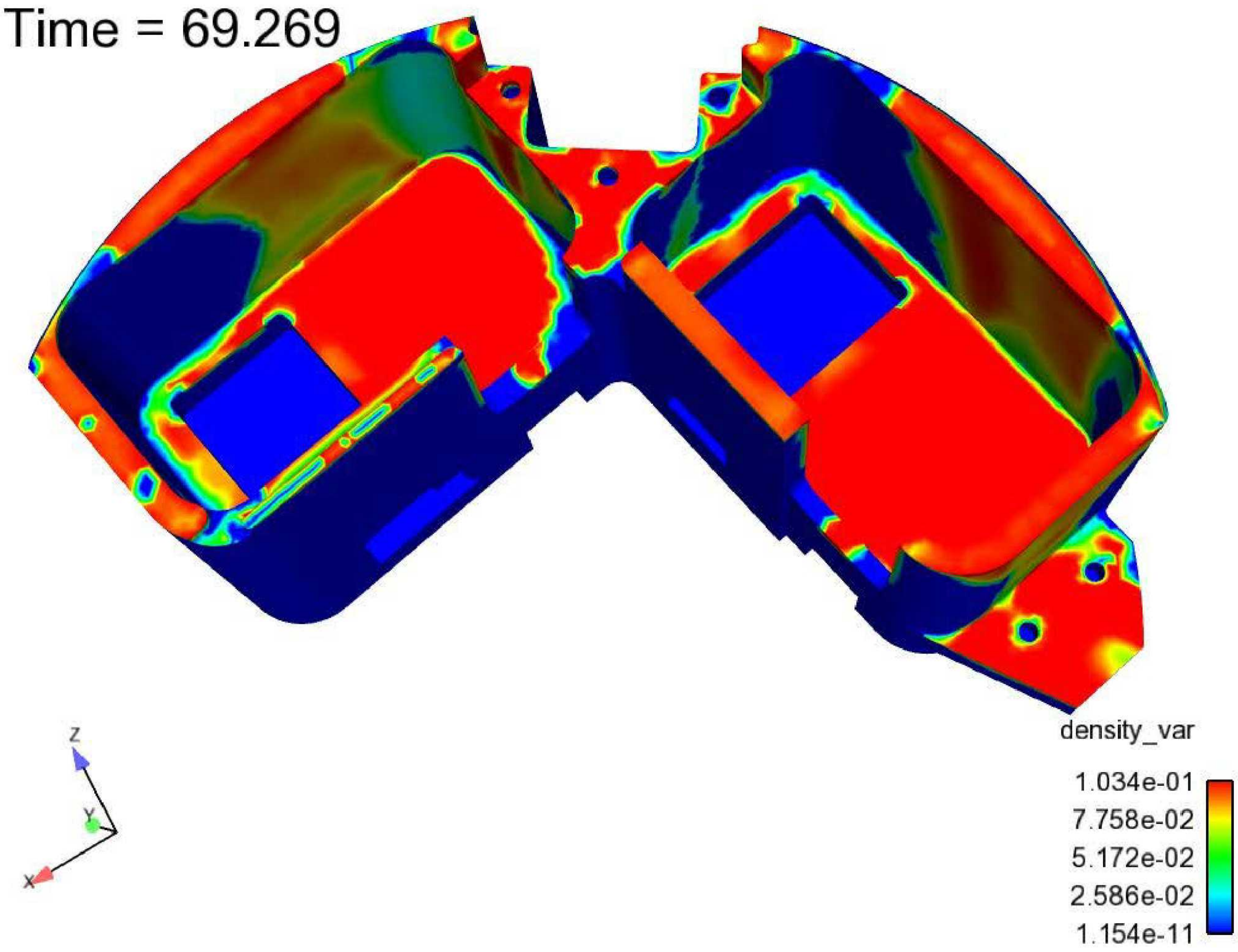
$$\int (\rho - \rho_{nom})^2 dV$$

$\rho_{nominal}$ = 240g/745ml
= 0.322g/ml

time=82.7s
voids = 3.6%
Int. var. = 2.81

Plot of Density Variation From Nominal

FLAT FILL HOT



Density Variation:
$(\rho_{local} - \rho_{nominal})^2$

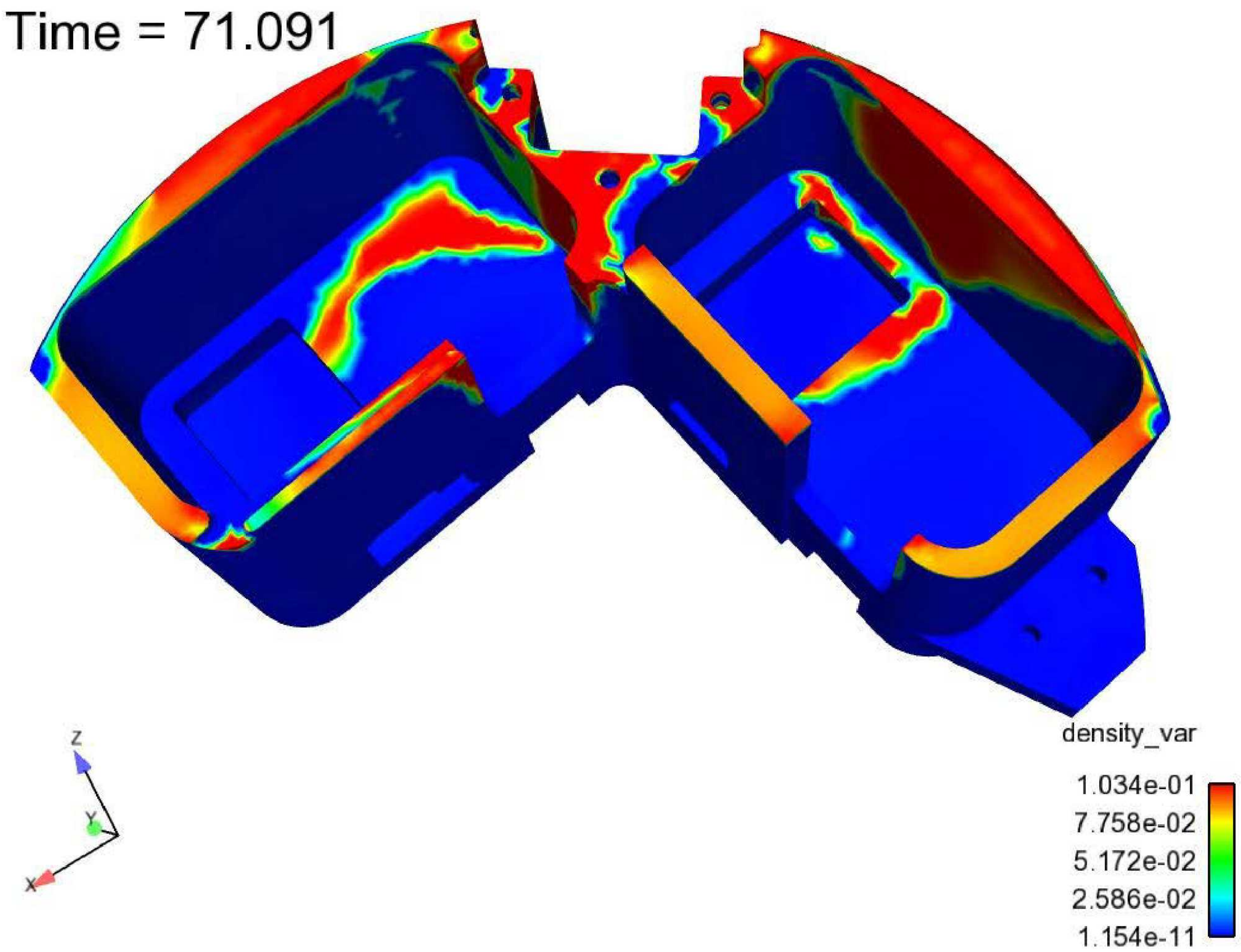
$$\int (\rho - \rho_{nom})^2 \, dV$$

$\rho_{nominal}$ = 240g/745ml
= 0.322g/ml

time=69.3s
voids = 4.5%
Int. var. =
3.56

Plot of Density Variation From Nominal

TILT 20 DEGREES FILL



Density Variation:
$(\rho_{local} - \rho_{nominal})^2$

$$\int (\rho - \rho_{nom})^2 dV$$

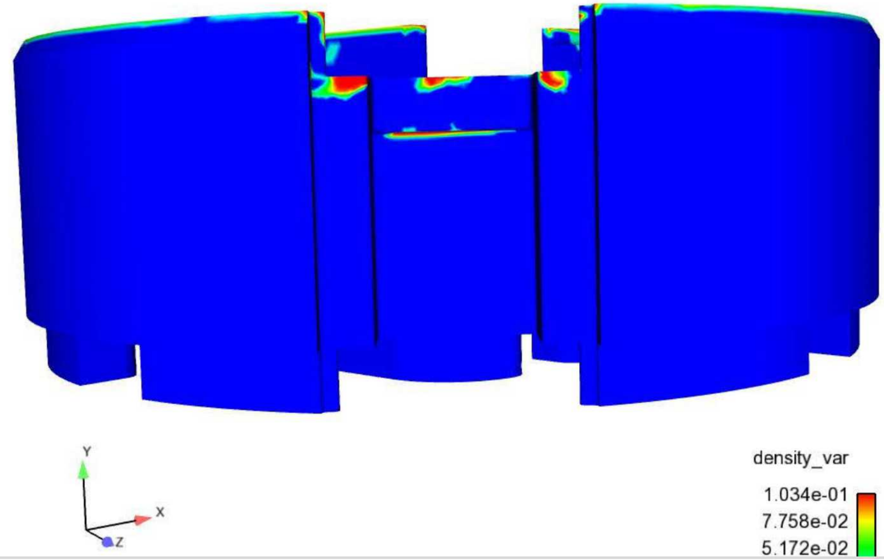
$\rho_{nominal}$ = 240g/745ml
= 0.322g/ml

time=71.1s
voids = 2.9%
int. var. = 2.87

Density Variations: Back View

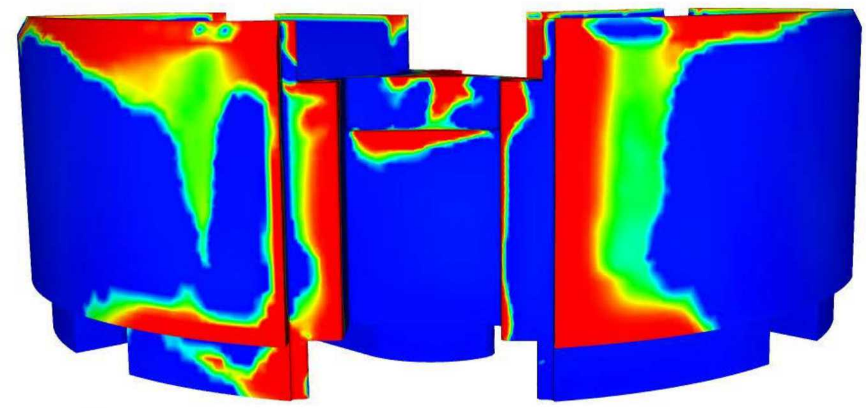
Time = 82.737

FLAT FILL



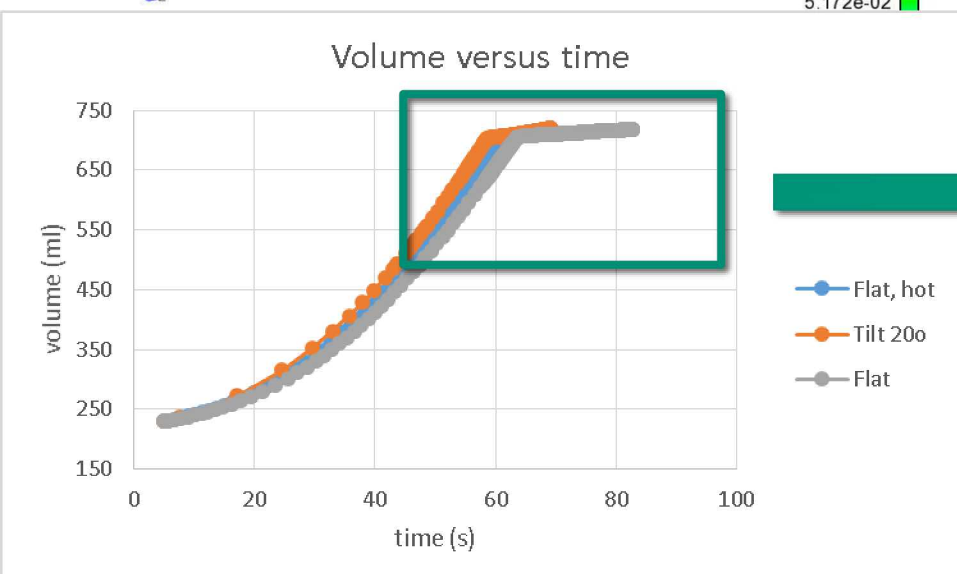
Time = 71.091

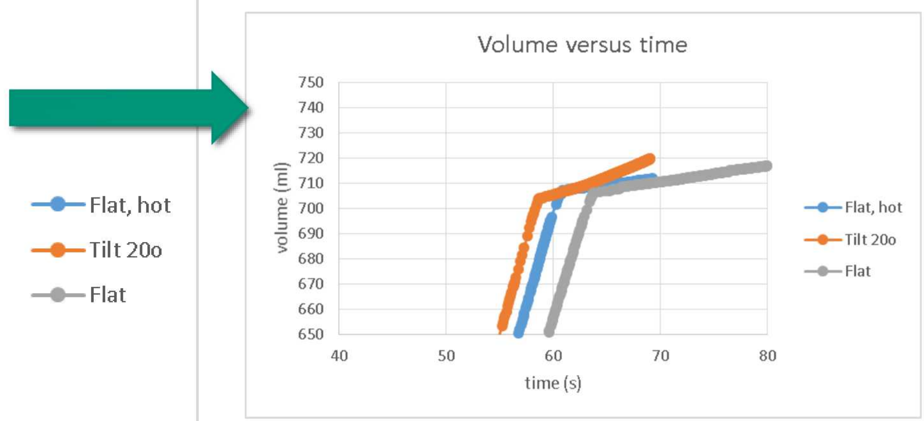
TILT 20 DEGREES FILL



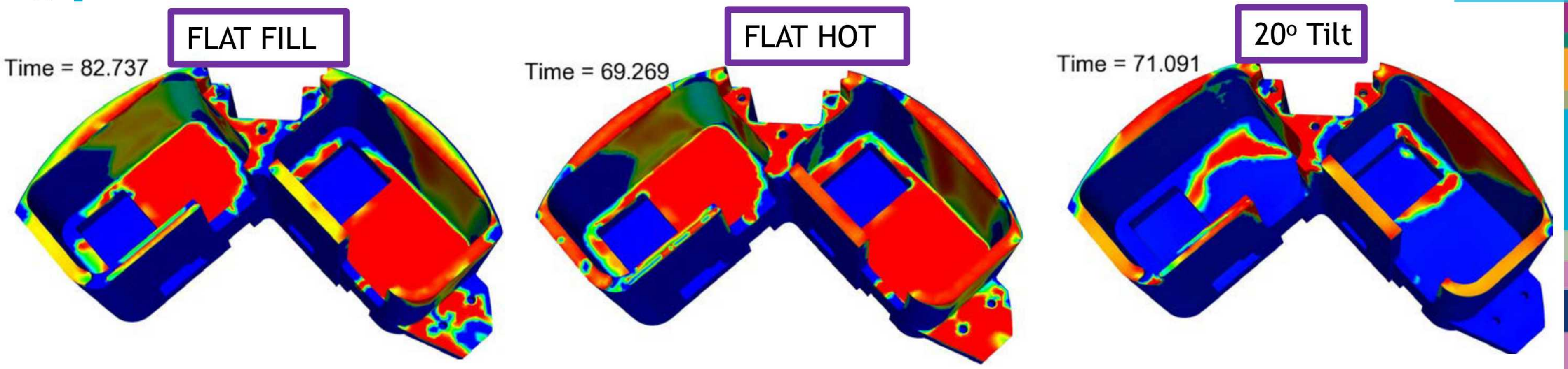
density_var
1.034e-01
7.758e-02
5.172e-02
2.586e-02
1.154e-11

- Forward tilt moves defects to the back part of the mold
- Tilt fills faster than flat

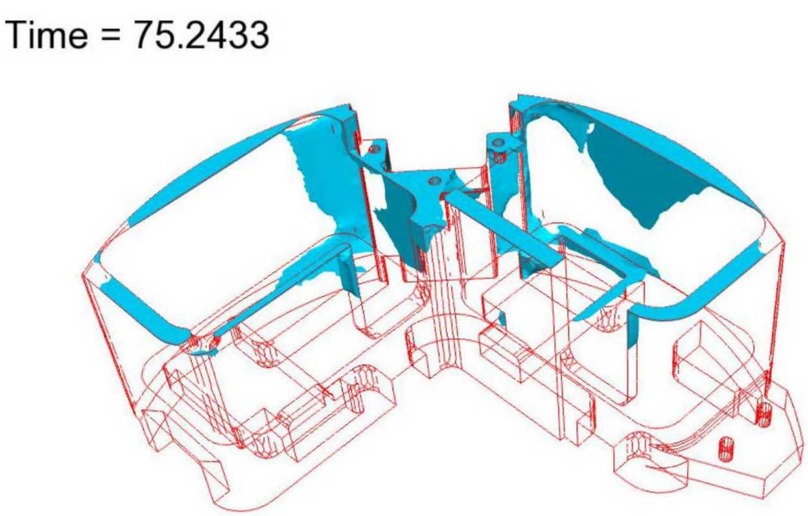




Computational Models of Foam



Density variations for three cases of interest



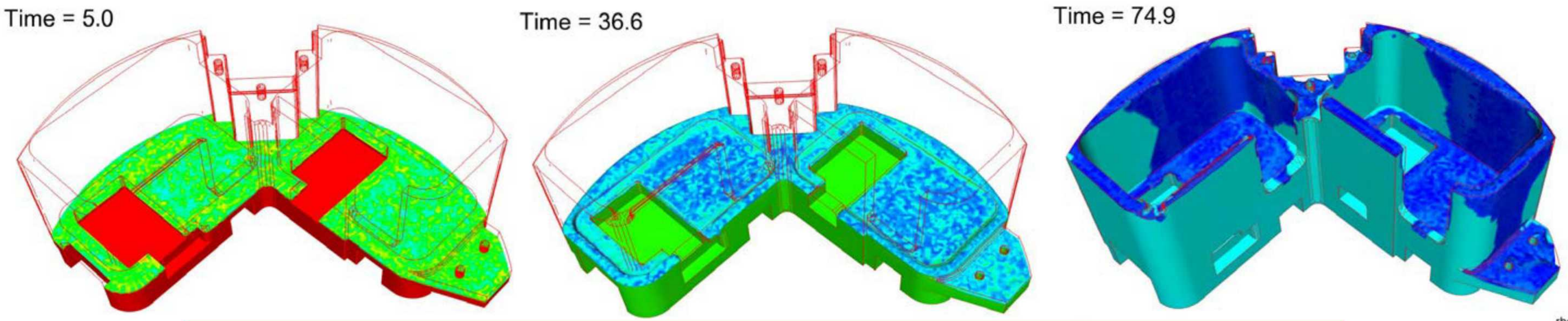
Foam filling for 20º tilt: the angled fill reduces voids on the new shelf

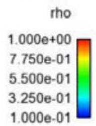
Case	Flat	Flat Hot	20º Tilt
Max. Time (s)	83s	70s	71s
Voids	3.6%	4.4%	2.9%
Density variation	2.8	2.9	3.6

All cases fill well!

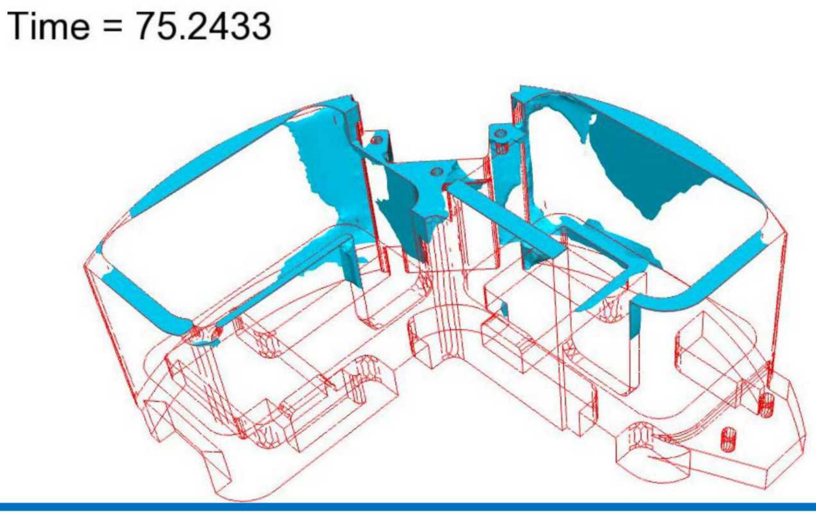
- Model over-predicts voids, but predictions are small
- Density variation greater with tilt

Computational Models of Foam



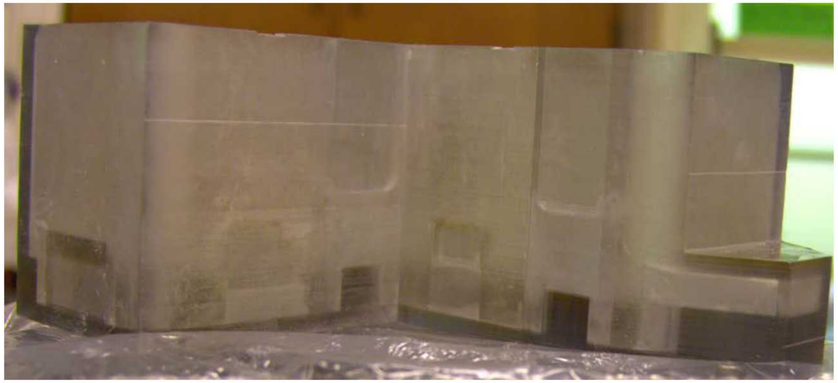


Evolution of density for flat mold with vent on the shelf feature

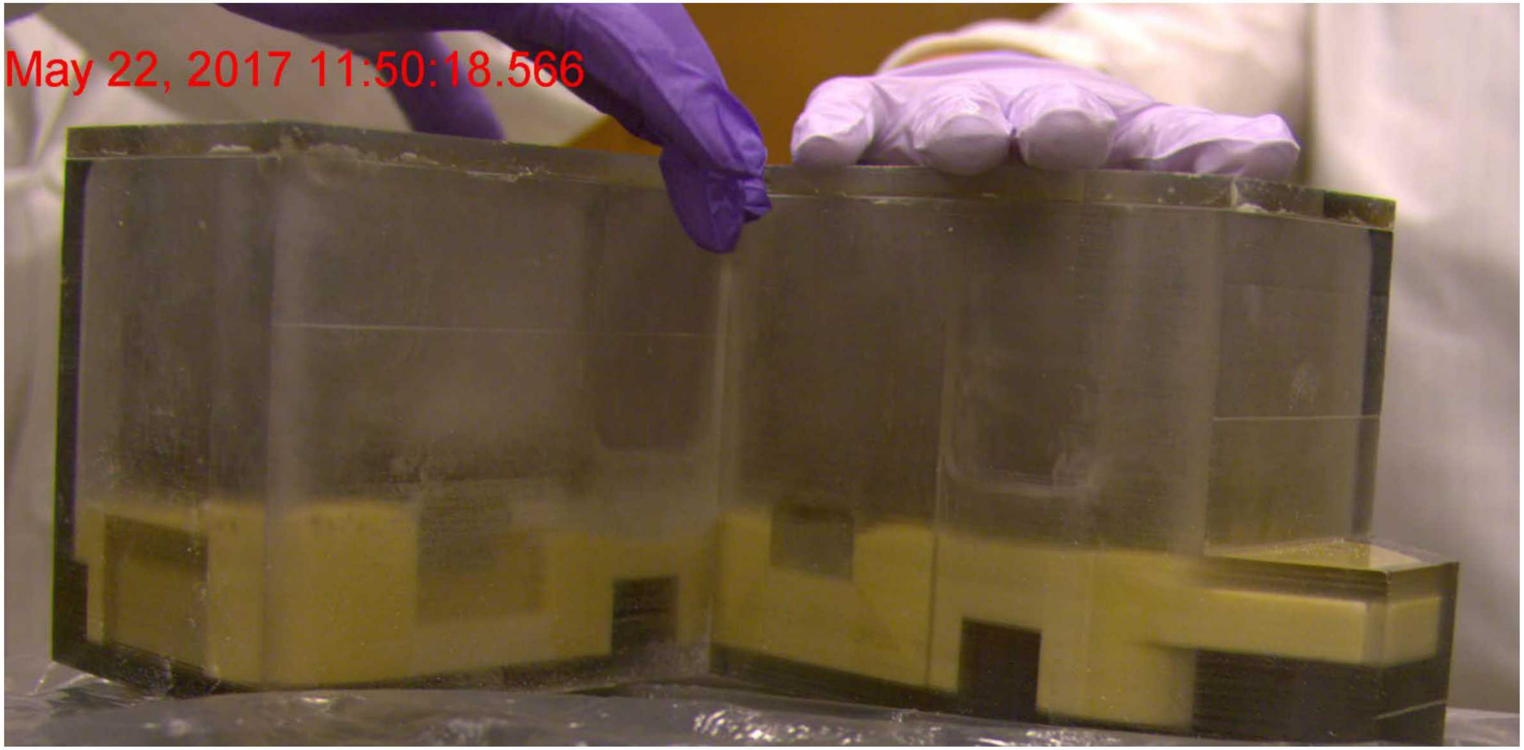


Foam filling for 20º tilt: the angled fill reduces voids on the new shelf

Flow visualization study supports computational conclusions



Validation Experiment: 5 Degree Tilt: Foam Fills Shelf and Levels Quickly

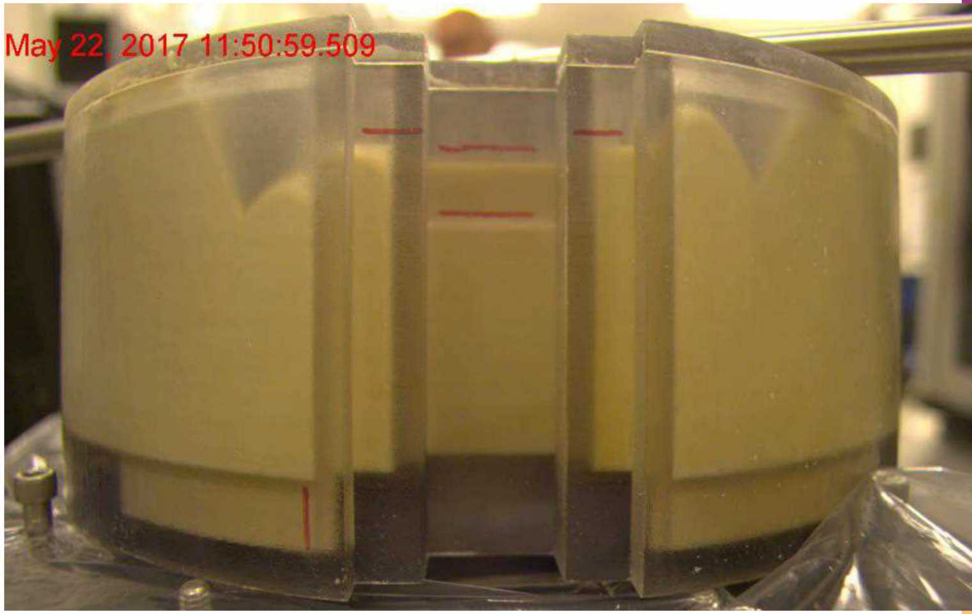


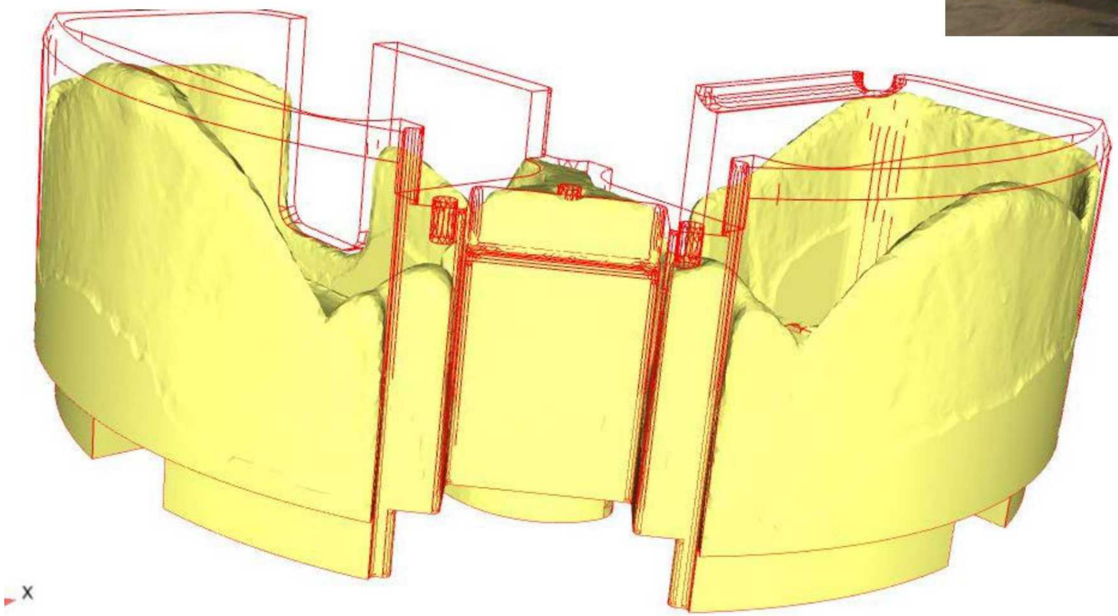
- New experiment using clear mold
- Room temperature mix of foam, which heats up to 24^{o}C
- Mold stays roughly 22^{o}C
- 5 degree tilt towards the front of the mold

Experimental Conditions: Back of Mold

Run model with similar initial conditions:

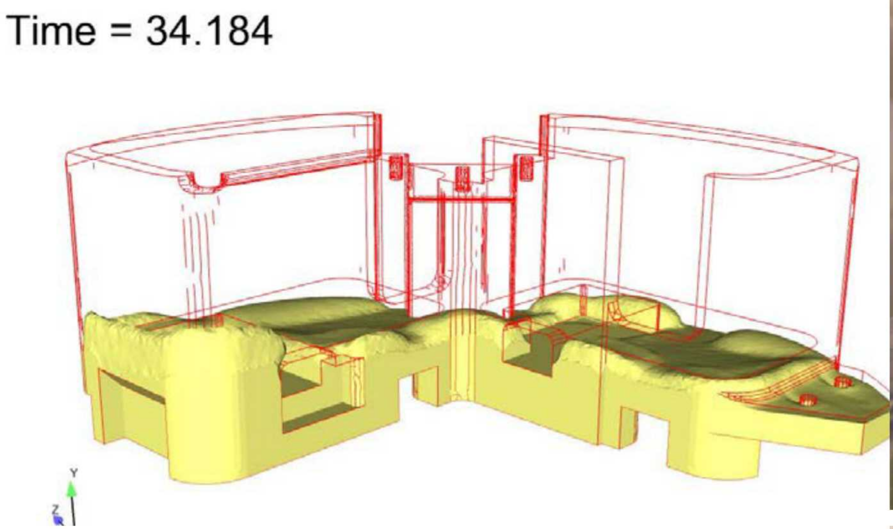
- 240g material
- 4 degree tilt
- Room temperature mold and foam

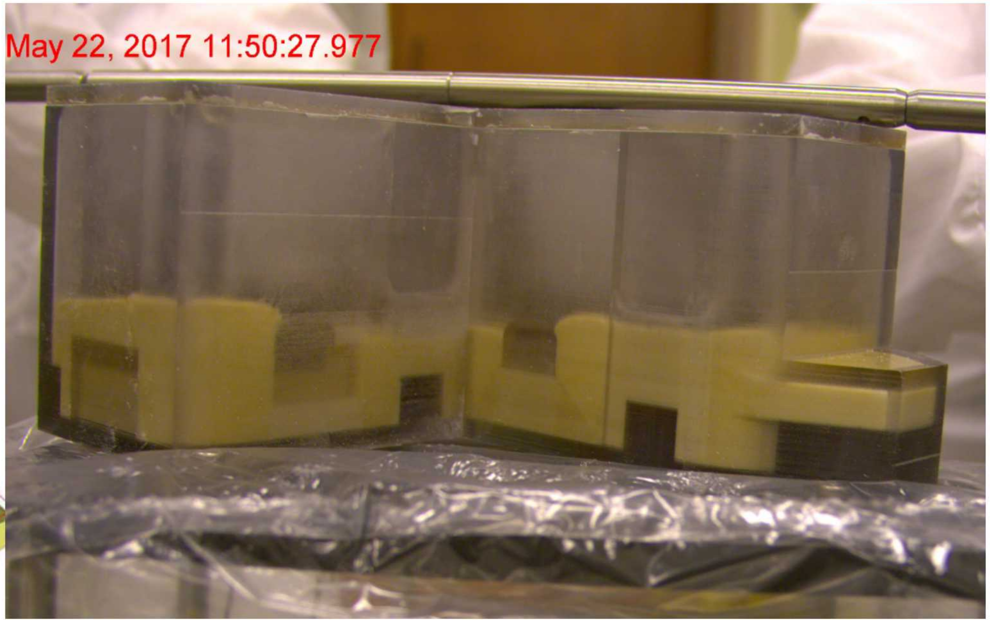


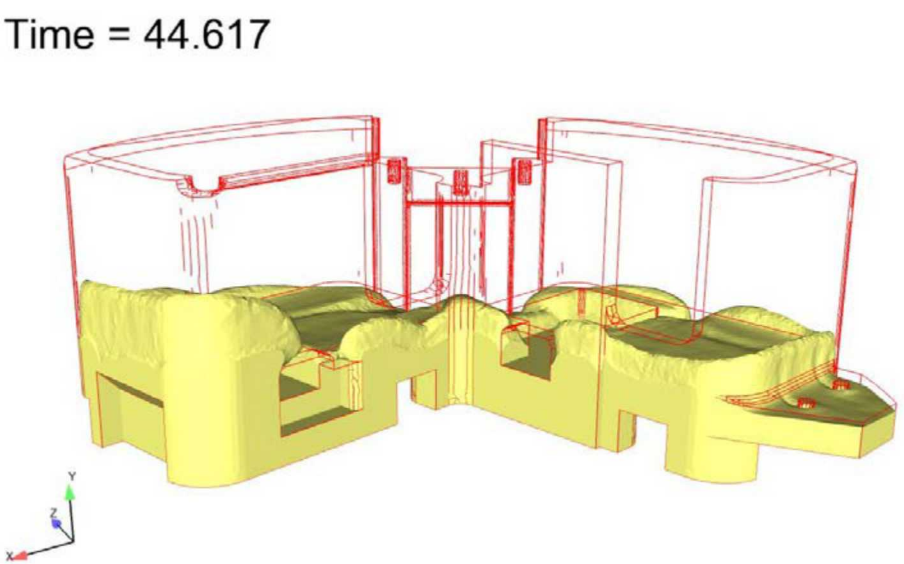


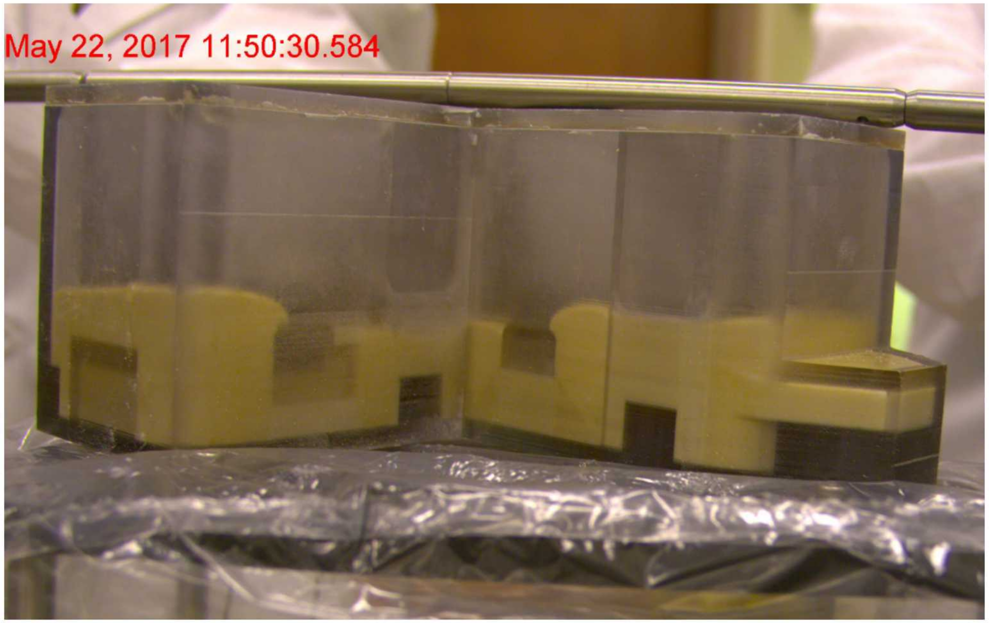
Shape of the model interface matches well with shape of experiment thought model fills back feature faster

Compare Mold Front: Early Times



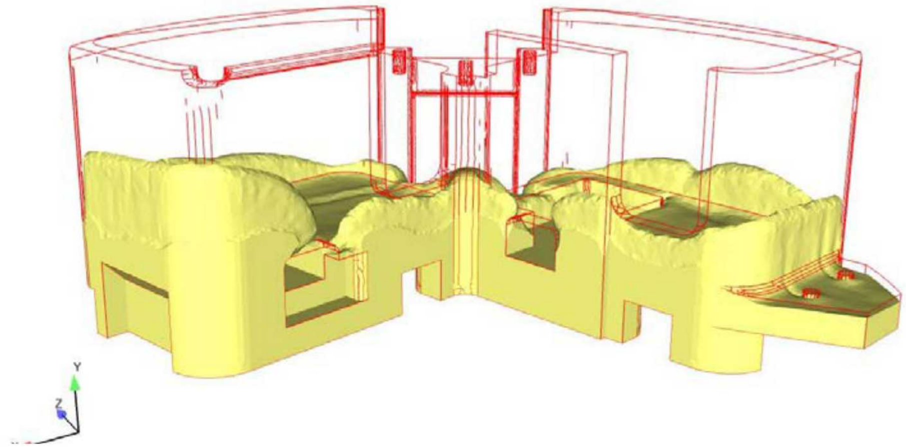


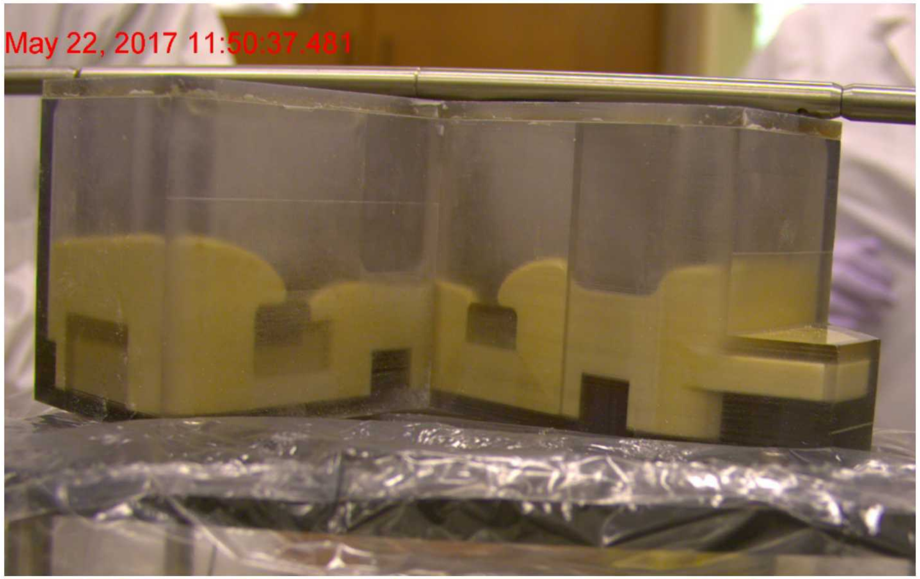




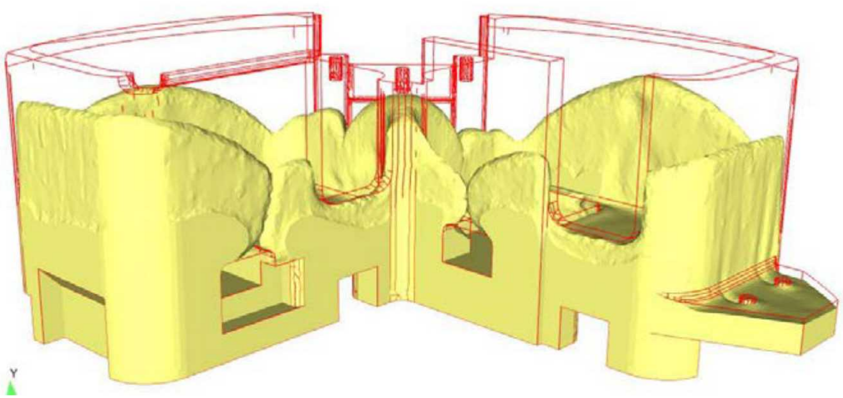
Compare Mold Front: Moderate Time

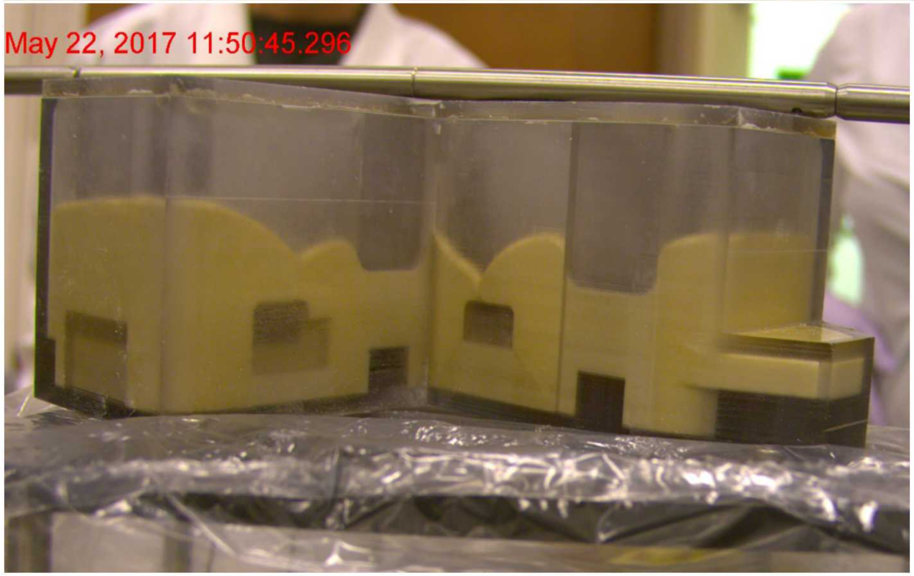
Time = 49.913



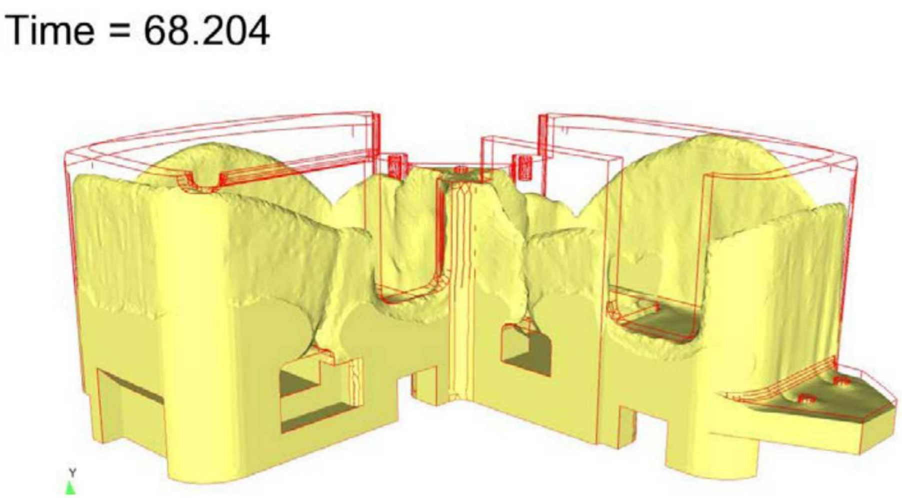


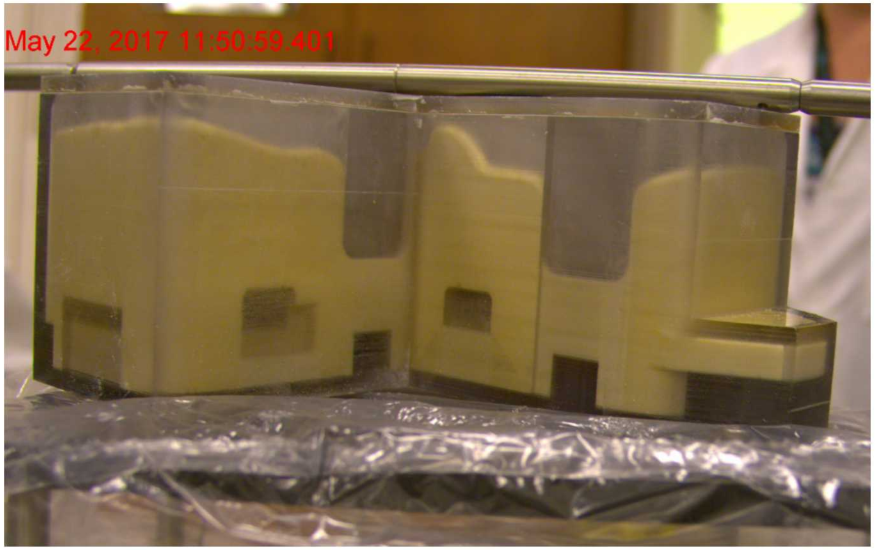
Time = 62.538





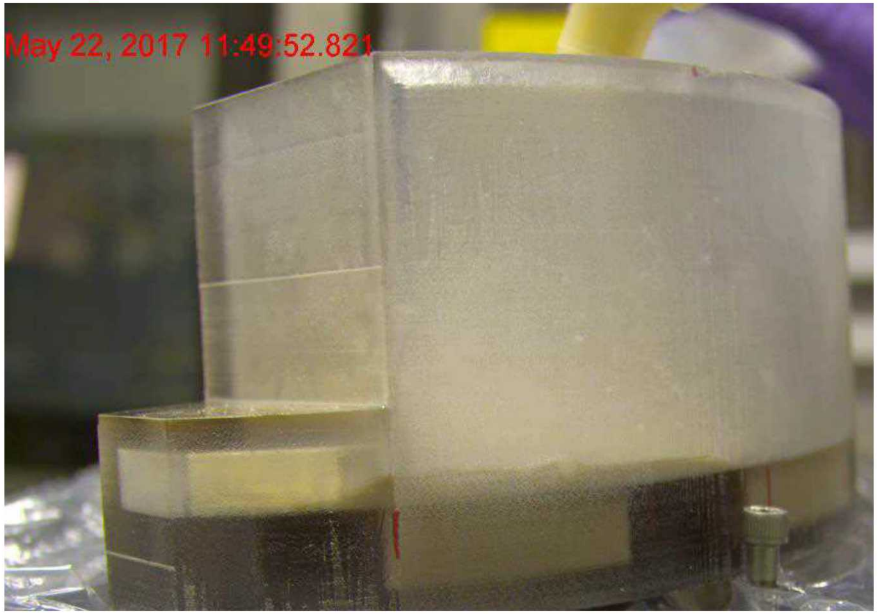
Compare Mold Front: Late Time

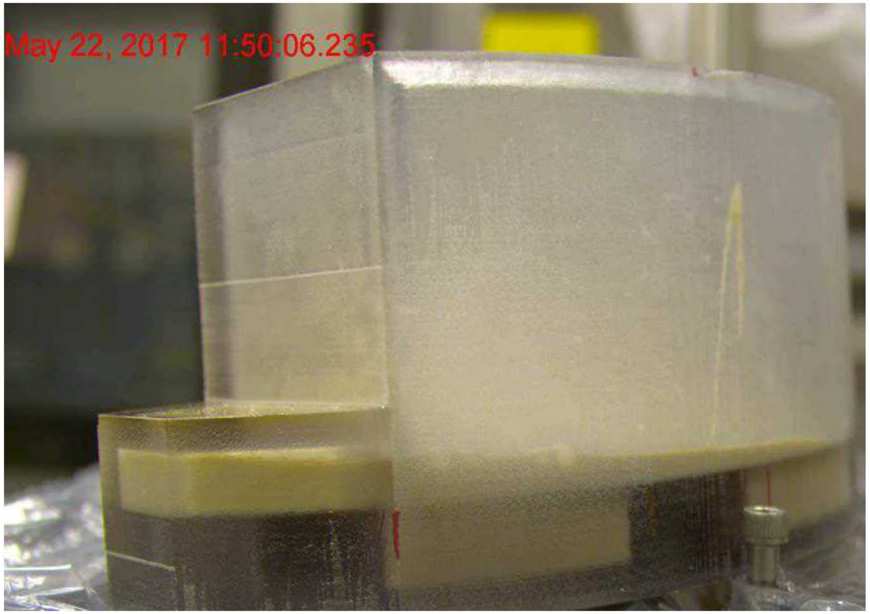


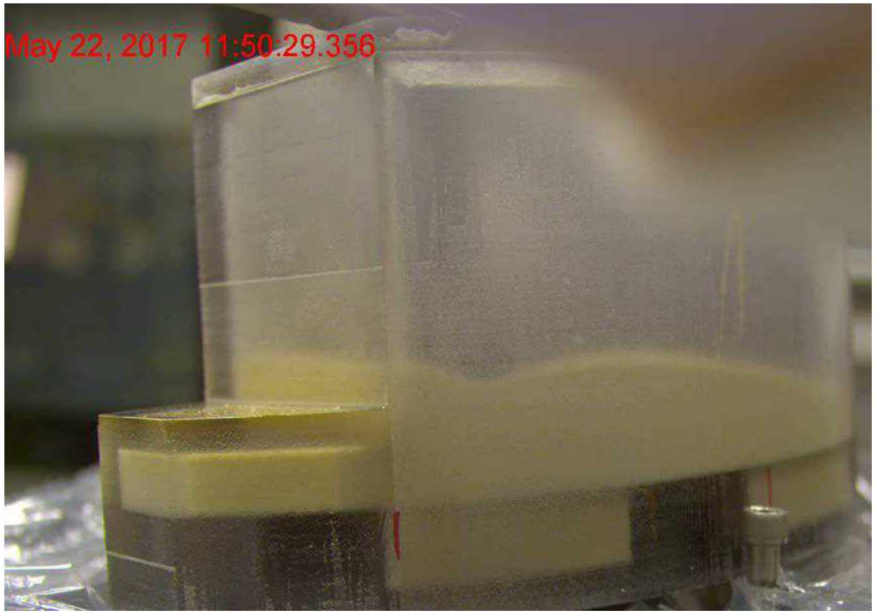


Shape of the model interface matches well with shape of experiment and the time-scale is similar

Shelf Feature Fills Well in Clear Mold

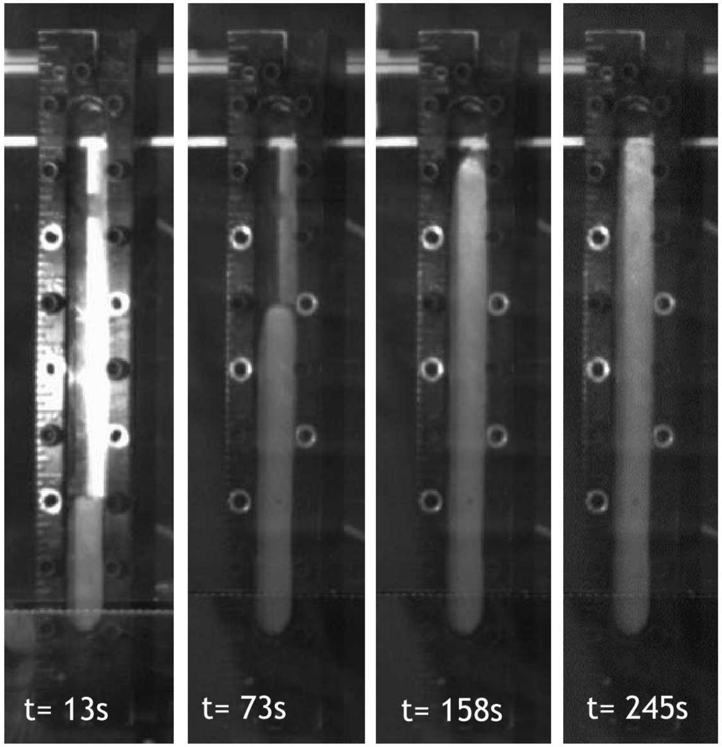




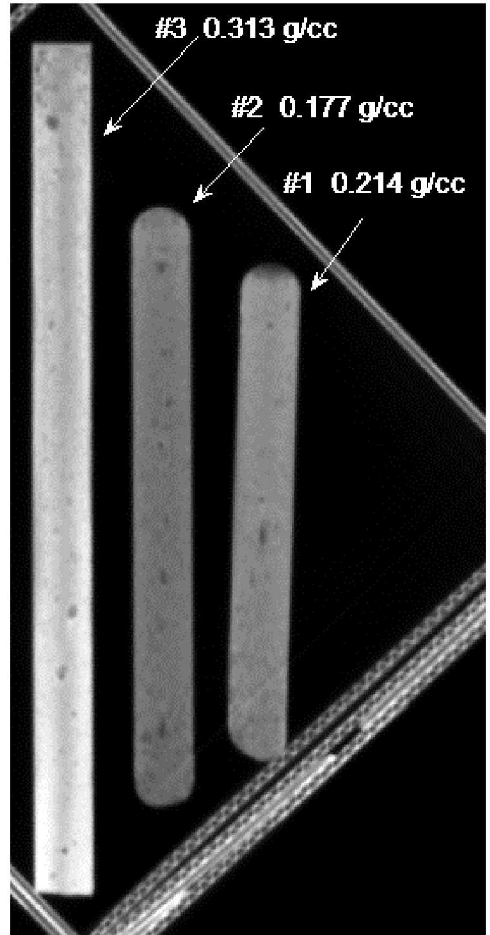


Experiment shows good filling of the shelf feature even at early times giving confidence in the foam model

Density Study for Structural Foam PMDI-10



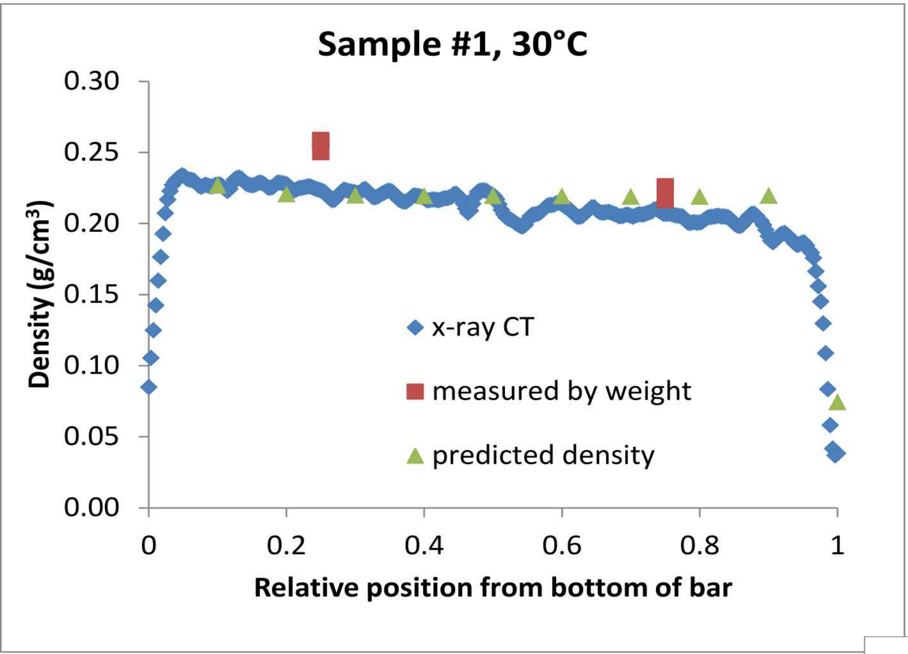
Foam expanding in a mold at 30°C. Time shown on frames is after the end of mixing the resin and the curative together for 45 seconds.

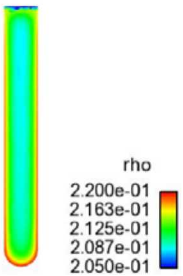


X-ray image of PMDI-10 foam bars: 1) free rise at 30°C, 2) free rise at 50°C, 3) over packed (1.5) at 30°C

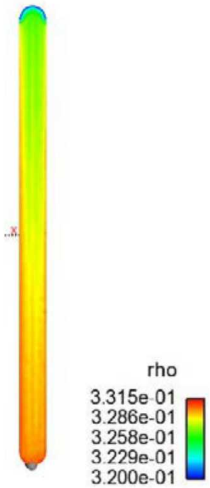
- Can the model predict the effects of over packing seen experimentally?
- Over-packed sample shows higher density and greater density variation
- 17% for free rise and 31% for over-packed foam bars

Density Study for Structural Foam PMDI-10

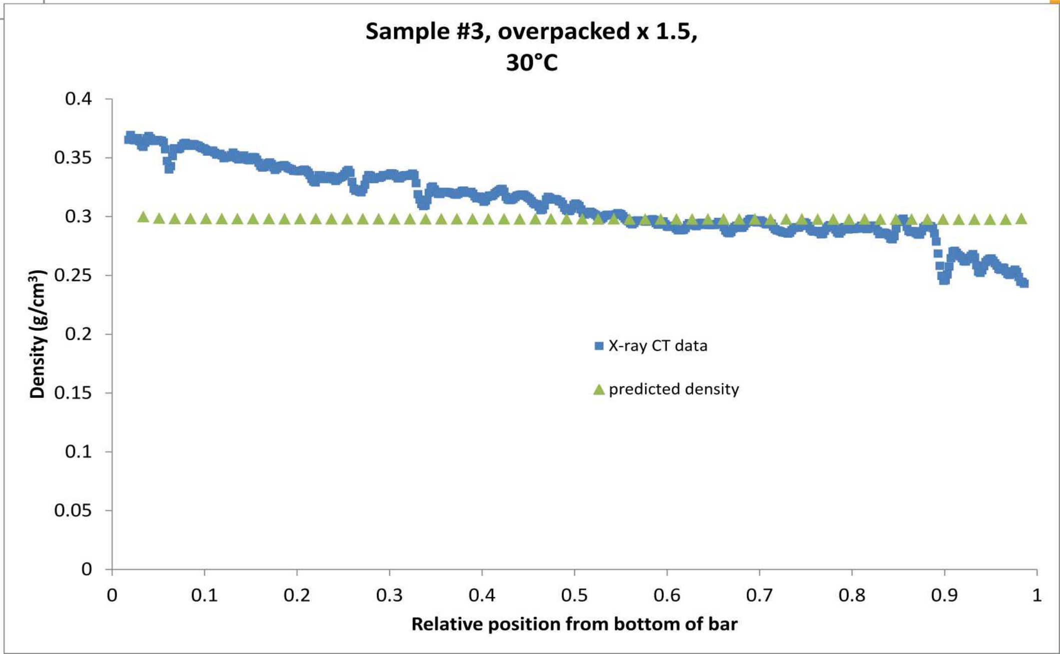




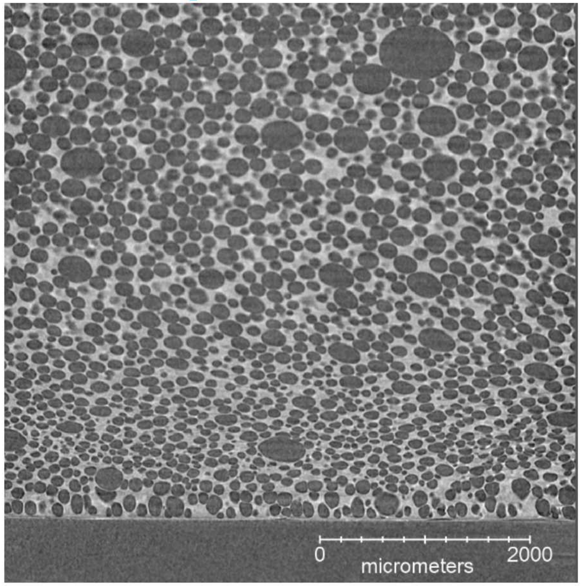
- Free rise foam density gradients. Plots are shown at the centerline of the foam cylinder
- Cylinder is under filled to give the free rise density

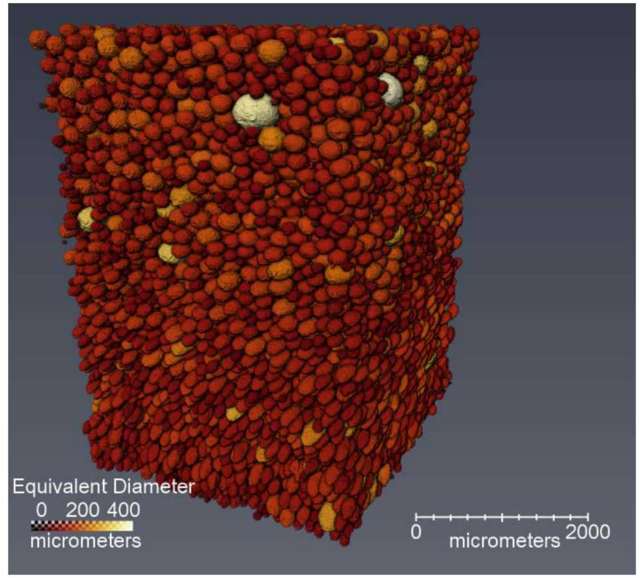


- Over packed (1.5) foam density gradients. Plots are shown at the centerline of the foam cylinder
- Self-closing vent lets air out, but keeps foam in for pressurization



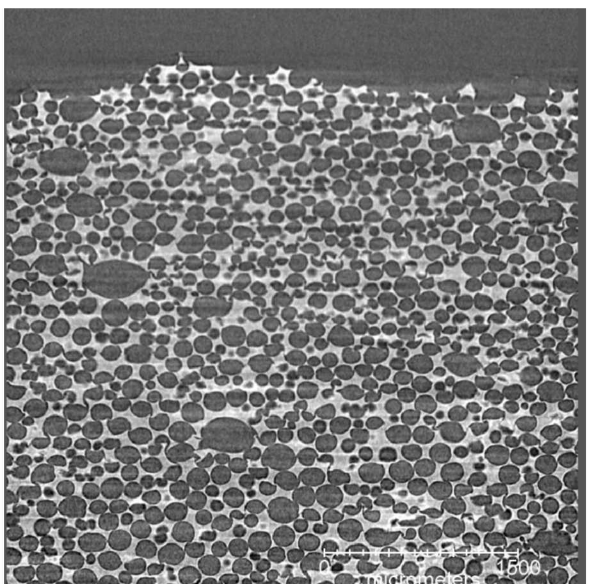
CT Microstructure of Bubbles from Large Complex Mold

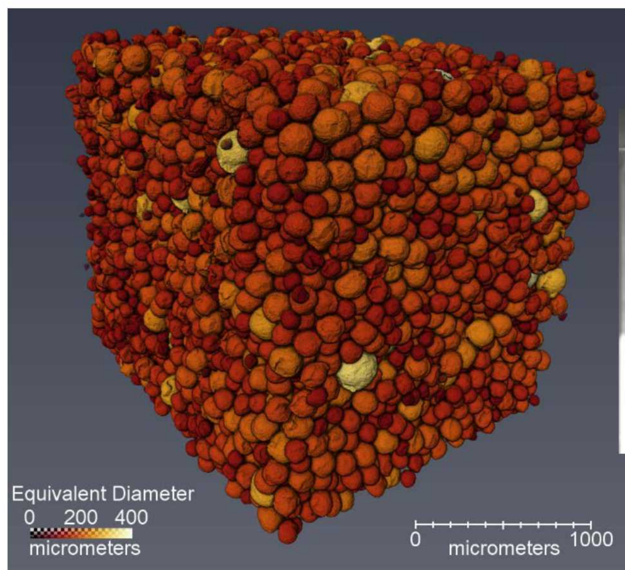


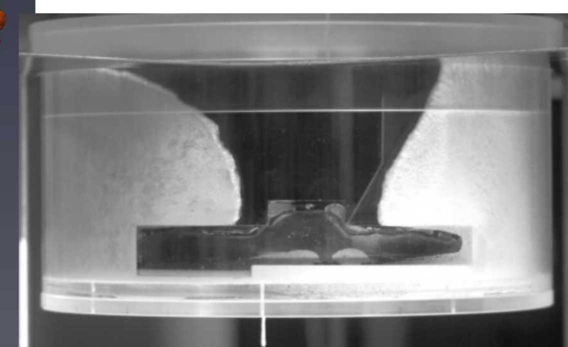


Sample 1 top

Foam microstructure
- Polydisperse bubble sizes
- Shear near boundaries cause elongated ellipsoidal bubbles



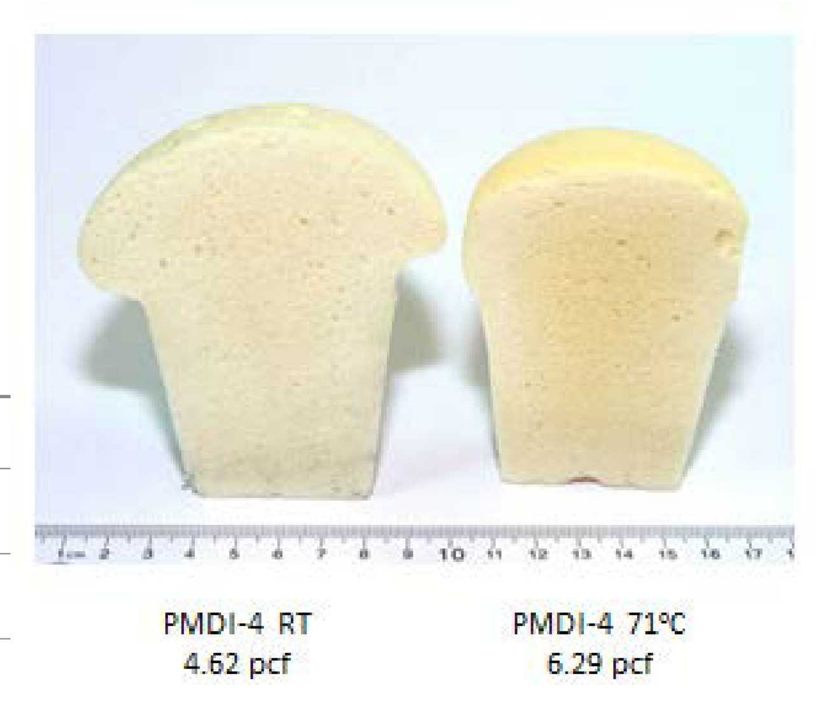


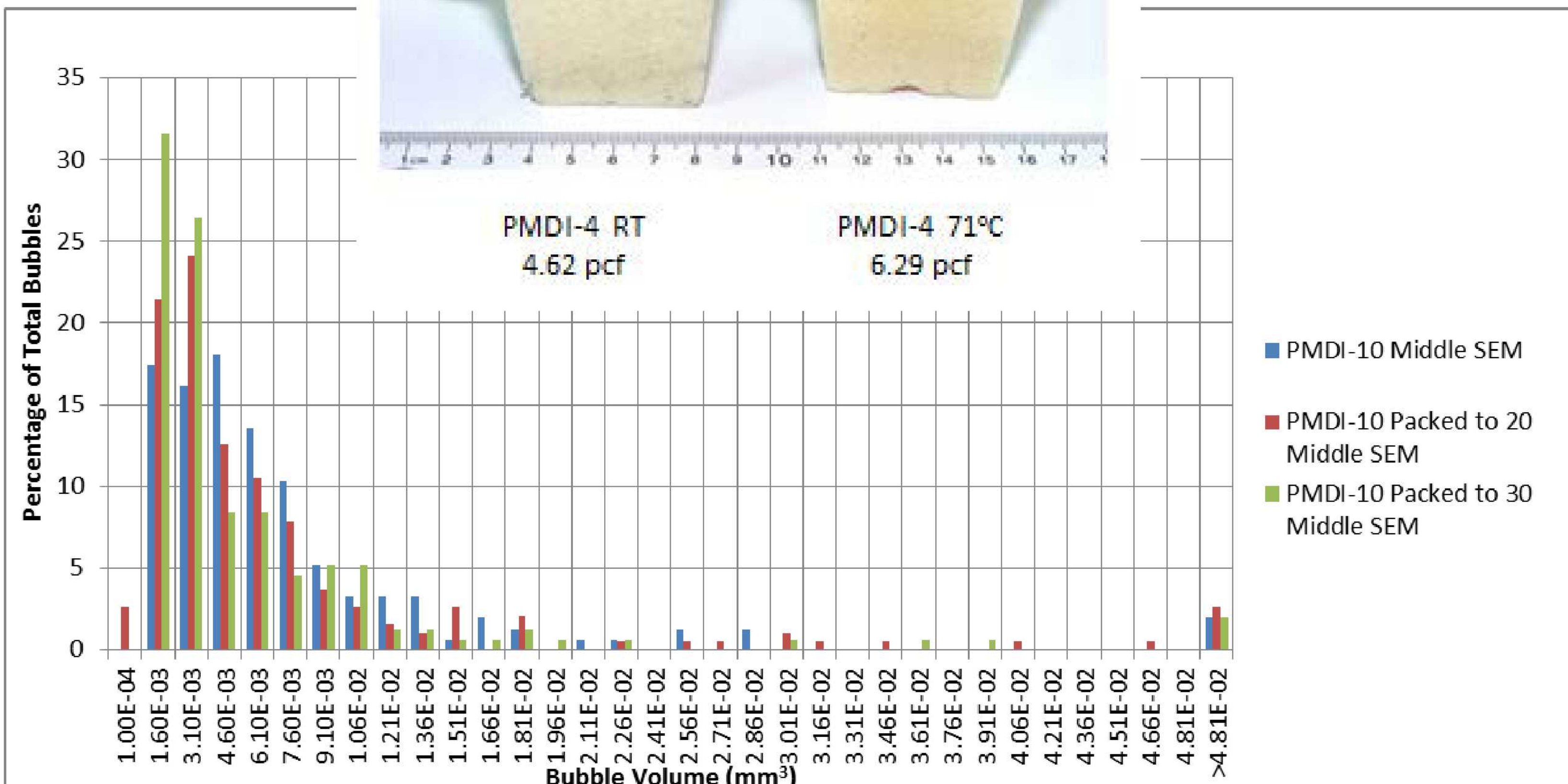


Sample 1 bottom

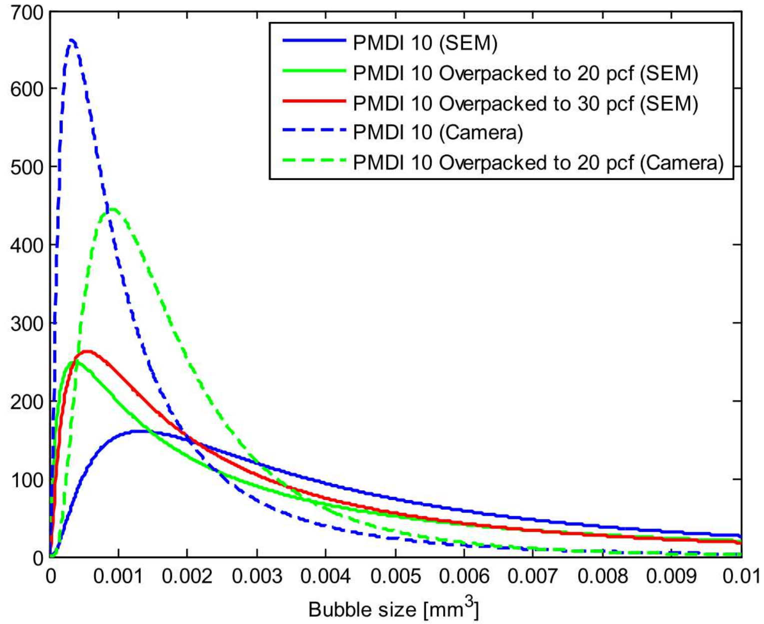
Brian M. Patterson, LANL, July 2016

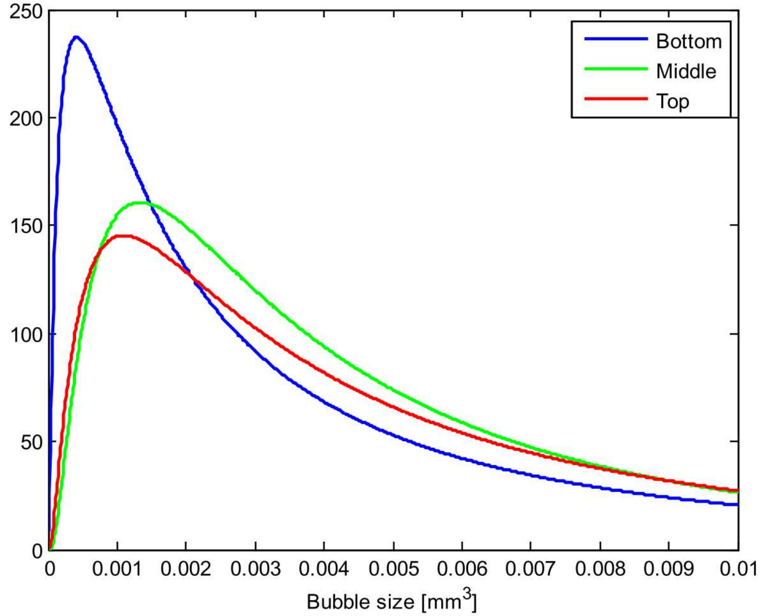
Processing Conditions Change Bubble-Size and Final Density

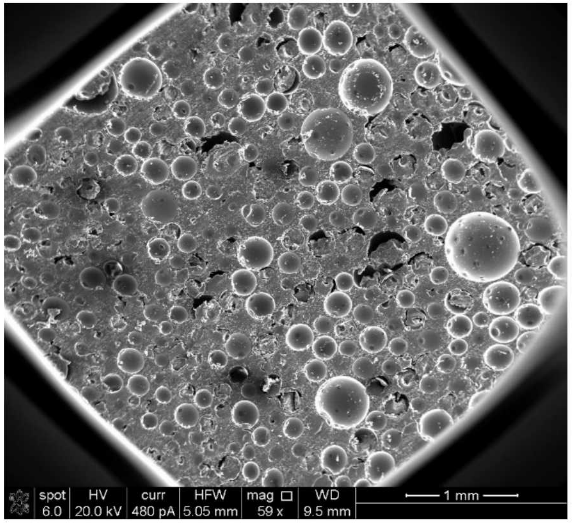




Bubble Size Data for PMDI-10 and Various Processing Conditions







Log-normal fits to bubble size measurements for (left) overpacked PMDI 10 foam and (right) PMDI 10 free rise foam of various channel height

Adding Bubble-Scale Information to Improve Model: Population Balance Equations

Population Balance Equation (PBE)

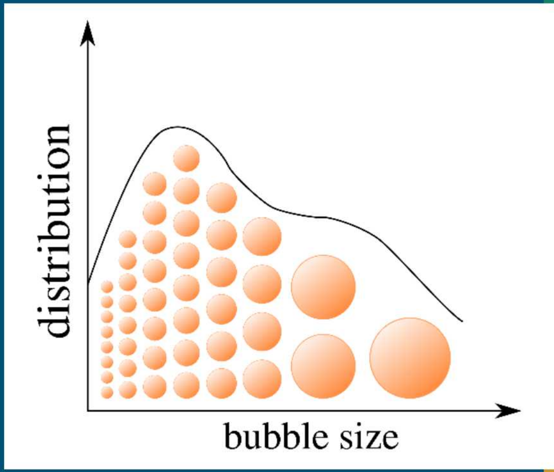
Bubble size distribution (BSD) is described by a number density function, $n(v)$, representing the number of bubbles per unit volume of liquid in volume between the range v and $v + dv$

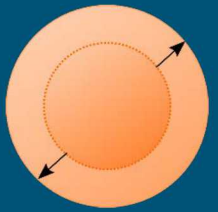
Evolution of the BSD is governed by the following Population Balance Equation

$$\frac{\partial n(v)}{\partial t} + \nabla \cdot (n(v)\boldsymbol{u}) + \frac{\partial}{\partial v}[n(v)G(v)]$$

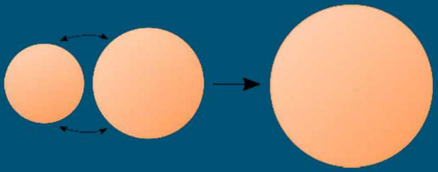
$$= \frac{1}{2}\int_0^v \beta(v', v - v')n(v')n(v - v')dv' - \int_0^\infty \beta(v, v')n(v)n(v')dv'$$

Where $\beta(\mathrm{v}', \mathrm{v})$ represents the coalescence kernel, and $G(v)$ represents the growth rate of bubbles.





Growth Rate Kernel, $G(v)$



Coalescence Kernel, $\beta(v, v')$

References
Karimi et al. 2017, Computer Physics Communications
Karimi et al. 2016 Macromolecular Symposia
Karimi et al. 2017 Computer Physics Communications

Transformation to Moment-Based Transport Equations

$$m_k(t,x) = \int_0^\infty n(v) v^k dv$$

Transformed PBE:

$$\frac{\partial m_k}{\partial t} + \boldsymbol{u} \cdot \nabla m_k = G_k + S_k , \qquad k = 0,1,2,3$$

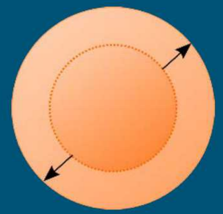
G_k is a source term relating to the growth rate, and S_k relates to coalescence

Quadrature method of moments (QMOM) is used to compute the source terms

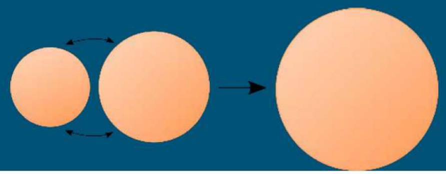
Use the first 4 moments to represent our PBE

Moments offer useful information:

- m_0, total number of bubbles per unit liquid volume
- m_1, total bubble volume per unit liquid volume
- m_2 and m_3 related to the variance and skewness of the BSD



$$\bar{G}_k \cong \sum_{i=1}^{N} w_i G(v_i) v_i^{k-1}$$



$$\bar{S}_k \cong \frac{1}{2} \sum_{a=1}^{N} \sum_{b=1}^{N} w_a w_b \left[(v_a + v_b)^k - v_a^k - v_b^k \right] \beta(v_a, v_b)$$

Volume fraction of gas

$$\frac{m_1}{1 + m_1}$$

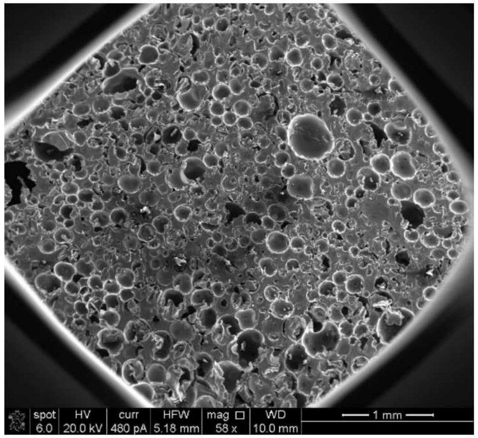
Mean bubble diameter

$$\left(\frac{m_1}{m_0} \frac{6}{\pi} \right)^{\frac{1}{3}}$$

References: Marchisio, Fox 2005 Journal of Aerosol Science, Karimi et al. 2016 Macromolecular Symposia, & Karimi et al. 2017 Computer Physics Communications

Improvements to PBE-QMOM Foam Model

- Initial model based on linking our kinetics with Karimi PBE-QMOM model could not simultaneously fit density and bubble size distribution
- New bubble growth kernel to account for decreased growth with increasing viscosity
- New coalescence kernels was added to account for bubble size and polymerizing viscosity
- Adaptive Wheeler integration model to eliminate negative moments
- With these changes, we were able to fit experimental data well.



SEM near middle of bar

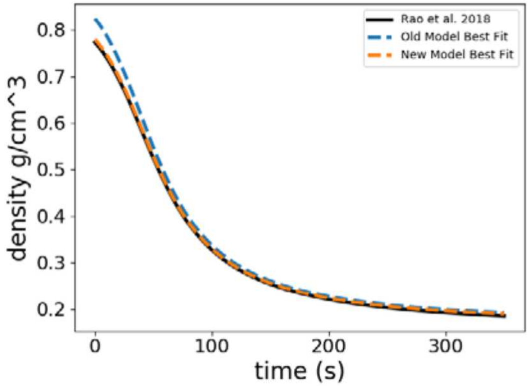
Population balance equation, which is solved using QMOM:

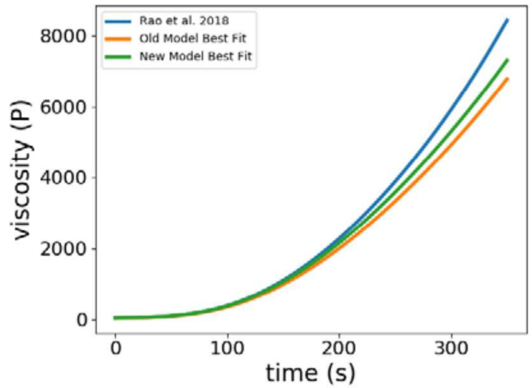
$$\frac{\partial n(v)}{\partial t} + \nabla \cdot (n(v)\boldsymbol{u}) + \frac{\partial}{\partial v}[n(v)G(v)]$$

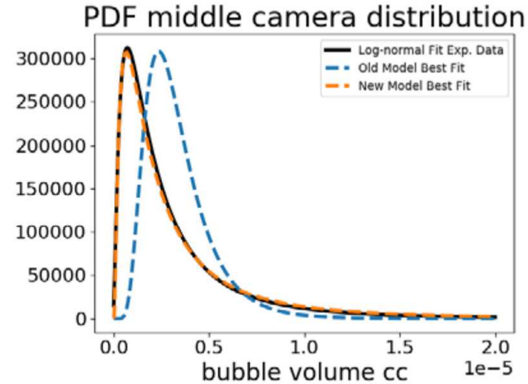
$$= \frac{1}{2}\int_0^v \beta(v', v - v')n(v')n(v - v')dv' - \int_0^\infty \beta(v, v')n(v)n(v')dv'$$

$\beta(v', v)$ isthe coalescence kernel, and $G(v)$ represents the growth rate

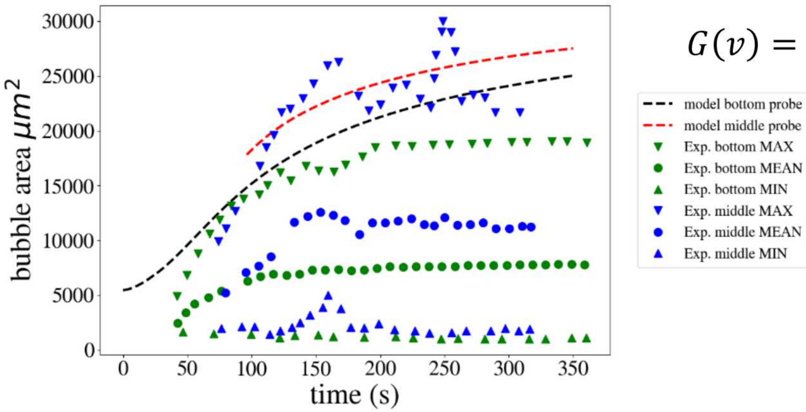
	Old Model	New Model
$G(v)$	$G_0\left(\max\left(0, \frac{w - w_{max}}{w_{max}}\right)\right)$	$G_0\frac{\mu_{ref}}{\mu}\left(\max\left(0, \frac{w - w_{max}}{w_{max}}\right)\right)$
$\beta(v', v)$	$\beta_0(v + v')$	$\beta_0\frac{\mu_{ref}}{\mu}(v + v')\max\left(\frac{v}{v'}, \frac{v'}{v}\right)$





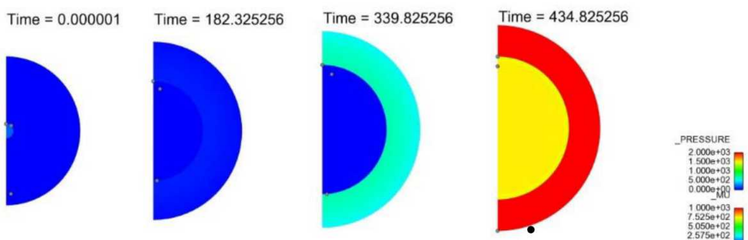


3D ALE Bar Modeling Results: New Pressure-Dependent Growth Term Mimics Local Bubble-Scale Effects



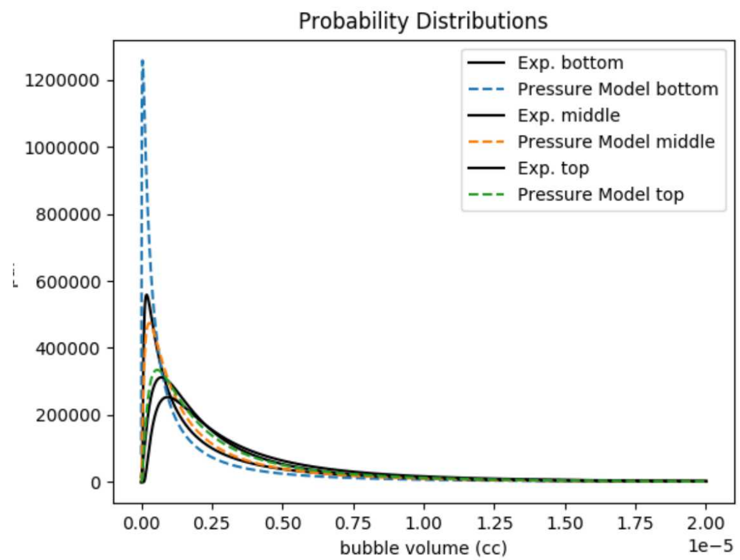
$$G(v) = G_0 \frac{\mu_{ref}}{\mu} \frac{(p_{CO_2} - 2\frac{\sigma}{R} - p_{ref})^2}{(p - p_{ref})^2} \left(\max\left(0, \frac{w_{CO_2} - w_{max}}{w_{max}}\right)\right)$$

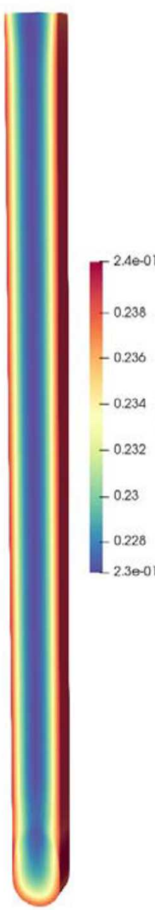
New growth term decreases with viscosity and pressure



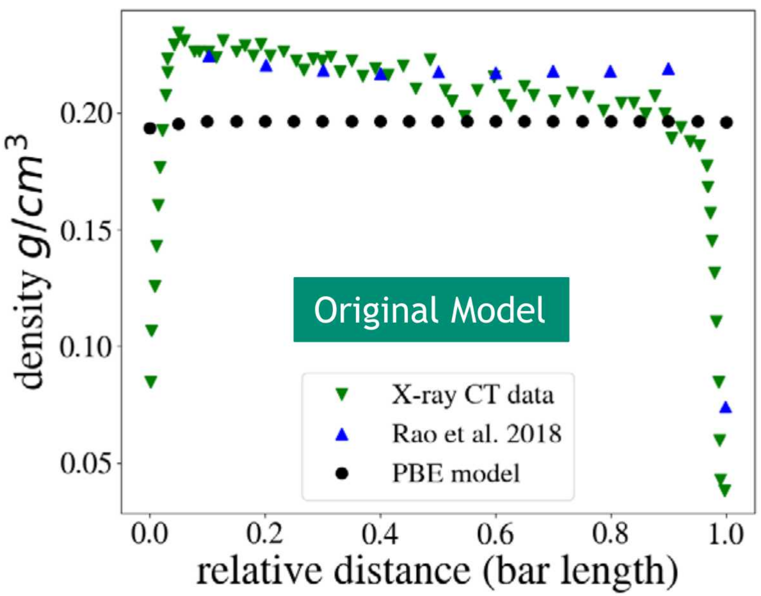
$$p_{gas} - p_{liq} - 2\frac{\sigma}{R} \approx 4\eta_{polymer} \frac{\dot{R}}{R}$$

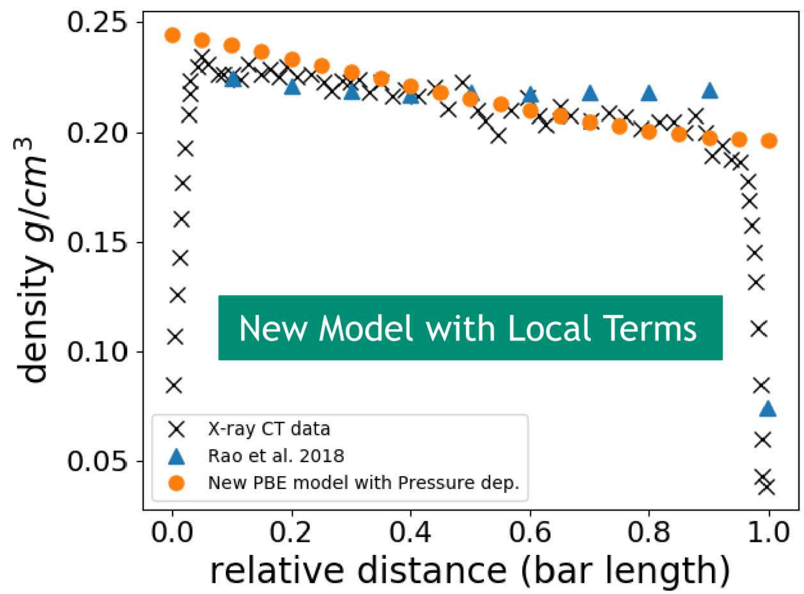
$$\frac{\dot{R}}{R} \approx \frac{\Delta p_{ref}}{4(\Delta p)^2 \eta_{polymer}}$$

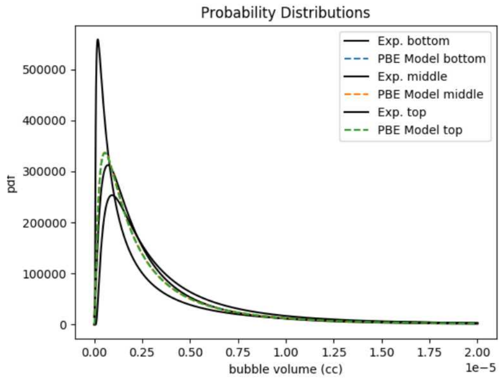


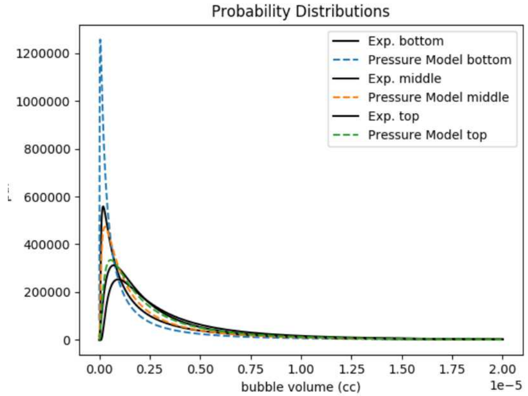


3D ALE Bar Modeling Results





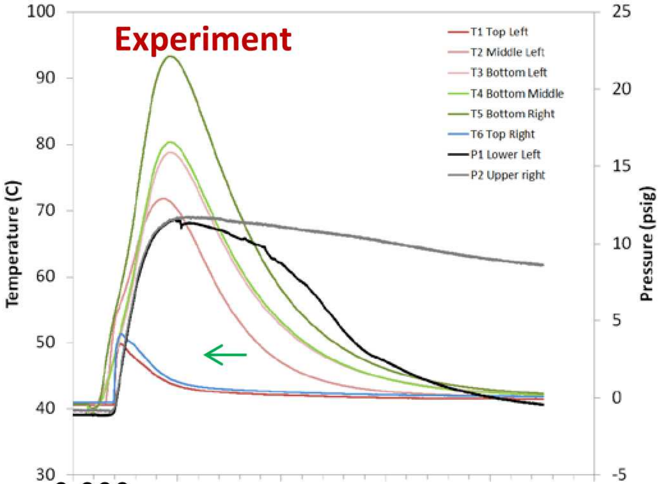


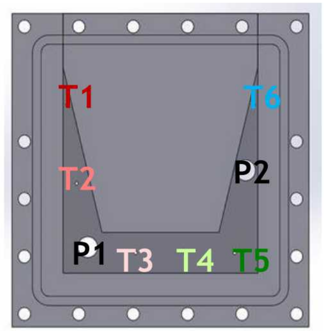


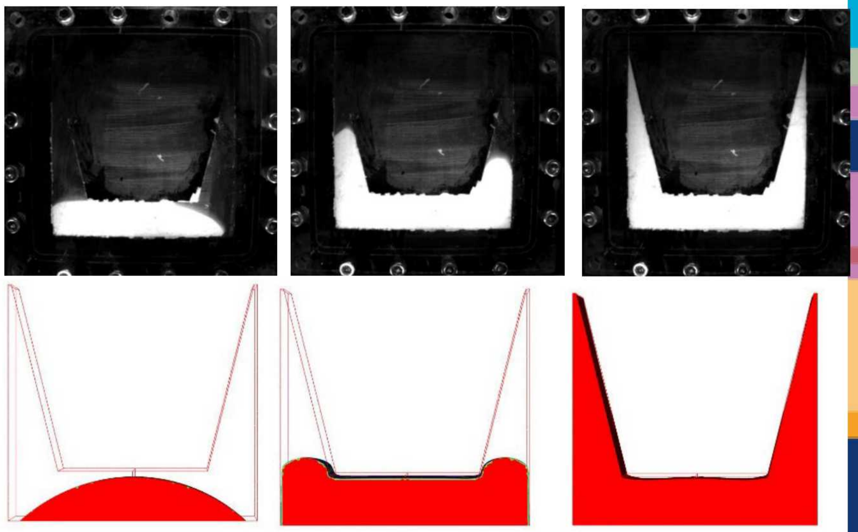
- Changes in bubble-size distribution from top to bottom can be seen if we use a pressure-dependent bubble growth kernel.
- The pressure-effect allows us to successfully predict the density gradient for the bar experiment for the first time!

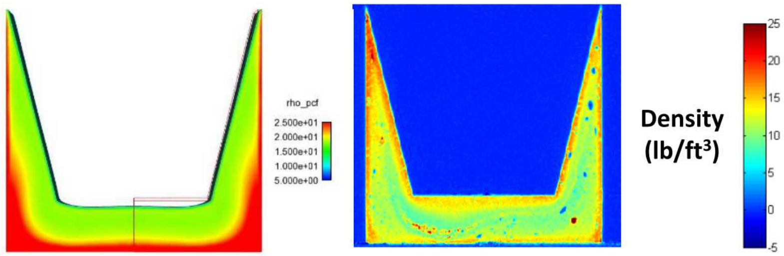
Lower Density Gradients from New Model

- 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.



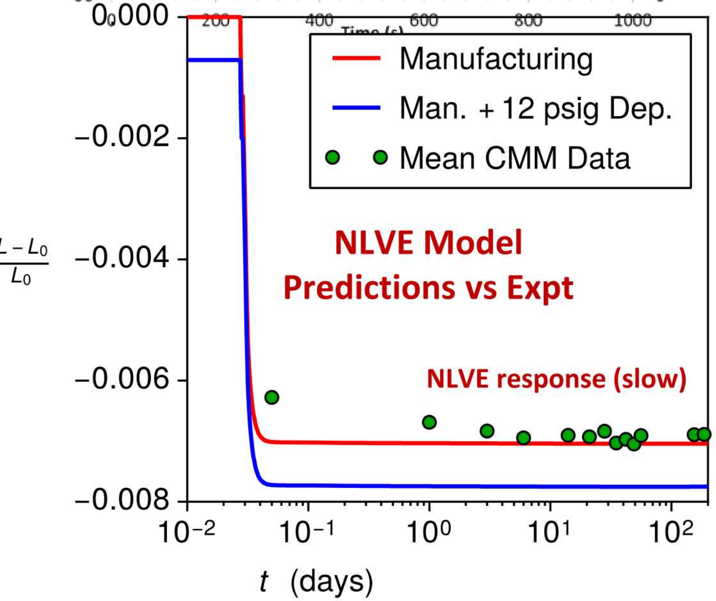






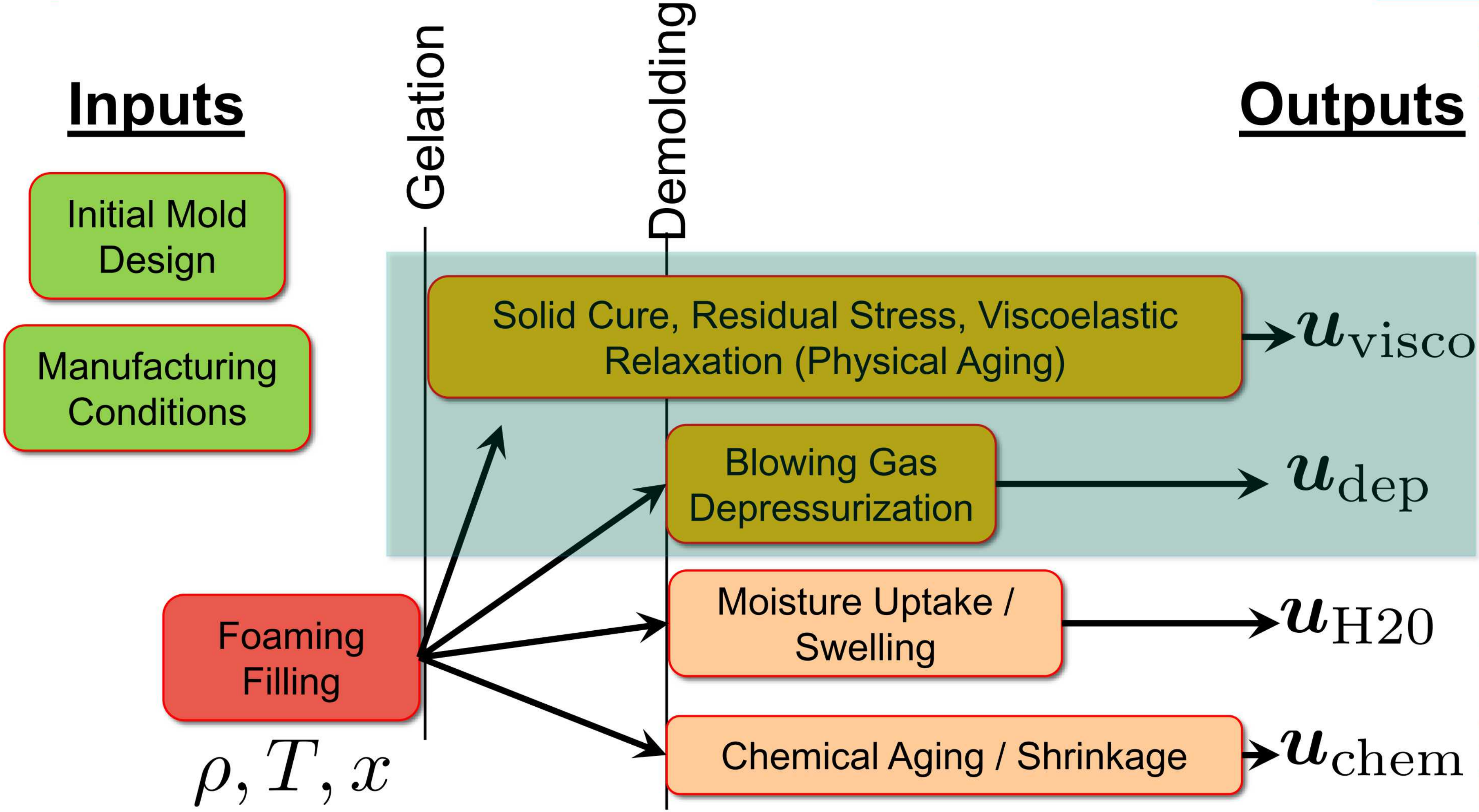
Model

X-ray CT Data (Thompson, 2016)



Model prediction captures thermal contraction
Relaxation of residual stress is extremely slow (eons)

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

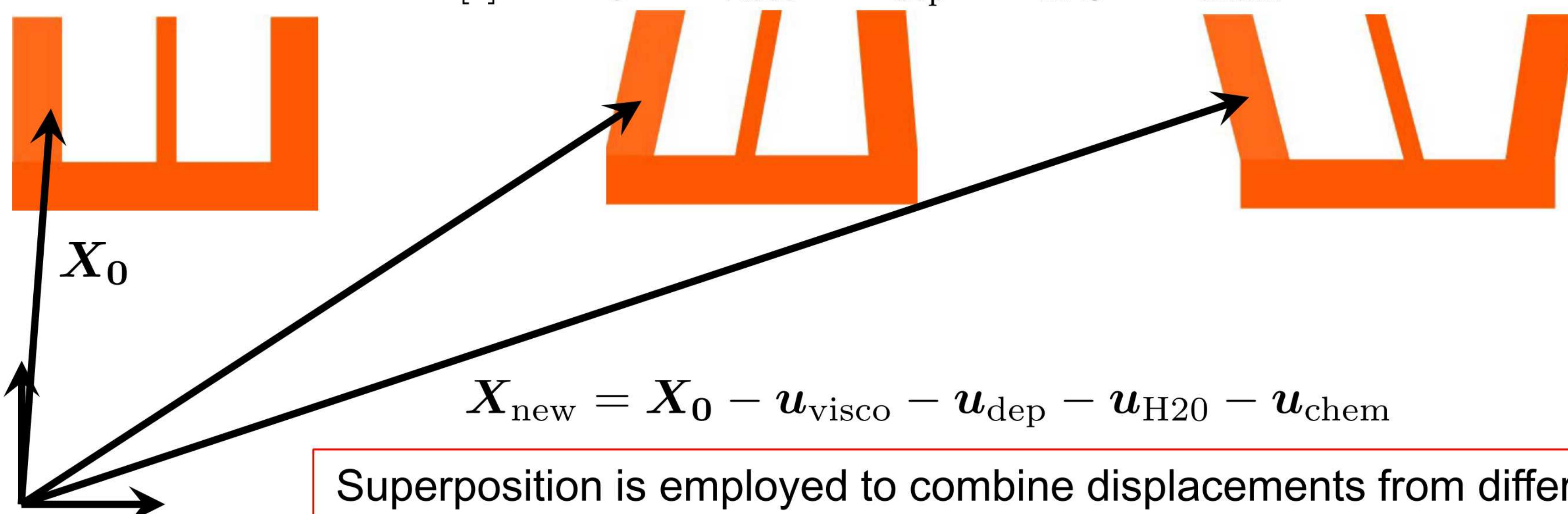
Inputs

- Manufacturing Conditions
- Initial Mold Design

→ Cradle-to-Grave Simulation → Final Mold Shape

Output

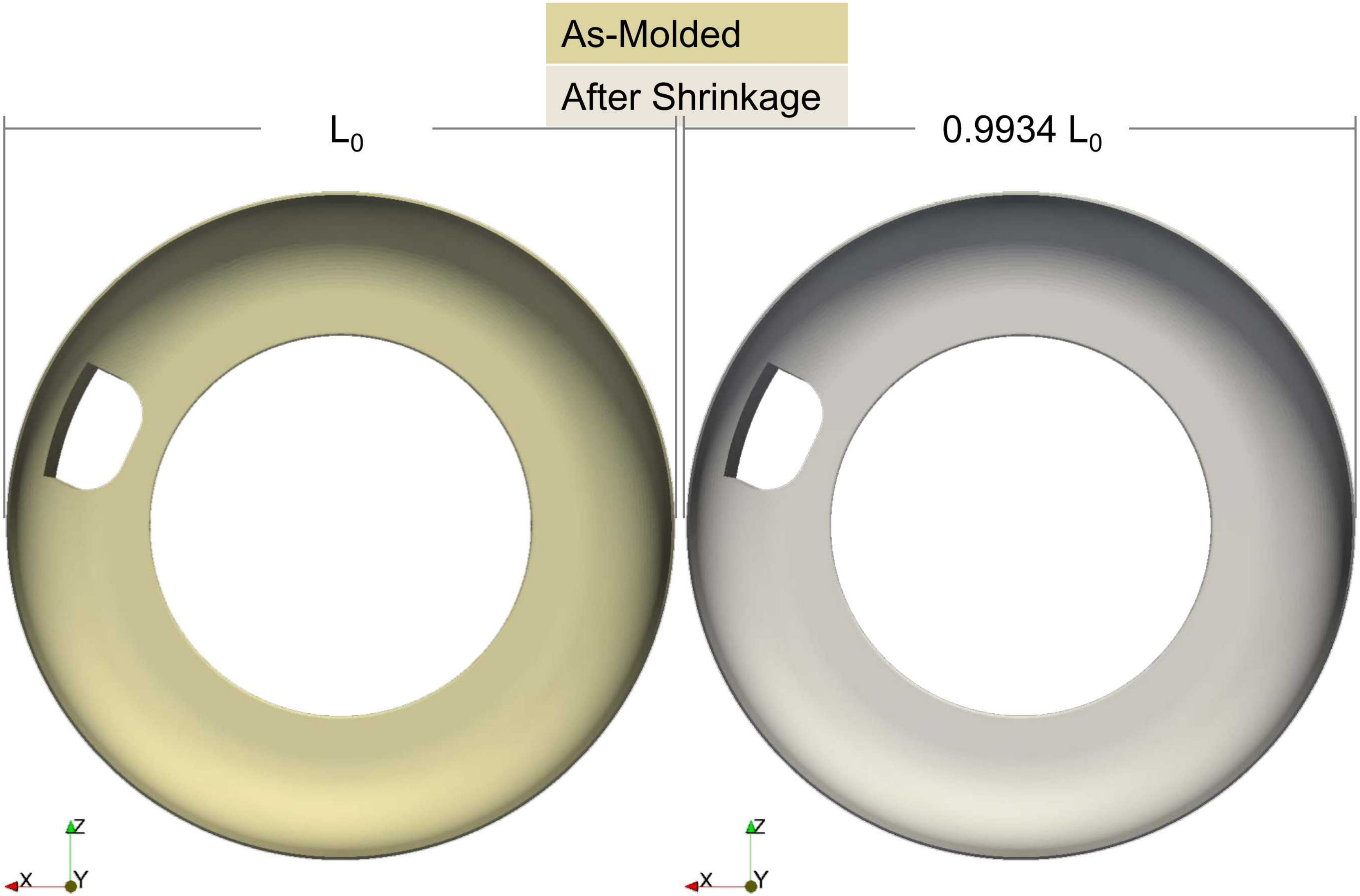
$$\boldsymbol{X}[t] = \boldsymbol{X_0} + \boldsymbol{u}_{\text{visco}} + \boldsymbol{u}_{\text{dep}} + \boldsymbol{u}_{\text{H20}} + \boldsymbol{u}_{\text{chem}}$$



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

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

Exemplar Part With Featured Regions



Warpage accentuated near holes and slender regions

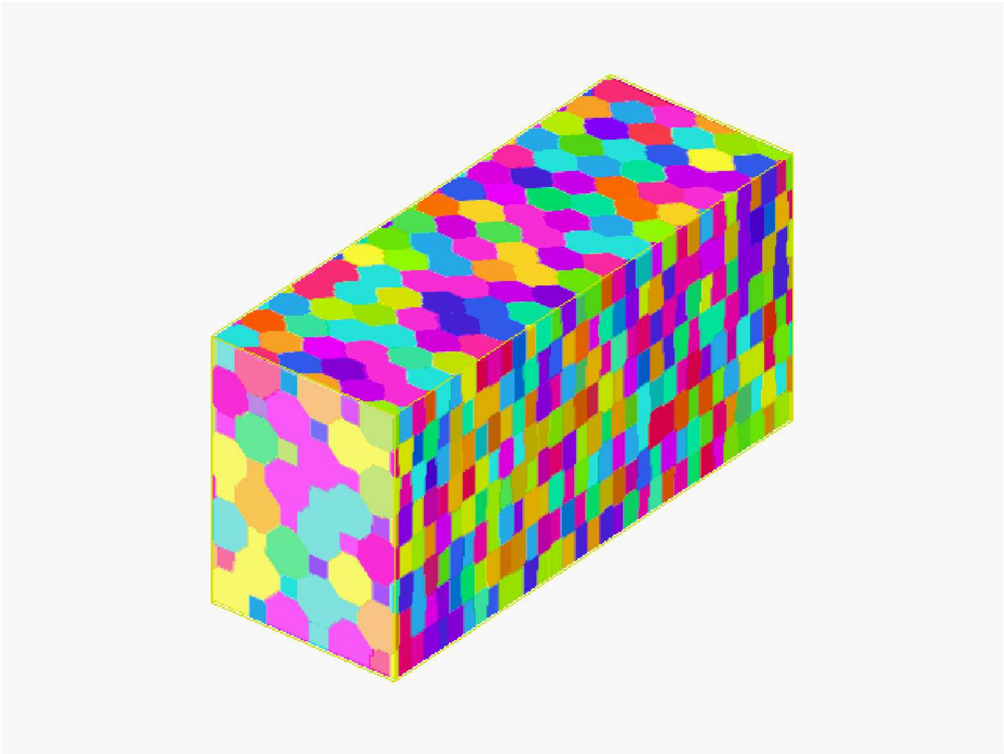
Displacement scaled 50x to emphasize shape change.

Conclusions and Future Work

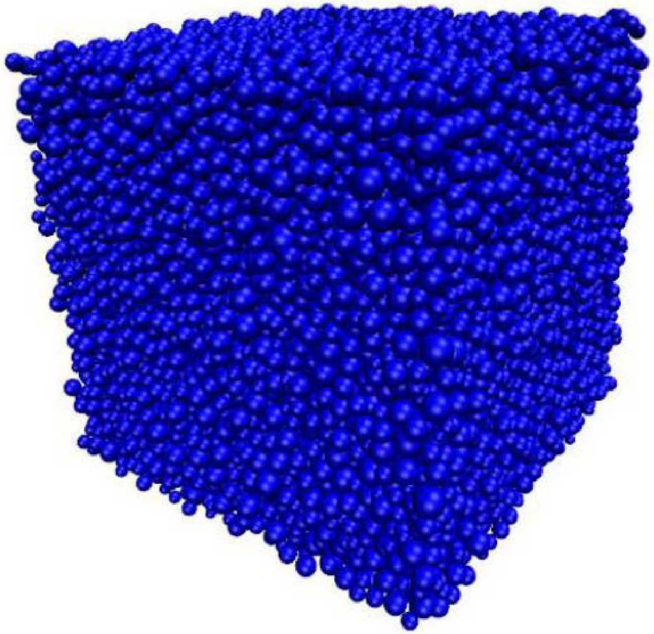
- **Current model is adequate for production calculation**
  - Determining metering, initial placement, voids, gate, and vent location, manufacturing stresses and initial foam shape
  - Current model is "first order." We are working to make the model more predictive
  - Model follows free surface of foam fairly well
  - Combination of experimental and computational work led to synergistic breakthroughs creating confidence in mold redesign
  - Density and density gradients are still not quantitative and give direction for future work -> bubble-scale modeling
- **Next generation model needs to include**
  - Equation of state for density approach for gas phase
  - Two-phase CO_2 generation model: solubilized CO_2 in the polymer and CO_2 gas in the bubbles
  - Population balance for bubble size evolution linked to single bubble model

Future work includes more multiphysics modeling to understand foam parts from manufacturing to 30 year.

Questions?



Pott's model of foam bubbles in shear flow (Veena Tikare, SNL)



Polydisperse bubble microstructure generated with LAMMPS and Aria/CDFEM (Dan Bolintineanu , SNL)