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Polyurethane Foam Manufacturing Models Using a FEM-Level Set-Population Balance Approach

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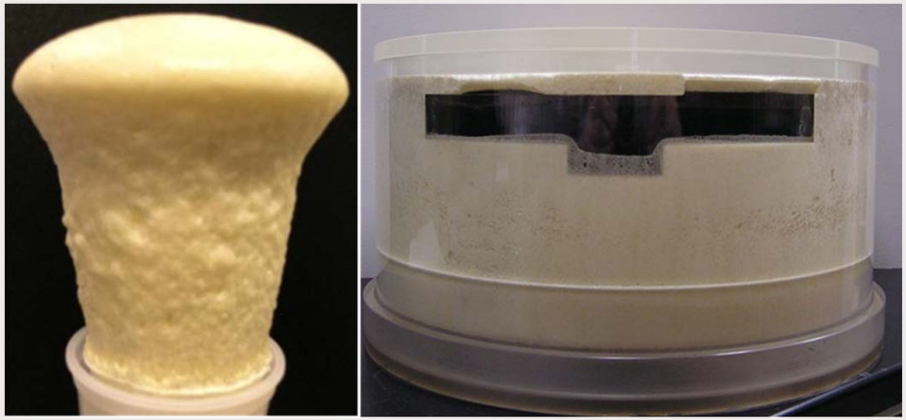
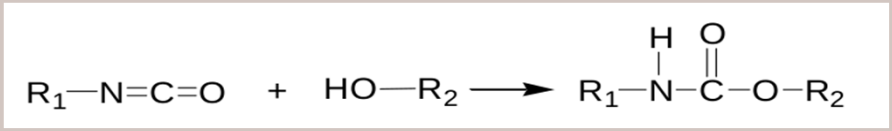
Polyurethane Foams



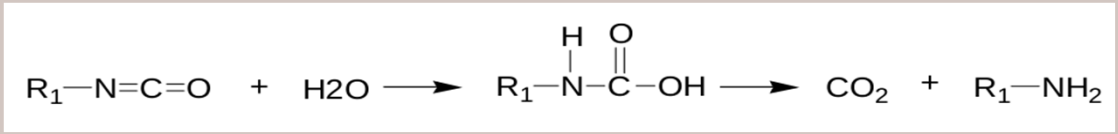
Polyurethane foams are widely used in manufacturing due to ease of use and useful material properties

We are focusing on modeling PMDI-10 a foam which is used for structural parts

Key reactions:

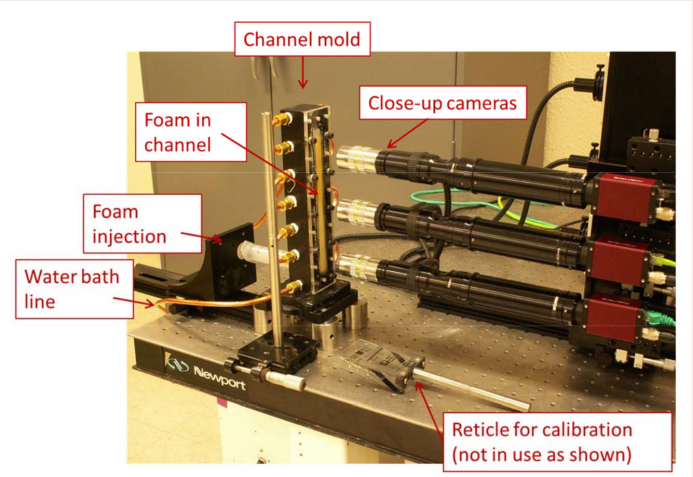


Isocyanate and Polyol -> polyurethane formation

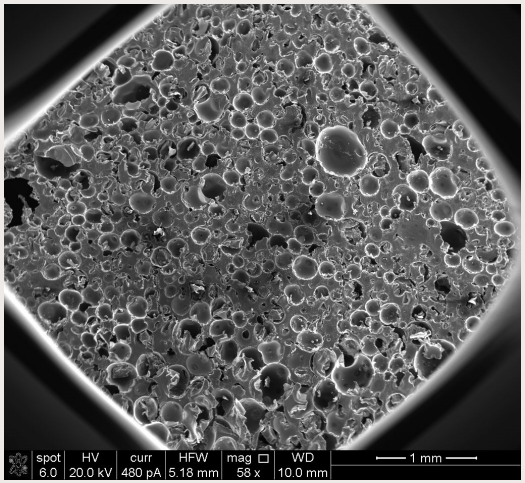


Isocyanate and Water -> CO_2 and an amine

Experimental Data



Experimental Setup



SEM near middle camera

Experimental data of foam rising in bar mold.

- rise over time
- bubble size over time from cameras
- X-ray CT data of final bar density
- SEM data of final bubble sizes.
- Diffusion wave spectroscopy (DWS) of bubble diameters over time.
- Various other experiments for measuring density and reactions over time

Mondy et al. (Submitted 2021 AIChE Journal)
Mondy et al. 2014 Tech. Report SAND2014-3292
Roberts et al. 2016 Tech. Report SAND2016-5445

Momentum and Mass Conservation

Continuity

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

Continuity is the main driver of flow in our problems as the density is decreasing over time due to foaming reactions

Conservation of Momentum

$$\rho\left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u}\right) + \nabla p - \nabla \cdot \left(\eta(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T) - \left(\frac{2}{3}\eta - \kappa\right)(\nabla \cdot \boldsymbol{u})\boldsymbol{I}\right) - \rho \boldsymbol{g} = \boldsymbol{0}$$

Rao et al. 2018 Computers & Fluids
Ortiz et al. (Submitted 2021 AICHe Journal)

Polymerization

We track polymerization as an extent of reaction as our isocyanate is always in excess for our foam

$$\frac{\partial \xi}{\partial t} + \nabla \cdot (\boldsymbol{u}\xi) - D_\xi \nabla^2 \xi = k(b + \xi^m)(1 - \xi)^n$$

Where k is an Arrhenius type equation with a Williams-Landal-Ferry shift factor:

$$k = \left(\frac{1}{(1 + w a_T)^\beta} \right) k_0 e^{E_\xi / RT}$$

Where T_g is the glass transition temperature following the Di Benedetto form.

Details can be found in Rao et al. 2018 Computers and Fluids

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

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

Energy Balance

We treat heat capacity and density as constants in our energy balance equation

Temperature increases as our foam reacts.

$$\rho C_p \left(\frac{\partial T}{\partial t} + \boldsymbol{u} \cdot \nabla T \right) - \nabla \cdot k \nabla T = \Delta H_{rxn} Y \rho \frac{\partial \xi}{dt}$$

Heat Capacity, C_p, and conductivity k are dependent on the foam gas liquid makeup and are fit using a mixture theory model

Rao et al 2018. Computers and Fluids

ΔH_{rxn}, Heat of Reaction

Y, liquid mass fraction

ξ, extent of polymerization

Population Balance

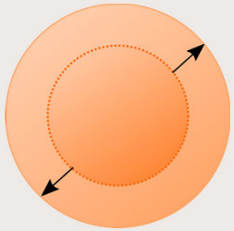
Bubble size distribution (BSD) is described by a number density function, $n(v)$, representing the number of bubbles per unit volume of liquid in volume between the range v and $v + dv$ (*Karimi et al. 2017, Computer Physics Communications*)

Evolution of the BSD is governed by the following Population Balance Equation (*Karimi et al. 2016 Macromolecular Symposia, Karimi et al. 2017 Computer Physics Communications*):

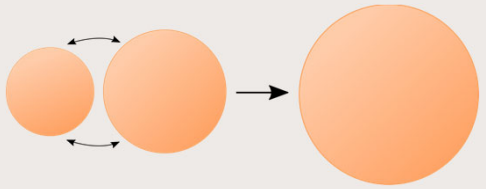
$$\frac{\partial n(v)}{\partial t} + \nabla \cdot (n(v)\boldsymbol{u}) + \frac{\partial}{\partial v}[n(v)G(v)]$$

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

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



Growth Rate Kernel, $G(v)$



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

Population Balance: Quadrature Method of Moments

Transformation into moments:

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

Transformed PBE:

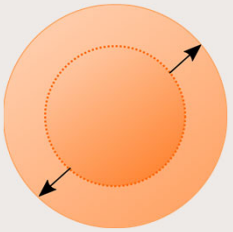
$$\frac{\partial m_k}{\partial t} + \nabla \cdot (\boldsymbol{u} m_k) = G_k + S_k\,, \qquad k = 0,1,2,\ldots,N_{moments}$$

- G_k is a growth rate source
- S_k is a source from coalescence of bubbles
- Quadrature method of moments (QMOM) is used to compute the source terms
- We use the first 4 moments to represent our PBE
- Moments offer useful information:

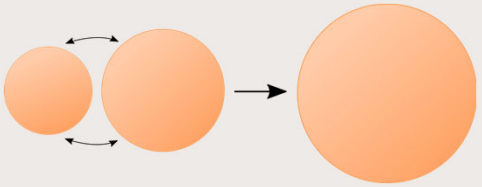
  m_0, total number of bubbles per unit liquid volume

  m_1, total bubble volume per unit liquid volume

  m_2 and m_3 related to the variance and skewness of the BSD
- Quadrature nodes/weights computed using Yuan and Fox's adaptive-Wheeler algorithm (Yuan, C., and R.O. Fox. 2011 Journal of Computational Physics)



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



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

Useful information from moments:

Volume fraction of gas	Mean bubble volume
$\frac{m_1}{1+m_1}$	$\frac{m_1}{m_0}$

Growth and Coalescence Kernels

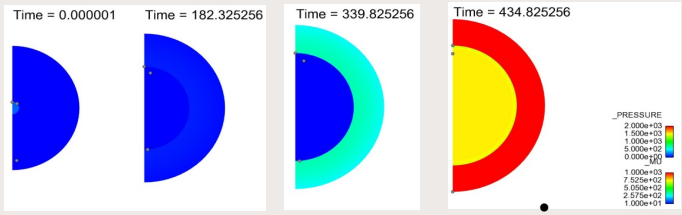
We try to capture variations in density along the height of experimental data by adding pressure and viscosity dependence to kernels from Karimi et al. 2017 (Computer Physics Communications) borrowing ideas from single bubble models

Our pressure scaling is based on system pressure as we do not track bubble pressure.

This seems to improve overall results while still being a pseudo bubble pressurization term.

Bubble growth and Coalescence are slowed by scaling with the inverse of the foam viscosity μ

Simplified Rayleigh-Plesset Equation



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

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

	Karimi et al. 2017	Pressure and Viscosity Dependent
$G(v)$	$C_0\left(\max\left(0, \frac{w - w_{max}}{w_{max}}\right)\right)$	$C_0\left(\frac{P_{ref}^2}{(P - P_{ref})^2}\right)\frac{\mu_{ref}}{\mu}\left(\max\left(0, \frac{w - w_{max}}{w_{max}}\right)\right)$
$\beta(v', v)$	$\beta_0(v + v')$	$\beta_0\frac{\mu_{ref}}{\mu}(v + v')$

Coalescence of $\beta(v', v) = \beta_0(v + v')$ represents bubbles of volume v and v' coalescing and creating a bubble of volume $v + v'$ at a rate β_0

C_0, β_0 constant coefficients
w_{max} maximum solubility
P_{ref} reference pressure (often atm.)
μ_{ref} reference viscosity

Governing Equations: Kinetics

$$\frac{\partial C_{H_2O}}{\partial t} + \boldsymbol{u} \cdot \nabla C_{H_2O} - D_{H_2O} \nabla^2 C_{H_2O} = -k_{H_2O} C^p_{H_2O}$$

$$\frac{\partial C^{liq}_{CO_2}}{\partial t} + \boldsymbol{u} \cdot \nabla C^{liq}_{CO_2} - D^{liq}_{CO_2} \nabla^2 C^{liq}_{CO_2} = k_{H_2O} C^p_{H_2O} - \bar{G}_1 \frac{P}{RT}$$

$$\frac{\partial C^{gas}_{CO_2}}{\partial t} + \boldsymbol{u} \cdot \nabla C^{gas}_{CO_2} - D^{gas}_{CO_2} \nabla^2 C^{gas}_{CO_2} = \bar{G}_1 \frac{P}{RT}$$

To account for growth rates of bubbles we have equations for both concentrations of liquid CO_2 and gaseous CO_2 and relate these based on growth rate determined by the QMOM

$$k_{H_2O} = A_{H_2O}\, e^{-E_{H_2O}/RT}$$

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

Where w_{CO_2} and w_{max} are mass fraction of liquid CO_2 and mass fraction related to the maximum solubility of liquid CO_2

$\bar{G}_1$ is the source for m_1 (total bubble volume per unit liquid volume)

Material Model: Density

We represent the density as a combination of the liquid and gas density found in the foam

$$\rho_{foam} = \rho_{gas}\psi + \rho_{liquid}(1 - \psi)$$

Volume fraction of gas

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

Where ψ represents a volume fraction of gas

$$\nu = \frac{V_{gas}}{V_{liquid}} = \frac{M_{CO_2} C_{CO_2}}{\rho_{gas}}$$

$$\psi = \frac{\nu}{1 + \nu}$$

The density of gas is based on the ideal gas law

$$\rho_{gas} = \frac{P M_{CO_2}}{RT}$$

Rao et al. 2018 Computers and Fluids
Ortiz et al. (Submitted 2021 AICHe Journal)

Material Model: Viscosity

Extra stress tensor:

$$\boldsymbol{\tau} = \eta(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T) - \left(\frac{2}{3}\eta - \kappa\right)(\nabla \cdot \boldsymbol{u})\boldsymbol{I}$$

The viscosity follows a Taylor-Mooney form derived from emulsion experiments

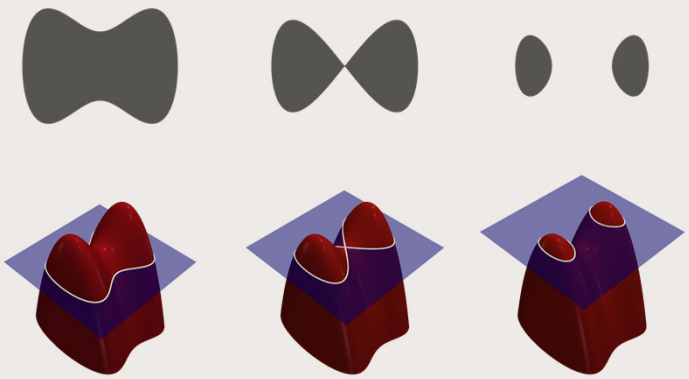
$$\eta = \eta_0 \exp\left(\frac{\psi}{1-\psi}\right)$$

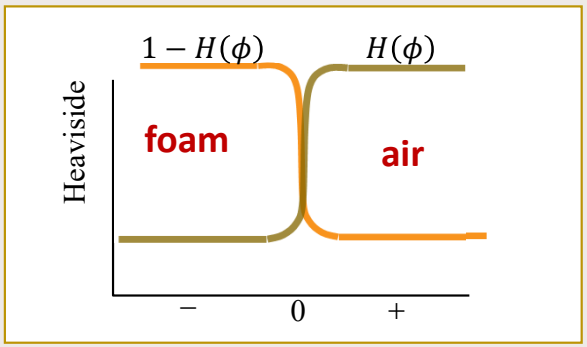
$$\eta_0 = \eta_0^0 \exp\left(\frac{E_\eta}{RT}\right)\left(\frac{\xi_c^p - \xi^p}{\xi_c^p}\right)^{-q}$$

$$\kappa = \frac{4}{3}\eta\left(\frac{1-\psi}{\psi}\right)$$

More details on the model can be found in Rao et al. 2018 Computers and Fluids

Level Set Boundary





Level Set Method

A signed distance function ϕ represents our interface at $\phi = 0$

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

Foam and gas phases are tracked, properties and source terms need to be smoothed to avoid instabilities

$$\rho(\phi) = \rho_{air} H(\phi) + \rho_{foam}\big(1 - H(\phi)\big)$$

$$S_{term} \rightarrow S_{term}(1 - H(\phi))$$

Where $\mathrm{H}(\phi)$ is a smoothed Heaviside and S_{term} is a source term for our species or moment equations

$$H(\phi) = \begin{cases} o & if\ \phi < \alpha \\ 0.5\left(1 + \frac{\phi}{\alpha} + \frac{\sin\left(\frac{\pi\phi}{\alpha}\right)}{\pi}\right) & if\ \alpha \le \phi \le \alpha \\ 1 & if\ \phi > \alpha \end{cases}$$

Discretization

We discretize our equation using the finite element method in open source software Goma (gomafem.com)

All elements are discretized using equal order P1 Tetrahedrons or Q1 Hexahedral elements depending on the mesh.

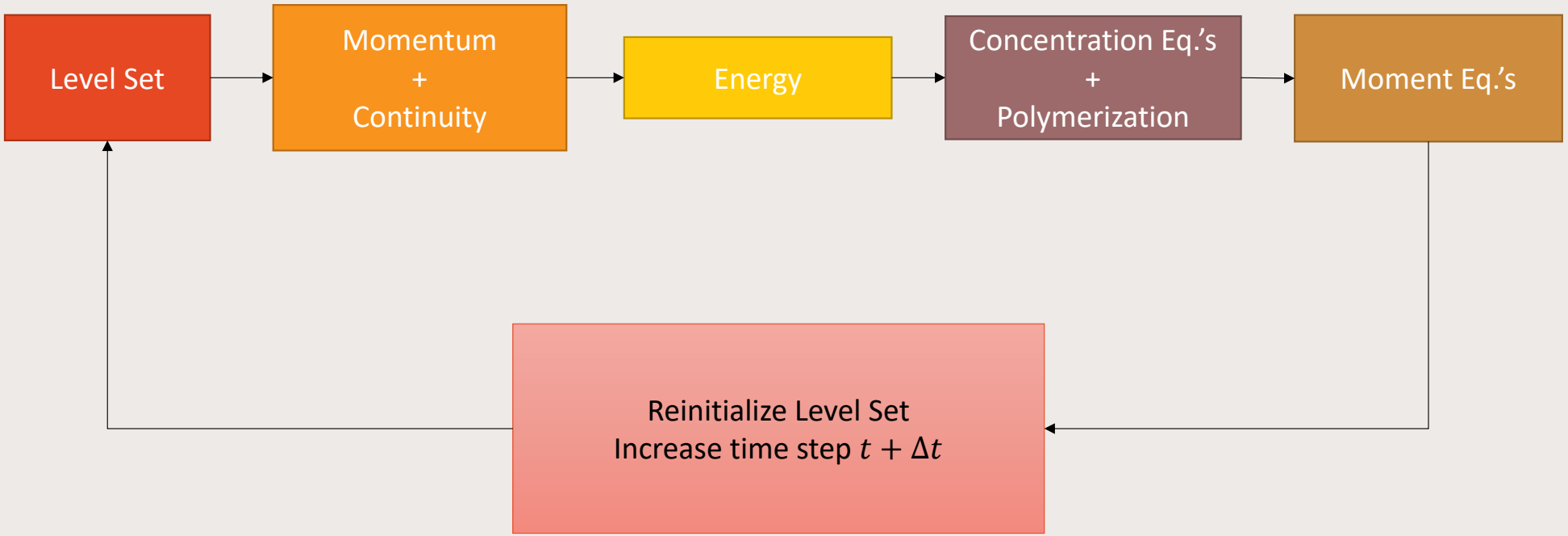
As we are using equal order we employ Pressure-Stabilizized Petrov-Galerkin (PSPG) stabilization for momentum and continuity

All convective-diffusion-reaction equations and momentum are stabilized using Streamwise-Upwind Petrov-Galerkin (SUPG)

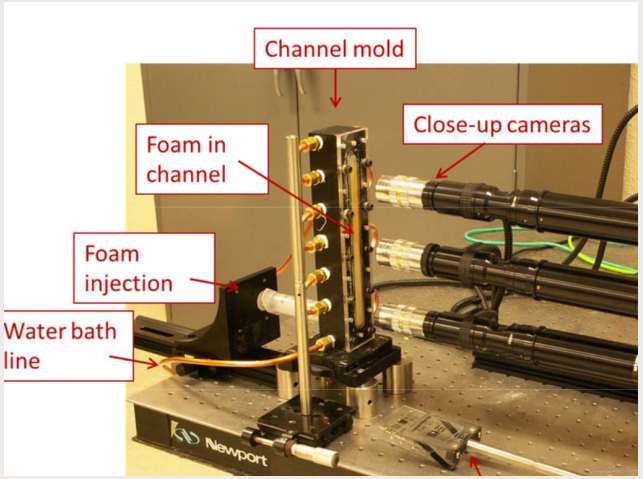
Time integration

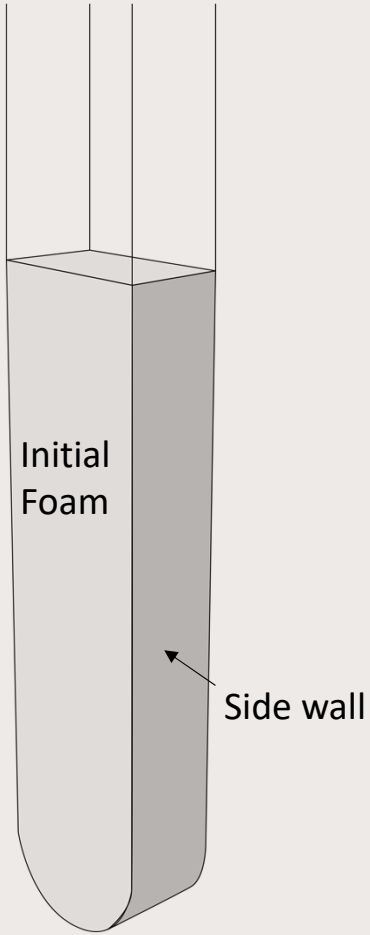
We employ a segregated approach to advance our solution in time

All terms are treated implicitly except for QMOM source terms which require a non-linear algorithm to compute the quadrature



Boundary Conditions and Initialization





Mold walls are restricted by a no penetration condition

$$\boldsymbol{u} \cdot \boldsymbol{n} = 0$$

And a slip condition due to foam typically slipping along walls

$$\boldsymbol{n} \cdot \boldsymbol{T} = \frac{1}{\beta(\phi)} \boldsymbol{u}$$

Molds are often preheated so we impose a constant Process Temperature on those walls and Adiabatic conditions elsewhere

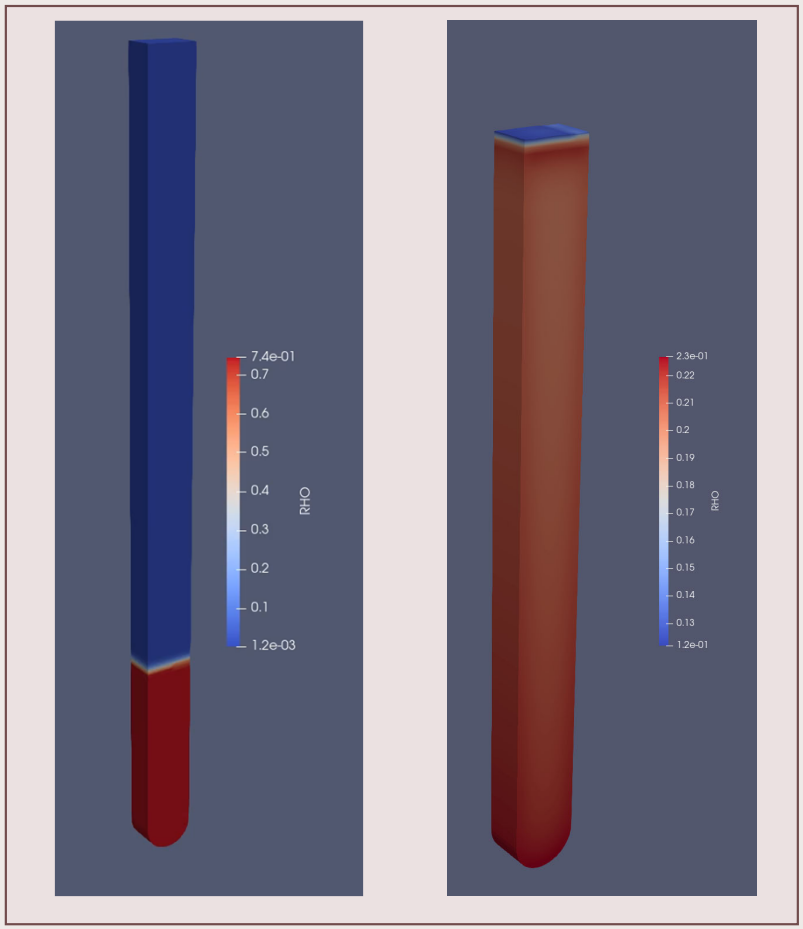
$$T = T_{process}$$

Foam is initialized to an initial foam state with many very small bubbles at an initial height

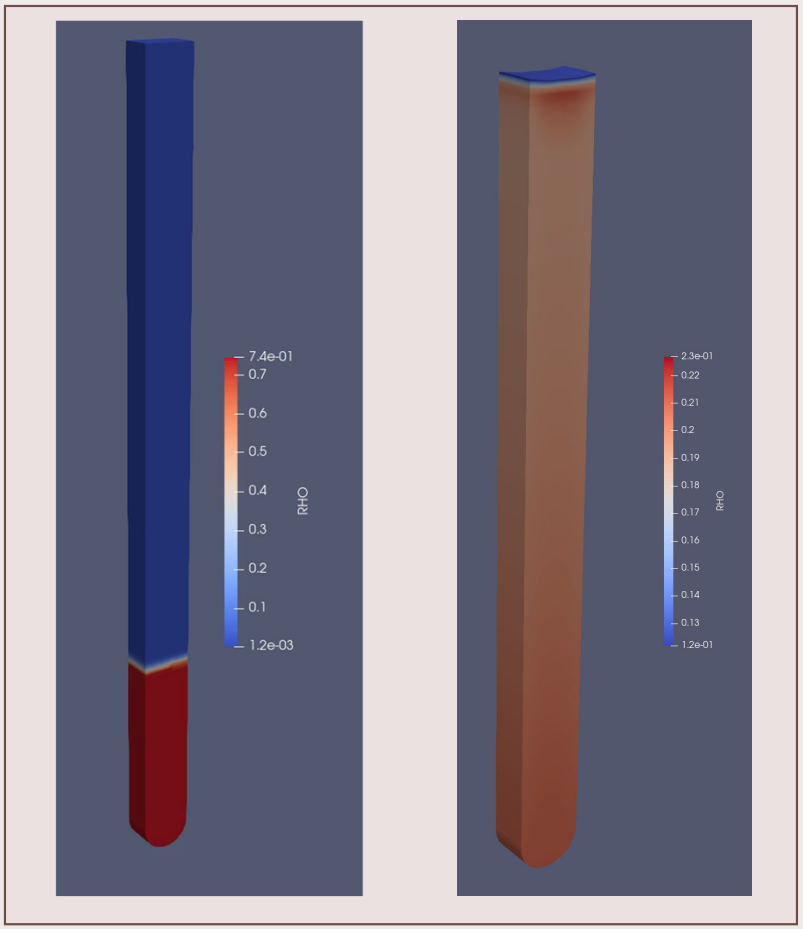
Foam is initialized uniformly with zero initial velocity

ALE Version: Ortiz et al. (Submitted 2021 AICHe Journal)

3D Bar at Two Process Temperatures



$30^\circ C$

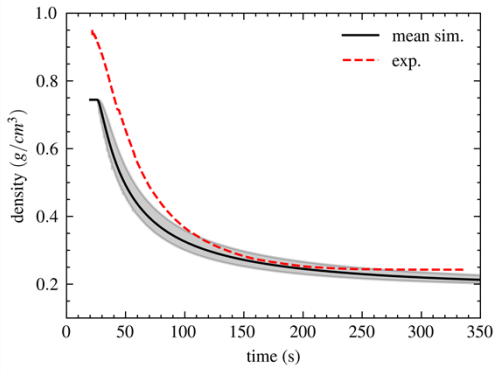


$40^\circ C$

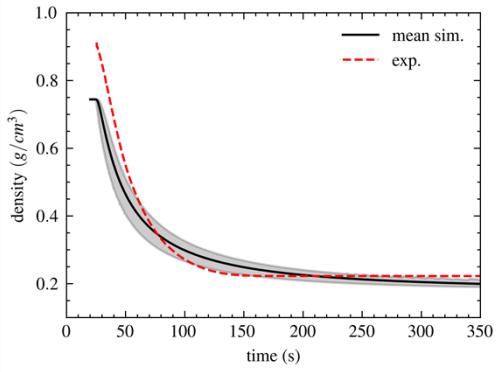
Level Set Model compared to Experimental Data

Density over time

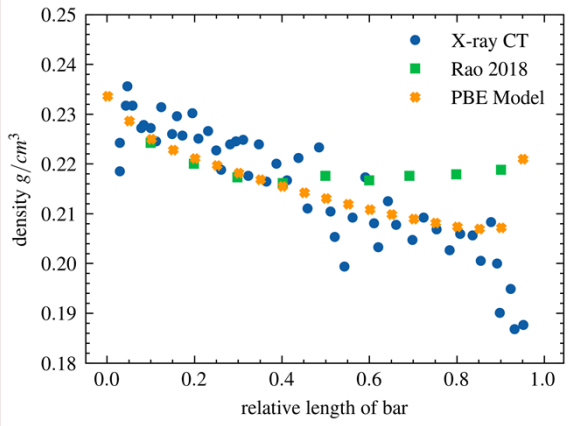
$30°C$



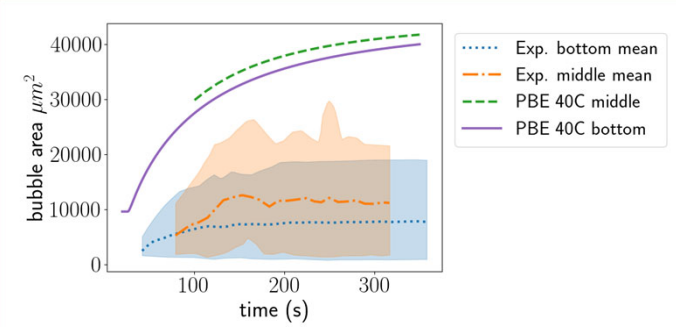
$40°C$



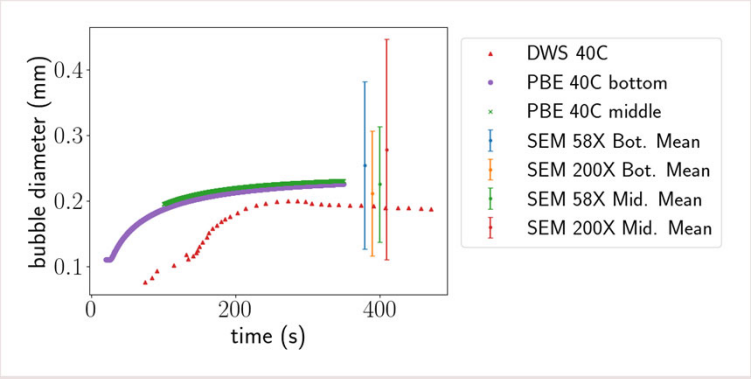
Final Bar Density at $30°C$



Simulation Bubble Area vs Camera

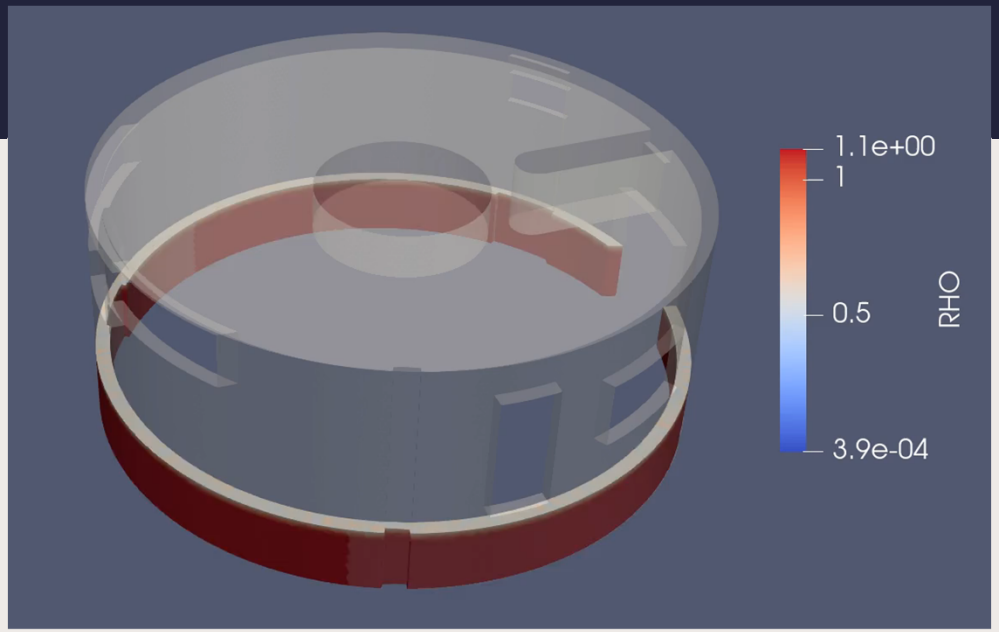


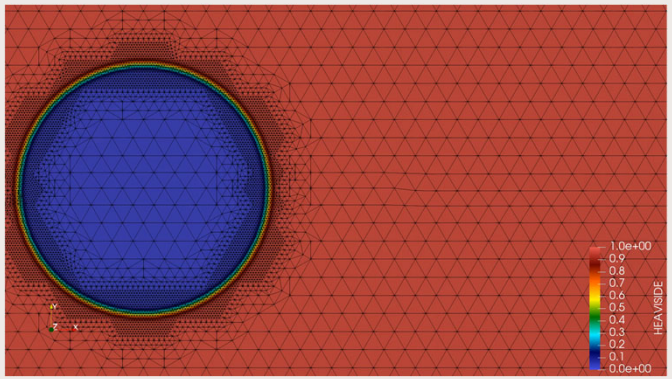
Simulation Bubble Diameter vs DWS+SEM



Future Work

- Complex mold comparisons
- Adaptive Meshing to alleviate level set issues like poor mass conservation
- More generic foam model which does not assume excess isocyanate
- Alternatives/Advances to Quadrature Method of Moments for tracking bubble distributions



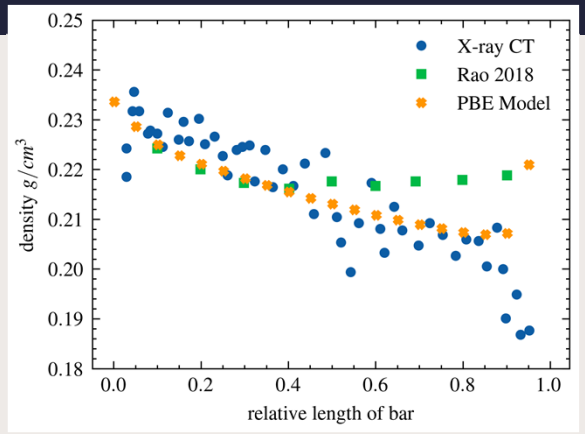


Conclusion

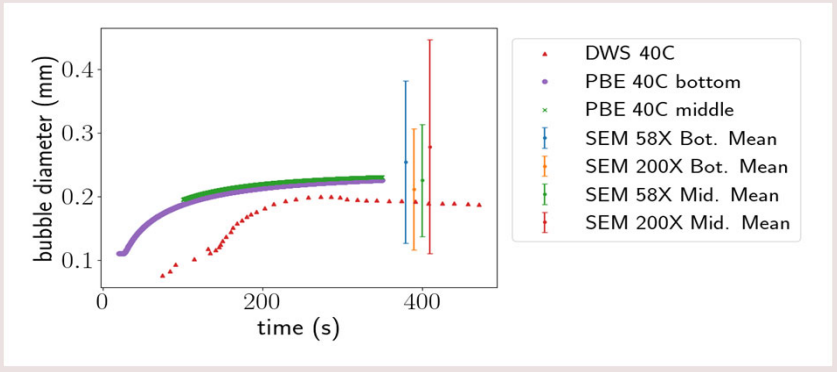
Presented a model for predicting polyurethane foam rise and final densities using a level set finite element method

We found good predictions when compared with experimental data

We plan to expand usage of this model to complex molds and exploring other techniques for tracking bubble distributions



Simulation Bubble Diameter vs DWS+SEM



Questions / Acknowledgements

Work was done using Goma an open source multiphysics finite element software (https://gomafem.com)

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EXTRA SLIDES

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Material Model: Heat Capacity and Conductivity

For Heat Capacity mixture theory is used to account for the effect of evolving gas

$$C_p = \frac{C_{p,liquid}\rho_{liquid}(1-\psi) + C_{p,CO_2}\rho_{gas}\psi}{\rho_{foam}}$$

Conductivity

$$k = \frac{2}{3}\left(\frac{\rho_{foam}}{\rho_{liquid}}\right)k_{liquid} + \left(1 - \frac{\rho_{foam}}{\rho_{liquid}}\right)k_{gas}$$

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Governing Equation: Concentrations

Concentration of water and carbon dioxide in the foam mixture:

$$\frac{\partial C_{H_2O}}{\partial t} + \boldsymbol{u} \cdot \nabla C_{H_2O} - D_{H_2O} \nabla^2 C_{H_2O} = -N k_{H_2O} C_{H_2O}^{p}$$

$$\frac{\partial C_{CO_2}}{\partial t} + \boldsymbol{u} \cdot \nabla C_{CO_2} - D_{CO_2} \nabla^2 C_{CO_2} = N k_{H_2O} C_{H_2O}^{p}$$

Where

$$k_{H_2O} = A_{H_2O} e^{-(E_{H_2O}/RT)}$$

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

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Moment equations source terms

The source terms after transformation are as follows, for Growth rate

$$\bar{G}_k = \int_0^\infty G(v) n(v) v^{k-1} dv$$

For Coalescence

$$\bar{S}_k = \frac{1}{2} \int_0^\infty \int_0^\infty [(v + v')^k - v^k - v'^k] \beta(v, v') dv dv'$$

Reference: Karimi and Marchisio 2015 Macromolecular Theory and Simulations

Quadrature Method of Moments (QMOM)

Approximation of the integrals is performed with Gaussian quadrature (*McGraw 1997 Aerosol Science and Tech.*)

$$k\int_0^\infty v^{k-1}\phi(v)n(v)dv = k\sum_{i=1}^{N} v_i^{k-1}\phi(v_i)w_i$$

For moments $k = 0$ through $2N-1$ our moment equations become

$$m_k = \int_0^\infty n(v)v^k dv \cong \sum_{i=1}^{N} w_i v_i^k$$

w_i weights
v_i nodes

Using this approximation quadrature points and weights are computed with Wheeler's algorithm (*Wheeler 1974 Journal of Mathematics*)

Quadrature applied to moment source terms

The quadrature approximation transform is also applied to the moment source terms (*Karimi et al. 2016 Macromolecular Symposia)*

Term for bubble growth rate

$$\bar{G}_k = \int_0^\infty G(v)n(v)v^{k-1}dv \cong \sum_{i=1}^{N} w_i G(v_i)v_i^{k-1}$$

$$G(v_i) = G_0(w_{CO_2} - w_{max})/w_{max}$$

Where w_{CO_2} and w_{max} are mass fraction of liquid CO_2 and mass fraction related to the maximum solubility of liquid CO_2

Term for bubble coalescence

$$\bar{S}_k = \frac{1}{2}\int_0^\infty \int_0^\infty [(v+v')^k - v^k - v'^k]\beta(v,v')dvdv$$

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

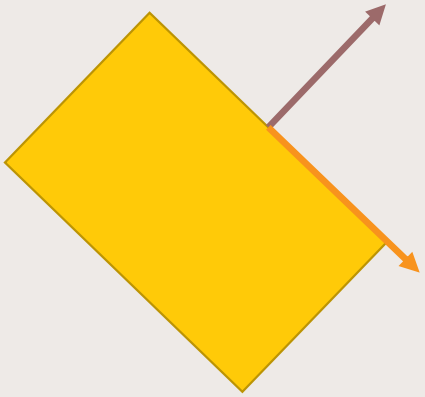
$$\beta(v_a, v_b) = \beta_0(v_a + v_b)$$

Constant coalescence rate kernel

What is a rotated boundary condition (2D)

no penetration conditions, $v \cdot n = 0$

We still want to be able to slip so we cannot use Dirichlet on something like a rotated domain:



So instead we use a rotated coordinate system to apply our boundary conditions

Then we will be able to specify slip in the tangential direction

Use a rotation matrix to change coordinate systems:

$$\begin{bmatrix} R_n \\ R_t \end{bmatrix} = \begin{bmatrix} n^T \\ t^T \end{bmatrix} \begin{bmatrix} R_x \\ R_y \end{bmatrix}$$

Now when we apply $v \cdot n = 0$ we still have freedom in the tangential direction which we can apply Navier slip boundary conditions (or free slip)

Solving the moment quadrature

Moment quadrature points and weights are dynamically calculated at each node at every time step.

A well behaved algorithm has proven essential to solution of these moment equations.

Yuan and Fox introduced an adaptive 1D quadrature algorithm which gives much better behavior in calculating moment quadrature weights and nodes.

Using Yuan and Fox's quadrature algorithm and following recommendations on parameters greatly reduces solution blow-up

Yuan, Cansheng, and Rodney O. Fox. "Conditional quadrature method of moments for kinetic equations." *Journal of Computational Physics* 230.22 (2011): 8216-8246.