Simulation of Polyurethane Foam Expansion

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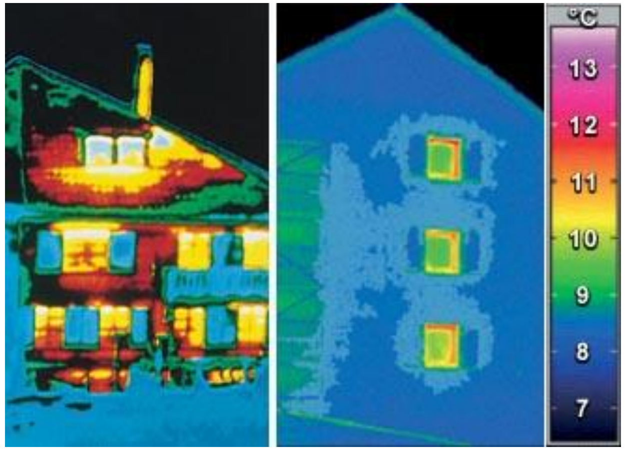
European Commission

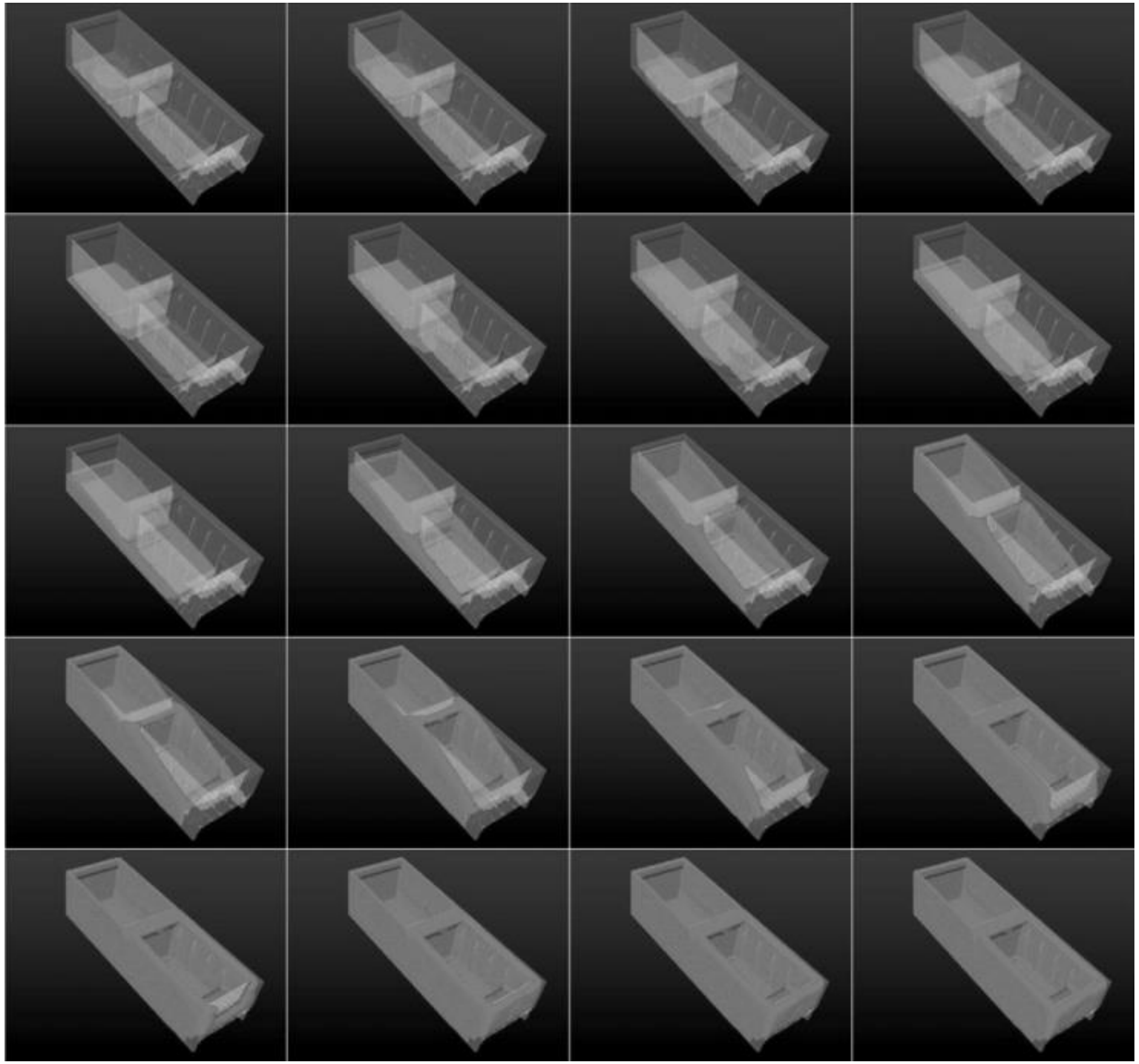
Prague, Czechia, December 2017

Motivation

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

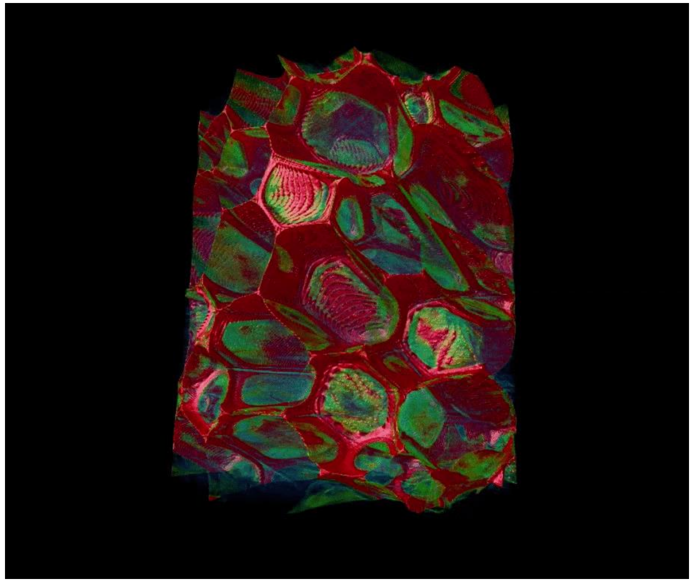


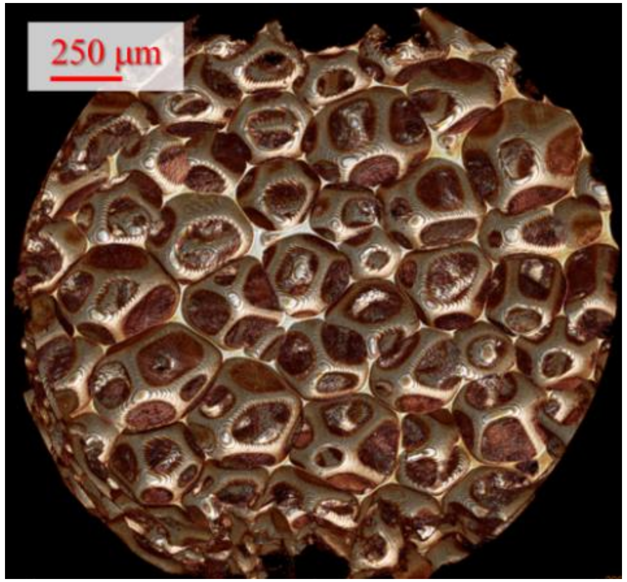
http://www.brinaco.cz/



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



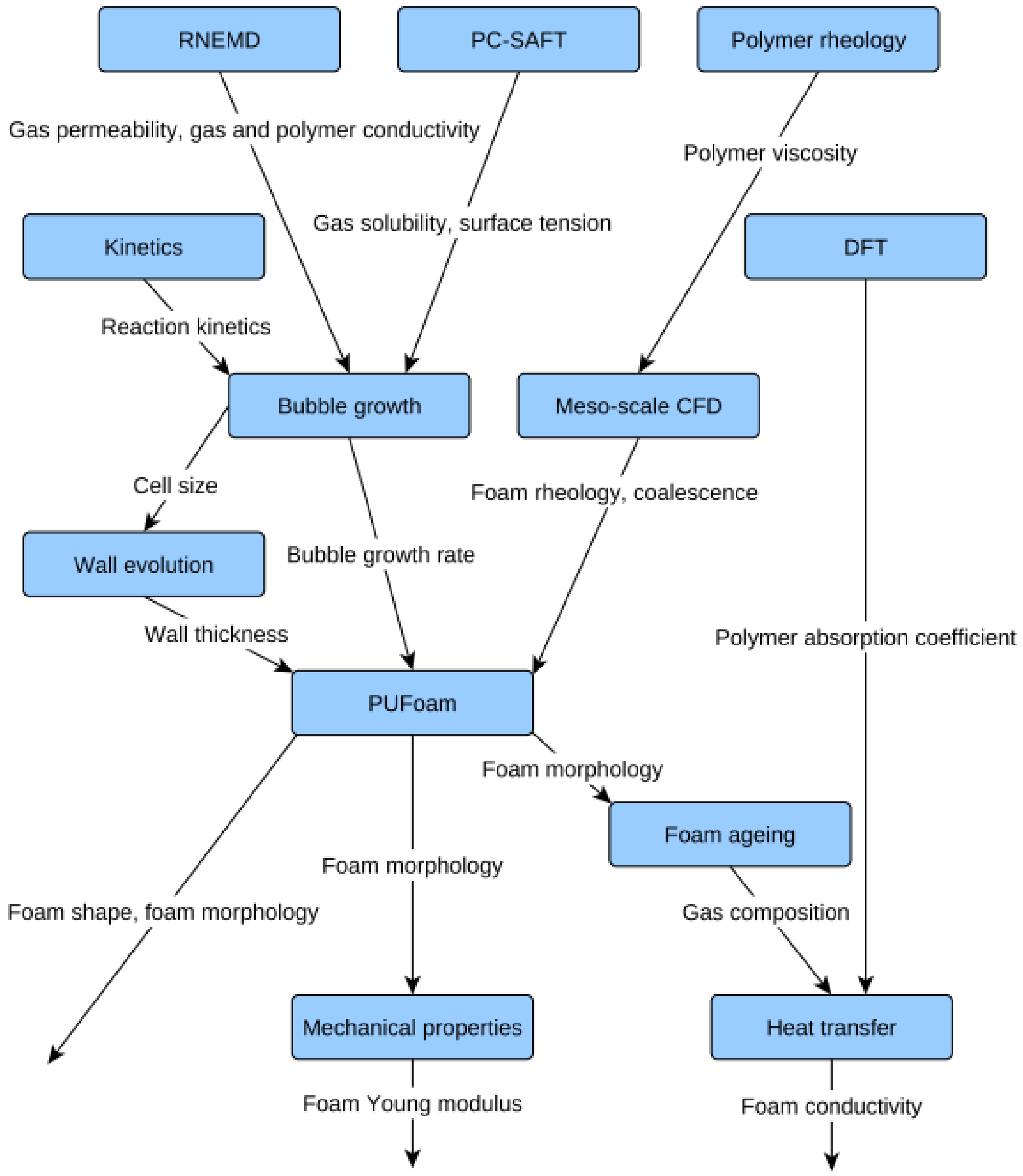


Multi-scale

- 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

$$\frac{\partial \alpha_a}{\partial t} + \boldsymbol{u} \cdot (\nabla \alpha_a) + \nabla \cdot \left(\boldsymbol{u_r} \alpha_a (1 - \alpha_a)\right) = \alpha_a \left((1 - \alpha_a) \left(\frac{1}{\rho_f} \frac{D\rho_f}{Dt} - \frac{1}{\rho_a} \frac{D\rho_a}{Dt} \right) \right)$$

  - Momentum balance

$$\frac{\partial}{\partial t}(\rho \boldsymbol{u}) + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla p + \nabla \cdot [\mu(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T)] + \rho \boldsymbol{g} + \boldsymbol{F}$$

$$\mu = \alpha_f \mu_f + (1 - \alpha_f)\mu_a$$

$$\rho = \alpha_f \rho_f + (1 - \alpha_f)\rho_a$$

  - Pressure-velocity coupling using PIMPLE loop

Polymerization

- Gelling reaction

$$\underset{\text{isocyanate}}{\mathrm{R-NCO}} + \underset{\text{polyol}}{\mathrm{R'-OH}} \longrightarrow \underset{\text{urethane bond}}{\mathrm{R-NH-CO-O-R'}}$$

$$\frac{\mathrm{d[OH]}}{\mathrm{d}t} = -A_{\mathrm{OH}}\mathrm{exp}\left(-\frac{E_{\mathrm{OH}}}{RT}\right)[\mathrm{NCO}][\mathrm{OH}]$$

- Blowing reaction

$$\underset{\text{isocyanate}}{\mathrm{2R-NCO}} + \underset{\text{water}}{\mathrm{H_2O}} \longrightarrow \underset{\text{urea bond}}{\mathrm{R-NH-CO-NH-R}} + \underset{\text{carbon dioxide}}{\mathrm{CO_2}}$$

$$\frac{\mathrm{d[W]}}{\mathrm{d}t} = -A_{\mathrm{W}}\mathrm{exp}\left(-\frac{E_{\mathrm{W}}}{RT}\right)[\mathrm{W}]$$

- Scalar transport equation

$$\frac{\partial X_i}{\partial t} + (\boldsymbol{u} - \alpha_a \boldsymbol{u_r}) \cdot \nabla X_i = S_i$$

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

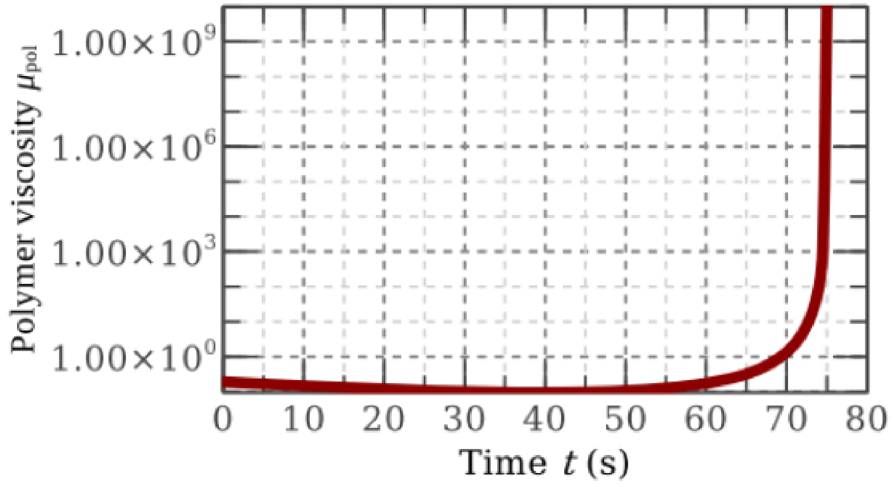
Rheology

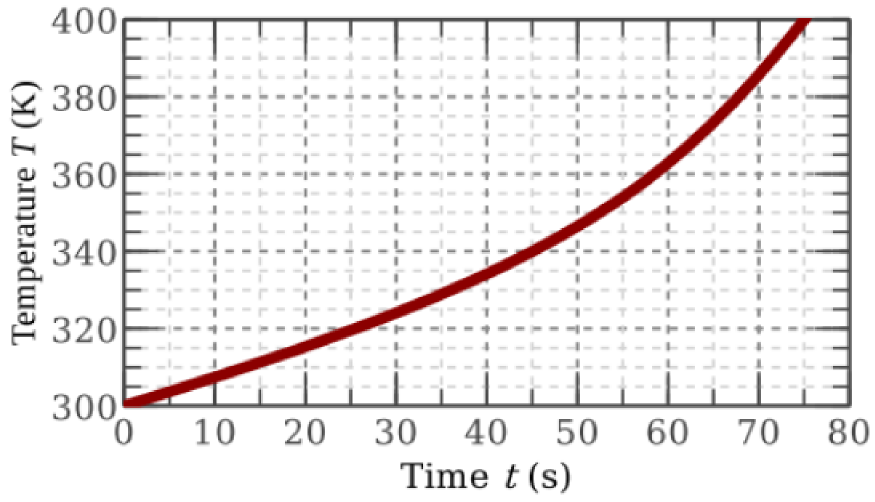
- Viscosity of reaction mixture
  - Castro-Macosko model

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

- Foam viscosity
  - Bird-Carreau model

$$\mu_f = \left(\mu_\infty + (\mu_0 - \mu_\infty)\left(1 + (\dot{\gamma}\bar{\Lambda})^\zeta\right)\right)^{\frac{n-1}{\zeta}}$$





Cell size distribution

- Population balance equation

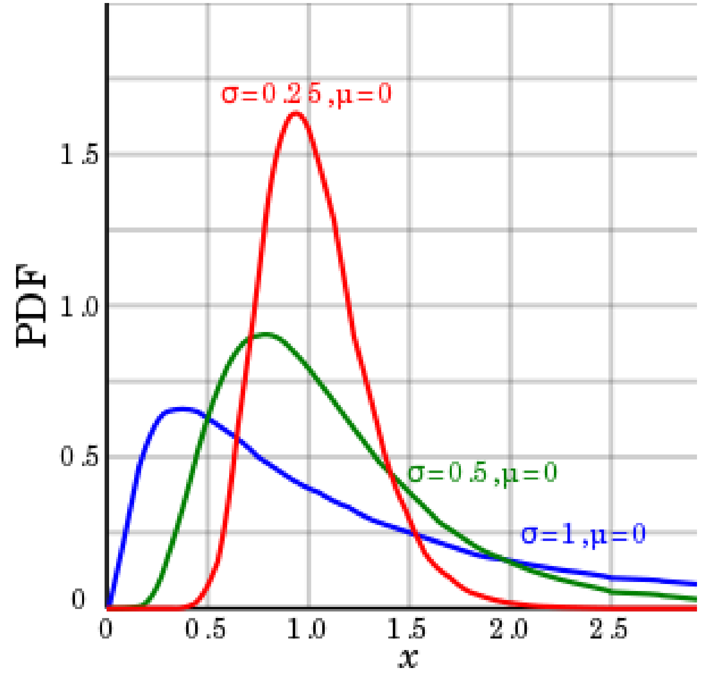
$$\frac{\partial n(\mathrm{v})}{\partial t} + \nabla \cdot (n(\mathrm{v})\boldsymbol{u}) + \frac{\partial}{\partial \mathrm{v}}[G(\mathrm{v})n(\mathrm{v})] = \frac{1}{2}\int_0^{\mathrm{v}} \beta(\mathrm{v}', \mathrm{v}-\mathrm{v}')n(\mathrm{v}')n(\mathrm{v}-\mathrm{v}')d\mathrm{v}' - \int_0^{\mathrm{v}} \beta(\mathrm{v}', \mathrm{v}-\mathrm{v}')n(\mathrm{v})n(\mathrm{v}')d\mathrm{v}'$$

- Quadrature method of moments

$$m_k = \int_0^{\infty} n(\mathrm{v})\mathrm{v}^k d\mathrm{v}$$

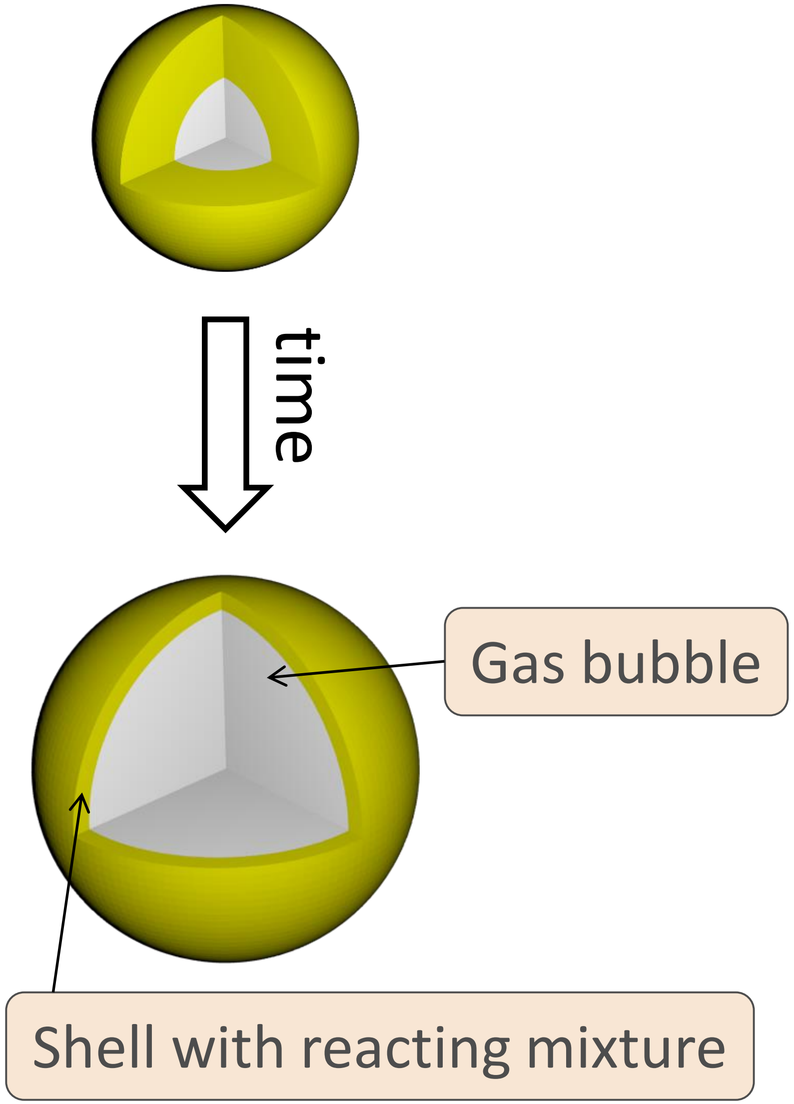
$$\frac{\partial m_k}{\partial t} + (\boldsymbol{u} - \alpha_a \boldsymbol{u_r}) \cdot \nabla m_k = k\sum_{i=1}^{z} G_k^i + S_k$$

$$\rho_f = \frac{\rho_b m_1}{1+m_1} + \frac{\rho_p}{1+m_1}$$



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



Bubble growth

- Momentum equation

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

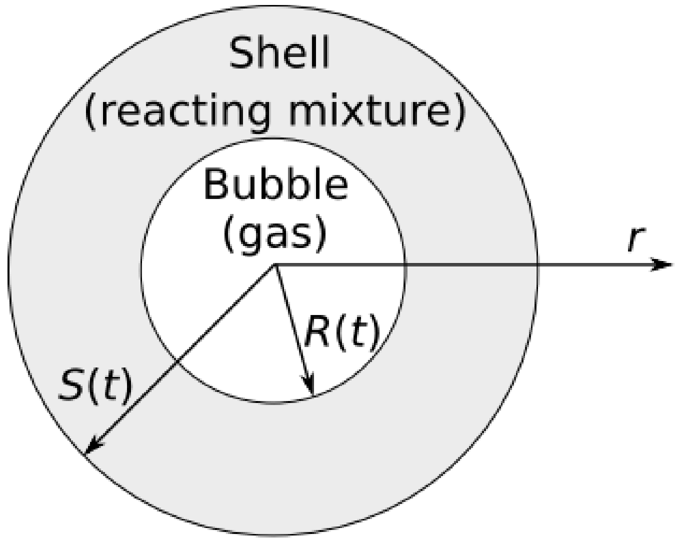
- Mass balance for gas in bubble

$$\frac{d}{dt}\left(\frac{p_\alpha R^3}{R_g T}\right) = 3D_\alpha R^2 \frac{\partial c_\alpha}{\partial r}\bigg|_{r=R}$$

- Mass balance for gas in shell

$$\frac{\partial c_\alpha}{\partial t} + \frac{R^2}{r^2}\frac{dR}{dt}\frac{\partial c_\alpha}{\partial r} = \frac{D_\alpha}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_\alpha}{\partial r}\right) + r_\alpha$$

- Reaction kinetics and enthalpy balance



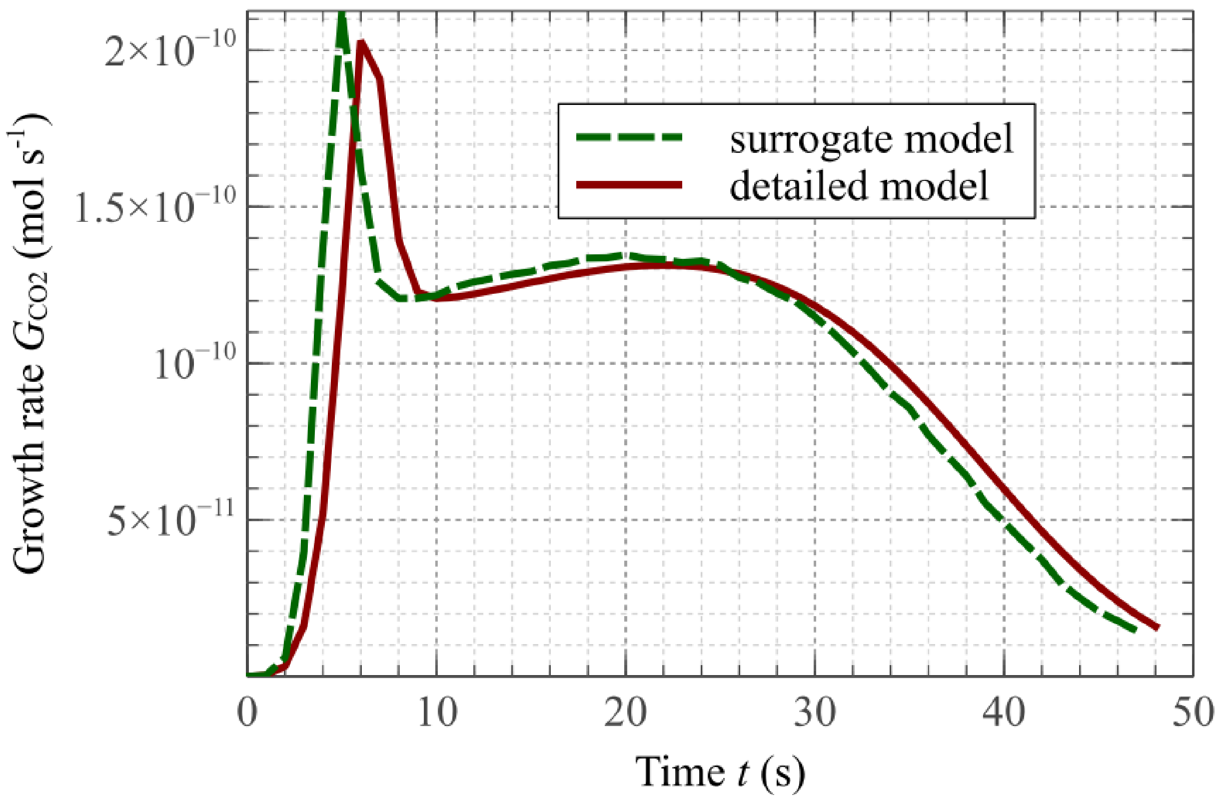
Bubble growth rate

- Detailed bubble growth model

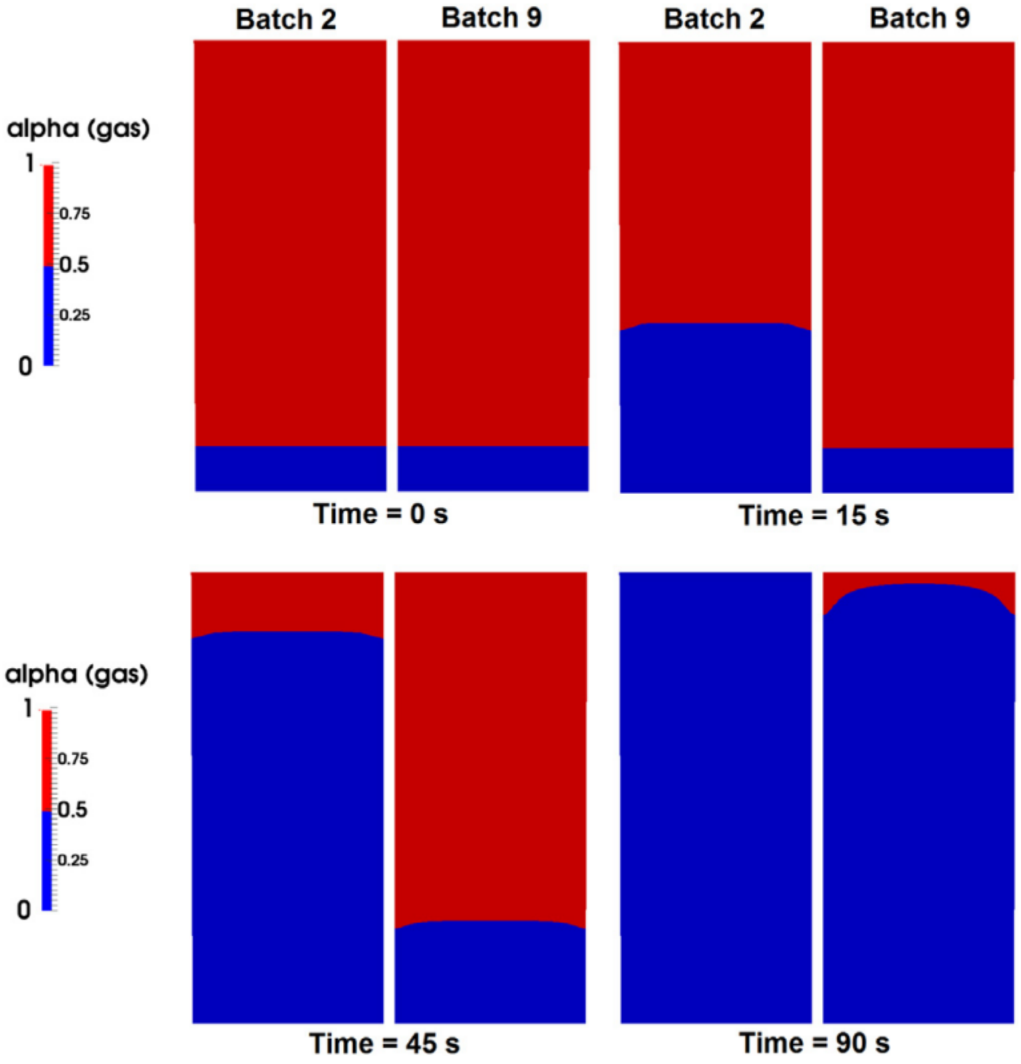
$$G_i = \frac{dn_i}{dt} = 4\pi D_i R^2 \left.\frac{\partial c_i}{\partial r}\right|_{r=R}$$

- Surrogate model

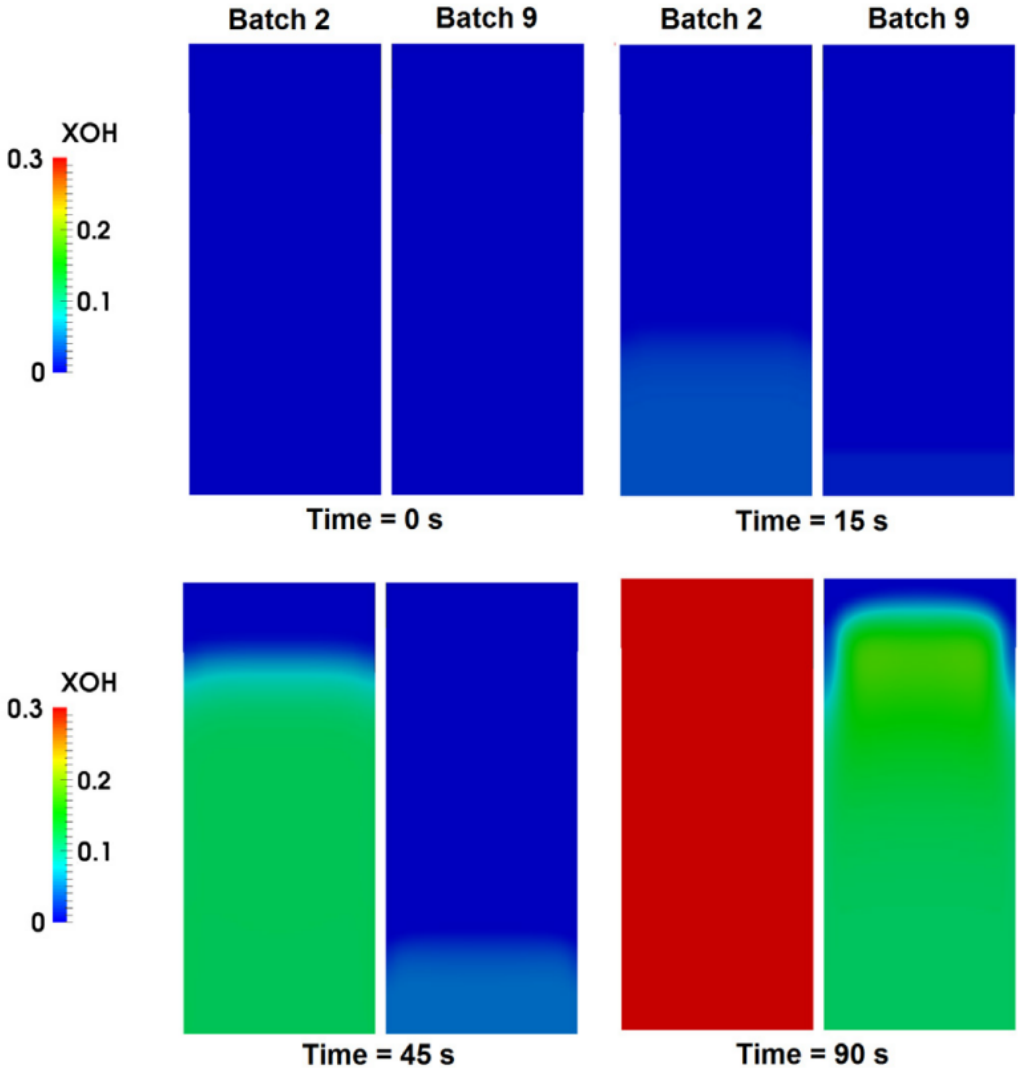
$$G_i = \frac{dn_i}{dt} = 4\pi R^2 k_{l,i}(c_i - H_i p_i)$$



Results



Batch 2
Batch 9
Batch 2
Batch 9
alpha (gas)
1
0.75
0.5
0.25
0
Time = 0 s
Time = 15 s
alpha (gas)
1
0.75
0.5
0.25
0
Time = 45 s
Time = 90 s

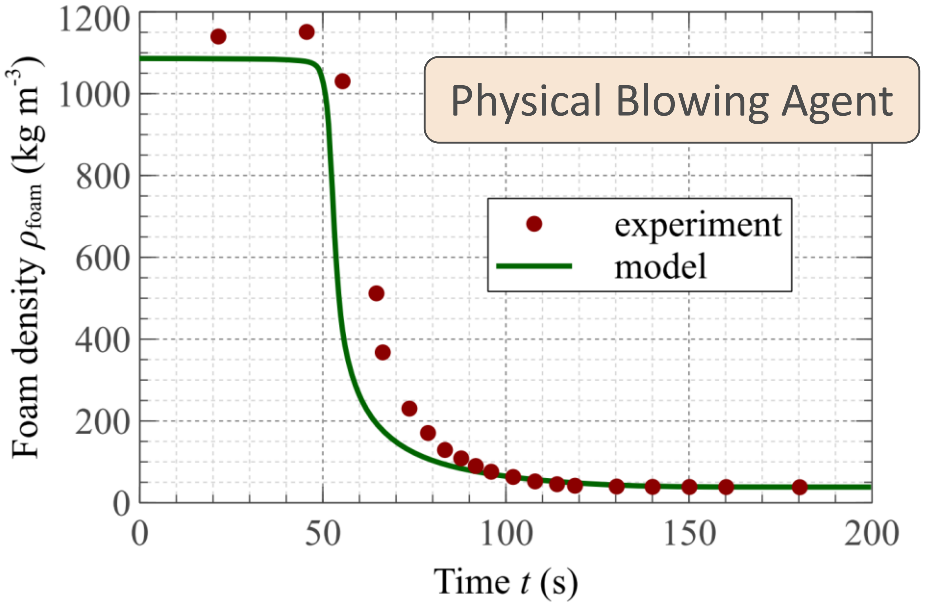


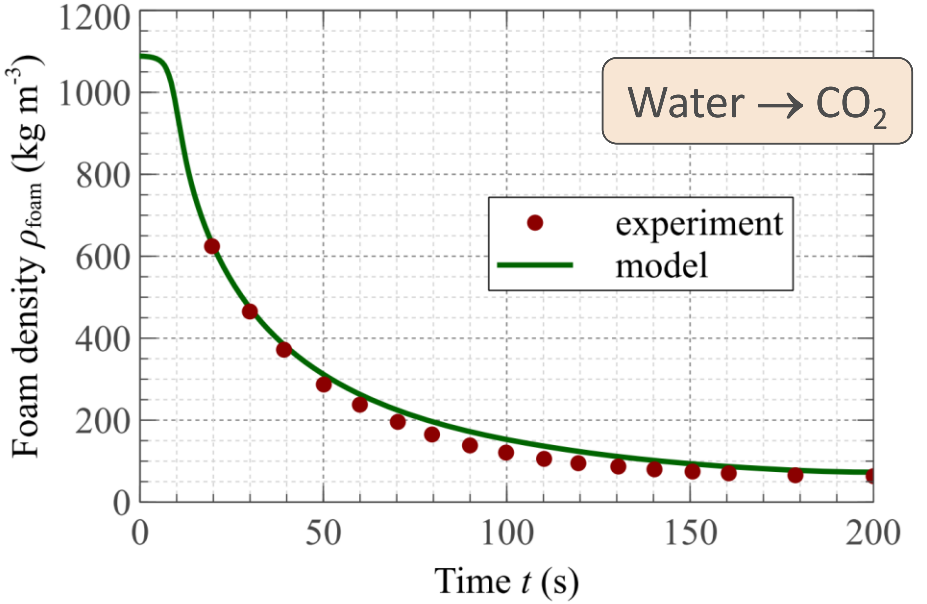
Batch 2
Batch 9
Batch 2
Batch 9
XOH
0.3
0.2
0.1
0
Time = 0 s
Time = 15 s
XOH
0.3
0.2
0.1
0
Time = 45 s
Time = 90 s

Bubble growth

Validation & future work

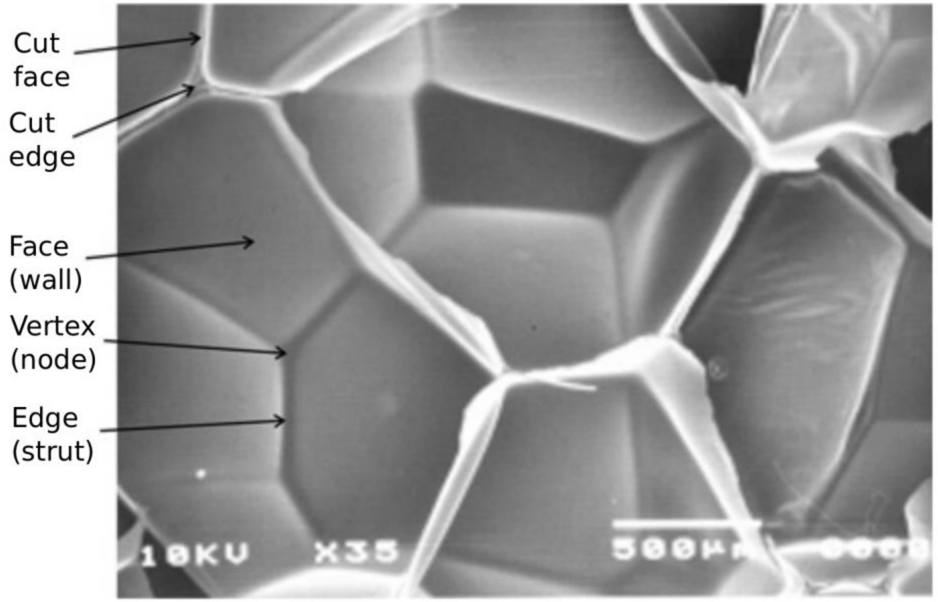
- Model described and compared to experimental results in Ferkl et al., Chem. Eng. Sci. 148, 55-64, 2016
- OpenFOAM solver described in Karimi et al., Comp. Phys. Comm. 217, 138-148, 2017
- Weak point is the initial BSD

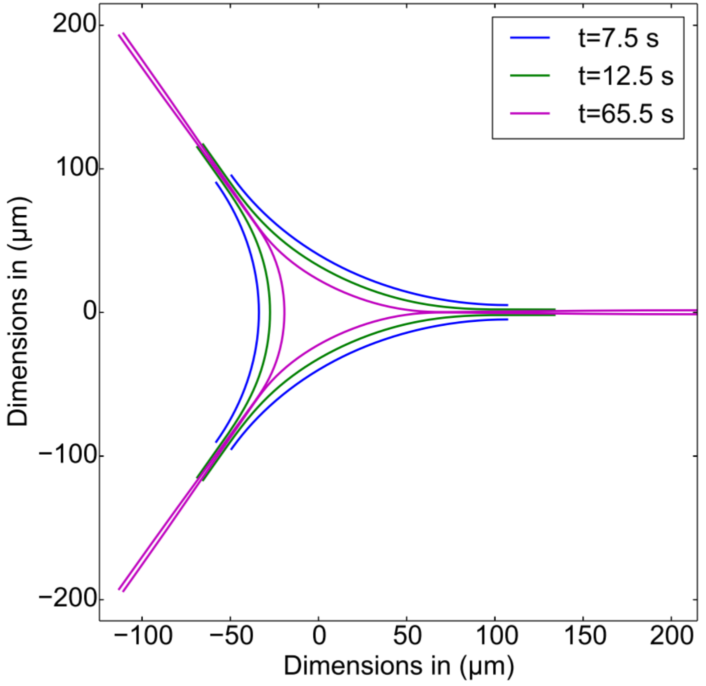


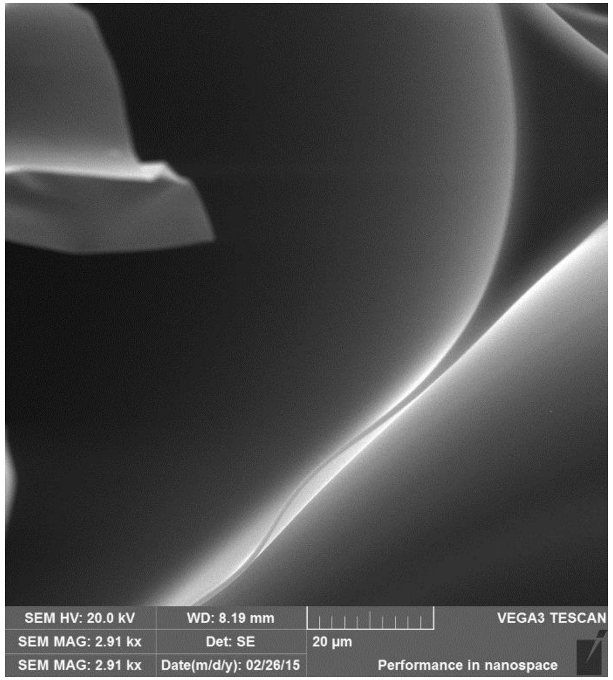


Wall evolution

- 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]

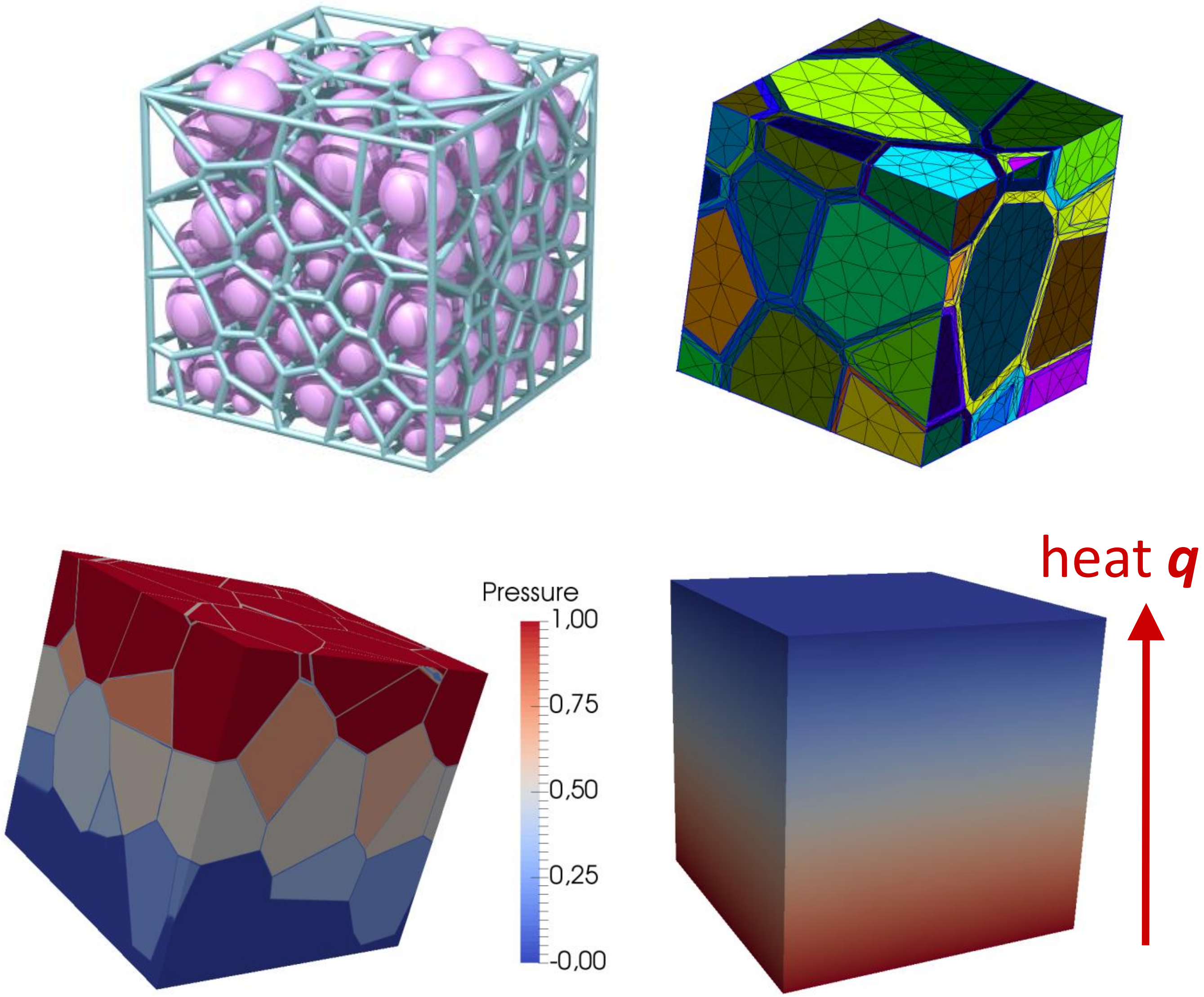






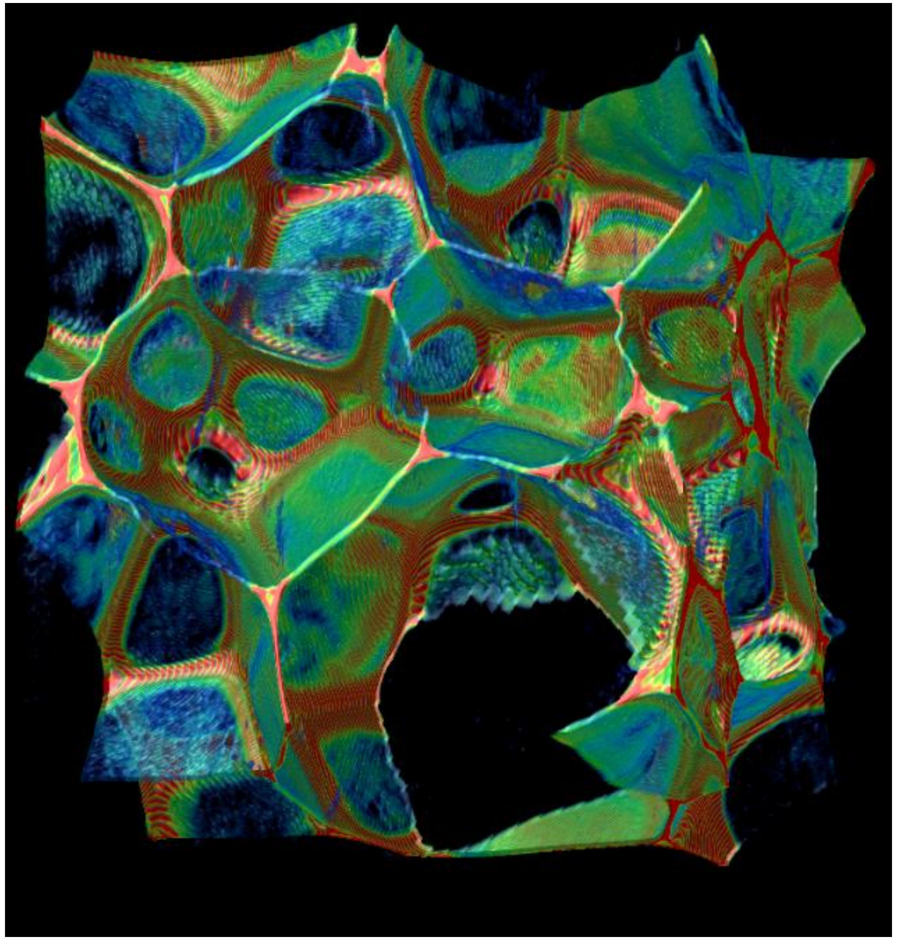
Foam conductivity

- 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
- Can be used to study physical mechanisms, determine influence of various parameters, optimize procedures, etc.



MoDeNa framework