

PUFOAM: a new OpenFOAM solver for the simulation of polyurethane foams

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Why are we modeling PU foams?

- Motivation & aims,
- Polyurethane foams,
- Modeling methods.

How are we modeling PU foams?

- Model development,
 - ◊ Computational Fluid Dynamics (CFD),
 - ◊ Population Balance Equation (PBE).
- Implementation and validations.

Did we model PU foams?

- Summary & concluding remarks.

Motivation

- Wide range of applications, e.g. construction, appliances and automotive industries.
- Economical contribution, in 2013, it created 235,200 jobs with \$71.9 billion outputs in U.S.
- Minimize the dependency of the final product to the operator's experience.

Aims

- Development of an open-source CFD solver dedicated for PU foams.
- Application of PBE to simulate bubble (or cell) size distribution, BSD, in PU foams.

Polyurethane nomenclature:

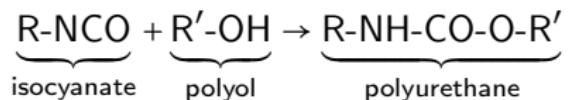
- **Polyurethane:** a wide class of polymers with one element in common, the presence of an urethane group $-\text{NH}-\text{CO}-\text{O}-$.
- **Foaming/expansion:** Mixing of polyols and isocyanates with water and additives ^a onsets a number of chemical reactions and physical phenomena leading to polymerization, gas formation and eventually foam expansion.



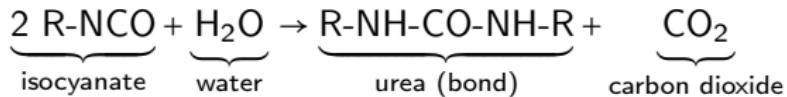
^awater, physical blowing agents, catalysts and surfactants

Polyurethane nomenclature:

- Gelling reaction:



- Blowing reaction:



What are the industrial concerns?

- Bubble size distribution (BSD),
- Polymerization progress,
- Foam expansion (mobile interface),
- Evolution of material properties.

What are the academic concerns?

- The foam is a multiphase system constituted by a continuous liquid phase (undergoing polymerization) and a disperse gas phase (gas bubbles or cells).
- The bubbles can growth and coalesce during the expansion.
- The foam rheology is very complex.
- The kinetics of chemical reactions is very complex.

Previous Models

Kinetics-based

- Gelling reaction → conversion of hydroxyl group,
- Blowing reaction → conversion of water,
- Temperature rise → energy equation,
- Foam density → based on kinetics,
- Expansion due to blowing agents → empirical expressions for maximum solubility,
- **Foam interface and BSD → not included!**

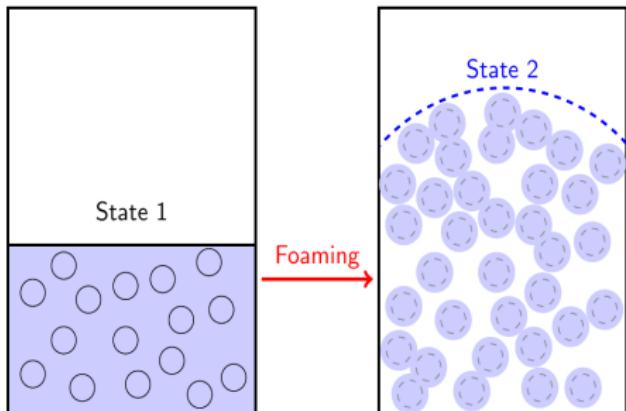
CFD-based

- Kinetics based models → additional partial differential equations,
- Interface capturing → volume of fluid (VOF),
- Foam rheology → Newtonian or non-Newtonian,
- **Evolution of BSD → not included!**

How to tackle the problem?

Polyurethane foam → **pseudo-fluid**

- Bubble / cell size distribution
 - ◊ Population Balance Model
- Interface capturing:
 - ◊ Volume-of-Fluid
- Material properties:
 - ◊ Variable density
 - ◊ Variable viscosity
 - ◊ Variable thermal conductivity
- Reactions of the components:
 - ◊ Kinetic model

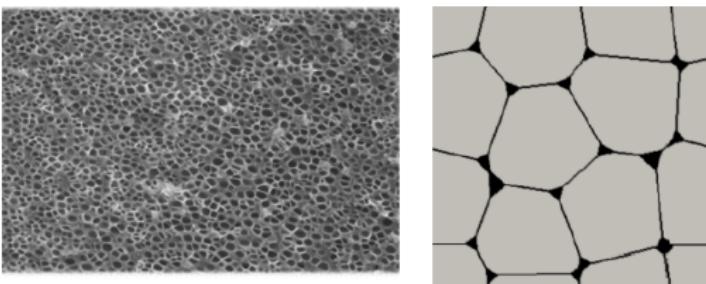


Why Population Balance Model?

- The micro-structure of the PU foam represented through a **bubble size distribution** (BSD), so:

$$n(t, x, v)dv \quad (1)$$

represents the number of bubbles (or cells), per unit volume of the liquid with volume between v and $v + dv$



- The evolution of BSD is governed by the population balance equation:¹

$$\underbrace{\frac{\partial n(v)}{\partial t}}_{\text{accumulation}} + \underbrace{\nabla \cdot (n(v) \mathbf{U}_f)}_{\text{convection}} + \underbrace{\frac{\partial}{\partial v} (n(v) G(v))}_{\text{growth}} = \\ \underbrace{\frac{1}{2} \int_0^v n(v-v') n(v') \beta(v-v', v') dv'}_{\text{coalescence}} - \underbrace{\int_0^\infty n(v) n(v') \beta(v, v') dv}_{\text{coalescence}} \quad (2)$$

- $G(v)$ is the growth rate due to the formation of carbon dioxide and the evaporation of blowing agent
- $\beta(v, v')$ is the coalescence kernel, namely the rate of coalescence of two bubbles with volumes equal to v and v'

¹Marchisio D.L., Fox R.O. (2013) Computational models for polydisperse multiphase and particulate flows. Cambridge University Press: Cambridge.

Instead of tracking the BSD evolution with the PBM, we track the evolution of some moments of BSD:

Moments of bubble size distribution (BSD)

$$M_k = \int_0^{\infty} n(v) v^k dv,$$

- M_0 : total number of bubbles per unit foam volume
- M_1 : total bubble volume per unit foam volume
- $M_2 \& M_3$: related to the variance and the skewness of BSD

Evolution of the moments of BSD

$$\frac{\partial M_k}{\partial t} + (\mathbf{U} - \alpha_a \mathbf{U}_r) \cdot \nabla M_k = \underbrace{\bar{S}_k}_{\text{coalescence}} + \underbrace{\bar{G}_k^{\text{BA}} + \bar{G}_k^{\text{CO2}}}_{\text{growth}} \quad (3)$$

Implementation of PU foam features

- Material properties:
 - ◊ Density,
 - ◊ Viscosity,
 - ◊ Thermal conductivity.
- Reactions kinetics:
 - ◊ Gelling reaction,
 - ◊ Blowing reaction,
 - ◊ Physical and chemical blowing agents.

Foam density

- Solving PBE \rightarrow total bubble volume per unit liquid volume, $m_1(t) \Rightarrow$

$$\rho_f = \rho_b \frac{m_1(t)}{1 + m_1(t)} + \rho_{PU} \left(1 - \frac{m_1(t)}{1 + m_1(t)} \right) \quad (4)$$

ρ_{PU} : reacting mixture density,

ρ_b : bubble density.

Foam viscosity

- Newtonian:

$$\mu_f(T, X_{\text{NCO}}) = \mu_\infty \exp\left(\frac{E_\mu}{RT}\right) \times \left(\frac{X_{\text{NCO, gel}}}{X_{\text{NCO, gel}} - X_{\text{NCO}}}\right)^{a+bX_{\text{NCO}}+cX_{\text{NCO}}^2} \quad (5)$$

- non-Newtonian:

$$\mu_F = \left\{ \mu_\infty + (\mu_0 - \mu_\infty) \left[1 + (\lambda \dot{\gamma})^\alpha \right]^{\frac{n-1}{\alpha}} \right\} A_\mu \exp\left(\frac{E_\mu}{RT}\right) \quad (6)$$

- Dependencies:

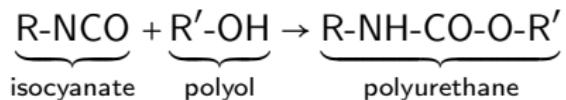
- Viscosities at the lowest and highest shear rates (i.e., μ_0 , μ_∞),
- Gelling point.

Foam thermal conductivity

- for n-pentane as blowing agent $\rightarrow \lambda_f \sim f(\rho_f)$

Simple kinetic scheme

- Gelling reaction:

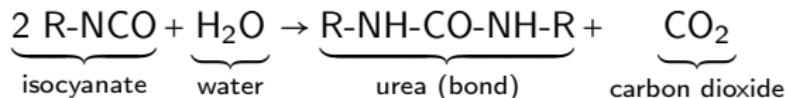


$$\frac{\partial X_{\text{OH}}}{\partial t} + (\mathbf{U} - \alpha_a \mathbf{U}_r) \cdot \nabla X_{\text{OH}} = A_{\text{OH}} \exp\left(\frac{-E_{\text{OH}}}{RT}\right) C_{\text{OH}}^0 (1 - X_{\text{OH}}) \left(\frac{C_{\text{NCO}}^0}{C_{\text{OH}}^0} - 2X_W \frac{C_{\text{W}}^0}{C_{\text{OH}}^0} - X_{\text{OH}} \right) \quad (7)$$

advancement of gelling reaction → conversion of OH group

Simple kinetic scheme cont'd

- Blowing reaction:



$$\frac{\partial X_W}{\partial t} + (\mathbf{U} - \alpha_a \mathbf{U}_r) \cdot \nabla X_W = A_W \exp\left(\frac{-E_W}{RT}\right) (1 - X_W) \quad (8)$$

advancement of blowing reaction \longrightarrow **conversion of water**

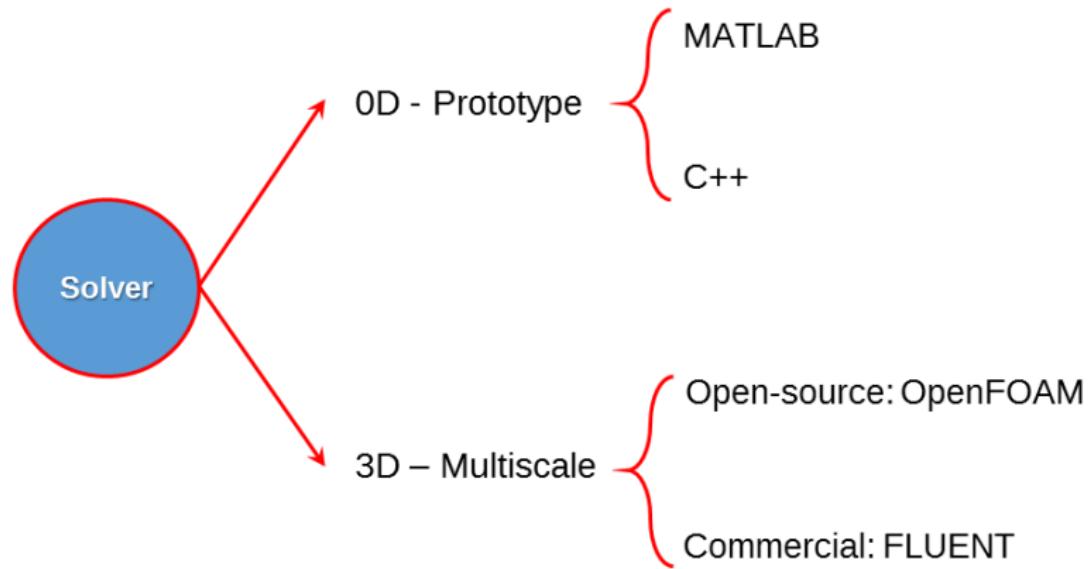
- Liquid blowing agent mass fraction:

$$\frac{\partial w_{BA}}{\partial t} + (\mathbf{U} - \alpha_a \mathbf{U}_r) \cdot \nabla w_{BA} = -\overline{G}_1^{\text{BA}} \frac{P}{RT} \frac{M_{BA}}{\rho_f}, \quad (9)$$

- Mass fraction of carbon dioxide in liquid:

$$\frac{\partial w_{\text{CO}2}}{\partial t} + (\mathbf{U} - \alpha_a \mathbf{U}_r) \cdot \nabla w_{\text{CO}2} = C_W^0 \frac{dX_W}{dt} \frac{M_{\text{CO}2}}{\rho_{\text{PU}}} - \overline{G}_1^{\text{CO}2} \frac{M_{\text{CO}2}}{\rho_f} \quad (10)$$

Implementation



Validation

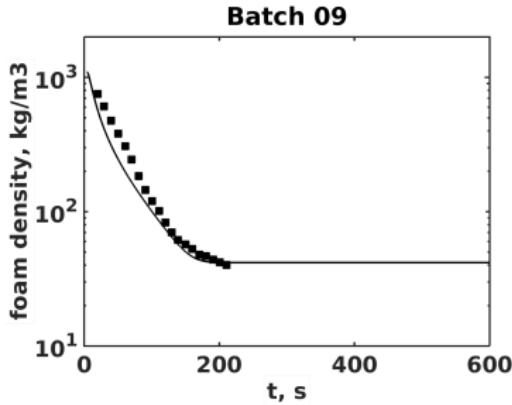
- Mixing cup experiments
- 12 different experiments with changing recipe:
 - ◊ Initial concentrations of isocyanate and polyol
 - ◊ Initial concentration of water
 - ◊ Initial concentration of blowing agent
 - ◊ Kinetics details
- Measurements:
 - ◊ Rising height of the foam
 - ◊ Temperature



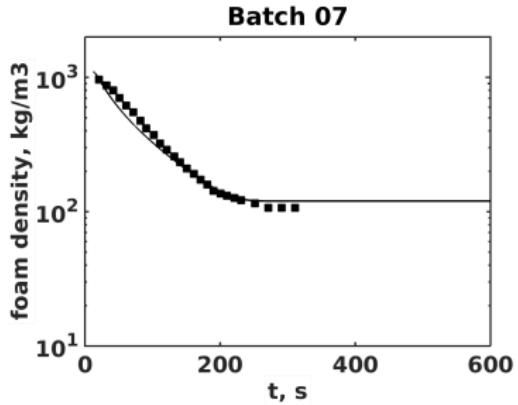
Validation (Model Prototype)

Density at highest and lowest amount of water

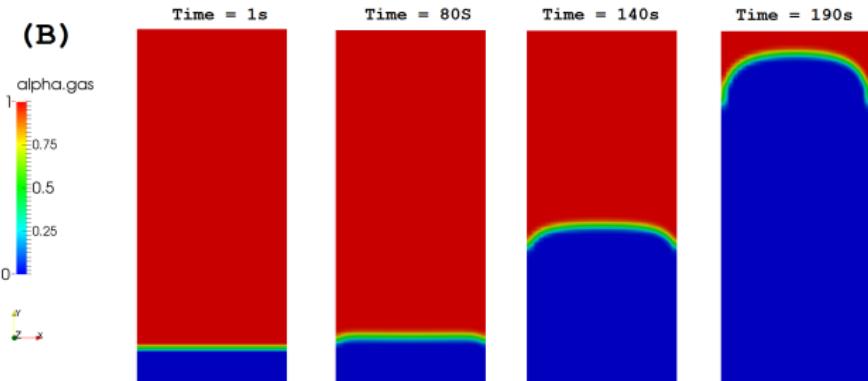
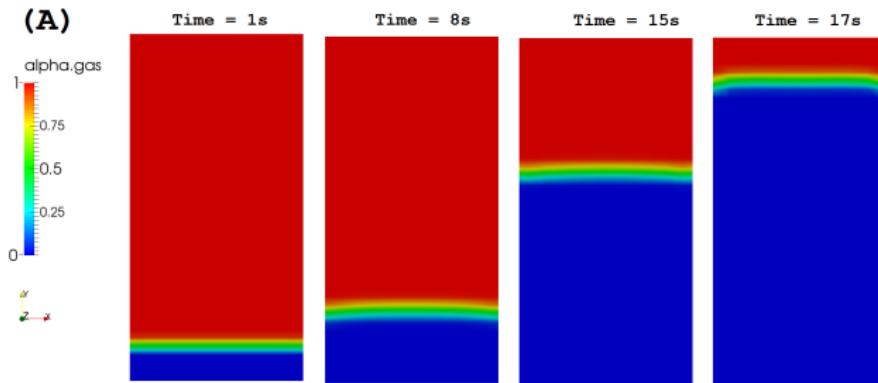
Highest amount of water
($C_W^0 = 915 \text{ mol} \cdot \text{m}^{-3}$)



Lowest amount of water
($C_W^0 = 305 \text{ mol} \cdot \text{m}^{-3}$)

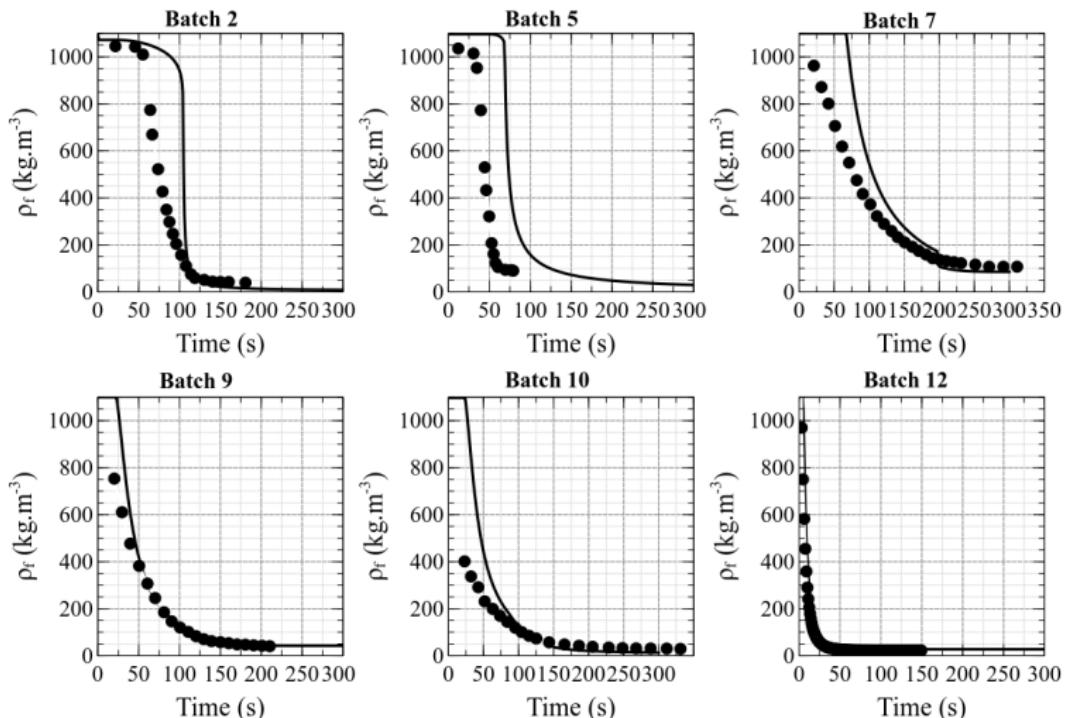


Foam expansion: (A) physically-blown & (B) chemically-blown



Validation (3D CFD Model) cont'd

Model predictions (line) against experimental data (symbols)



Conclusions

- Development of a CFD model coupled with PBE,
- The following features of PU foams have been included:
 - ◊ Evolution of bubble size distribution,
 - ◊ Kinetics of reactions,
 - ◊ Fate of different blowing agents,
 - ◊ Material properties such as thermal conductivity.
- Validation of model for various PU recipes,
- Link to the associated article: <https://doi.org/10.1016/j.cpc.2017.03.010>

Thank you