Simulation of Polyurethane Foam Expansion

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Motivation

- Polymer foam products
  - Heat insulation materials
  - Bed mattresses
  - Shoe soles
  - Automotive parts

http://www.brinaco.cz/
Problem

- Chemical reactions
  - Isocyanates, polyols, water
- Thermodynamic properties
  - Solubility, diffusivity, viscosity
- Morphology evolution
  - Bubble growth
  - Wall evolution
- Foam expansion
  - Foam rheology
  - Foam density, temperature
- Material properties
  - Mechanical, heat insulation
Multi-scale

- MoDeNa project
  - Development of multi-scale framework
  - Model coupling between quantum, molecular, and continuum models
  - Prediction of application properties using first principle modelling

MoDeNa

MoDeNa FP7 project (2014 – 2016)
Foam flow

- VOF approach
  - Foam treated as pseudo-homogeneous material on macro-scale
  - Based on compressibleInterFoam
    \[
    \frac{\partial \alpha_a}{\partial t} + \mathbf{u} \cdot (\nabla \alpha_a) + \nabla \cdot (\mathbf{u} \alpha_a (1 - \alpha_a)) = \alpha_a \left(1 - \alpha_a\right) \left(\frac{1}{\rho_f} \frac{D \rho_f}{Dt} - \frac{1}{\rho_a} \frac{D \rho_a}{Dt}\right)
    \]
  - Momentum balance
    \[
    \frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \left[\mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)\right] + \rho \mathbf{g} + \mathbf{F}
    \]
    \[
    \mu = \alpha_f \mu_f + (1 - \alpha_f) \mu_a
    \]
    \[
    \rho = \alpha_f \rho_f + (1 - \alpha_f) \rho_a
    \]

- Pressure-velocity coupling using PIMPLE loop
Polymerization

- **Gelling reaction**
  \[ \text{R-NCO} + \text{R'-OH} \rightarrow \text{R-NH-CO-O-R'} \]
  isocyanate + polyol \rightarrow urethane bond

  \[ \frac{d[\text{OH}]}{dt} = -A_{\text{OH}} \exp \left( - \frac{E_{\text{OH}}}{RT} \right) [\text{NCO}][\text{OH}] \]

- **Blowing reaction**
  \[ 2\text{R-NCO} + \text{H}_2\text{O} \rightarrow \text{R-NH-CO-NH-R} + \text{CO}_2 \]
  isocyanate + water \rightarrow urea bond + carbon dioxide

  \[ \frac{d[\text{W}]}{dt} = -A_{\text{W}} \exp \left( - \frac{E_{\text{W}}}{RT} \right) [\text{W}] \]

- **Scalar transport equation**

  \[ \frac{\partial X_i}{\partial t} + (\mathbf{u} - \alpha_a \mathbf{u}_r) \cdot \nabla X_i = S_i \]

- Alternatively, detailed kinetic model exported from Predici as C code
Rheology

- Viscosity of reaction mixture
  - Castro-Macosko model

\[ \mu_{rm} = A \mu \exp \left( - \frac{E_\mu}{R_g T} \right) \left( \frac{X_{gel}}{X_{gel} - X_p} \right)^{m+nX_p} \]

- Foam viscosity
  - Bird-Carreau model

\[ \mu_f = \left( \mu_\infty + (\mu_0 - \mu_\infty)(1 + (\dot{\gamma} \Lambda)^\zeta) \right)^{\frac{n-1}{\zeta}} \]
Cell size distribution

- **Population balance equation**

\[
\frac{\partial n(v)}{\partial t} + \nabla \cdot (n(v)u) + \frac{\partial}{\partial v} [G(v)n(v)] = \frac{1}{2} \int_{0}^{v} \beta(v',v-v')n(v')n(v-v')dv' - \int_{0}^{v} \beta(v',v-v')n(v)n(v')dv' 
\]

- **Quadrature method of moments**

\[
m_k = \int_{0}^{\infty} n(v)v^k dv \\
\frac{\partial m_k}{\partial t} + (u - \alpha_u u_r) \cdot \nabla m_k = k \sum_{i=1}^{z} G_k^i + S_k \\
\rho_f = \frac{\rho_b m_1}{1 + m_1} + \frac{\rho_p}{1 + m_1}
\]
Bubble growth

- Simulation of growth of a single bubble and its immediate surroundings
- Supports both physical and chemical blowing
- Models diffusion of blowing agents in the shell and evaporation at phase interface
- Simple model based on momentum and mass balances
  - Runtime in seconds

Simulation of Polyurethane Foam Expansion
Bubble growth

- **Momentum equation**
  \[
  \sum_{\alpha=1}^{N} p_{\alpha} + p_{\text{air}} - p_{\text{rm}} = \rho_{\text{rm}} \left[ R \frac{d^2 R}{dt^2} + \frac{3}{2} \left( \frac{dR}{dt} \right)^2 \right] + \frac{2\gamma}{R} + \frac{4\mu_{\text{rm}} dR}{R dt}
  \]

- **Mass balance for gas in bubble**
  \[
  \frac{d}{dt} \left( \frac{p_{\alpha} R^3}{R_g T} \right) = 3D_\alpha R^2 \frac{\partial c_\alpha}{\partial r} \bigg|_{r=R}
  \]

- **Mass balance for gas in shell**
  \[
  \frac{\partial c_\alpha}{\partial t} + \frac{R^2}{r^2} \frac{dR}{dt} \frac{\partial c_\alpha}{\partial r} = D_\alpha \frac{\partial}{\partial r} \left( r^2 \frac{\partial c_\alpha}{\partial r} \right) + r_\alpha
  \]

- **Reaction kinetics and enthalpy balance**
Bubble growth rate

- Detailed bubble growth model
  \[
  G_i = \frac{dn_i}{dt} = 4\pi D_i R^2 \frac{\partial c_i}{\partial r}\bigg|_{r=R}
  \]

- Surrogate model
  \[
  G_i = \frac{dn_i}{dt} = 4\pi R^2 k_{li}(c_i - H_i p_i)
  \]
Results

Simulation of Polyurethane Foam Expansion
Bubble growth

Validation & future work

- Model described and compared to experimental results in Ferkl et al., Chem. Eng. Sci. 148, 55-64, 2016
- Weak point is the initial BSD
Wall evolution

- Wall thickness is influenced by stretching (bubble growth) and drainage (capillary forces)

- Data for validation are relatively limited - μCT for strut shape and SEM for wall thickness

- Model described in Ferkl et al., Chem. Eng. Sci. 176, 50-58, 2018
Foam conductivity

- Developed algorithms for reconstruction of foam morphology
- Model for diffusion of blowing agents out of foam
- Coupled conduction-radiation model for heat insulation properties
- Validation against experimental data in Ferkl et al., Chem. Eng. Sci. 172, 323-334, 2017
Summary

- Developed models for PU foaming
- VOF OpenFOAM for foam expansion
- Lower-scale models for reaction kinetics, bubble growth rate, foam conductivity, etc.
- Tools are available on [github](https://github.com)
- Can be used to study physical mechanisms, determine influence of various parameters, optimize procedures, etc.
MoDeNa framework
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