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Multi-scale framework for the simulation of polyurethane foam morphology and heat insulation properties

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Highlights

- Foam morphology and its application properties are predicted from foam recipe.
- Foam density, bubble size distribution, and wall thickness are predicted.
- Coupled conduction-radiation heat transfer in polymer foams is solved.
- Effective transfer of information across scales is implemented.

1. Introduction

Polyurethane (PU) foams are typically produced by reaction injection molding process, in which the foam expansion and the polymerization take place simultaneously. Due to the large variety of types and concentrations of reactants, blowing agents, catalysts, and surfactants it is possible to create foams tailored to specific purpose. Thus, PU foams find application as heat insulating materials, various car parts, bed mattresses, and many other products. Predictive mathematical model provides valuable insight into the foaming process and it is instrumental in easing the process design, optimization of its parameters and reduction of human dependencies.

However, first principle modeling of application properties of PU foams is quite complex. It involves several intertwined processes on different length and time scales. Thus, predictive model must incorporate precise description of the polymerization reaction kinetics, the diffusion of blowing agents in reaction mixture, the evolution of small spherical bubbles to large polyhedral cells, the development of cell walls and foam interface during foam expansion, and heat transfer by conduction and radiation in the foam. Under this perspective, the aim of this work is to develop a multi-scale framework for the prediction of foam morphology and its heat insulation properties by improving existing modelling tools, and developing surrogate models for scale coupling.

2. Mathematical model

The multi-scale model can be conceptually divided into several blocks. Each block represents a mathematical model that simulates part of the overall process from given inputs. First, starting from the lower length scales, at the scale of individual phases we have models for reaction kinetics [1], rheology of reaction mixture [2], and thermal conductivity of polymer and gas mixtures [3]. Second, at the scale of individual bubbles, we implement models for bubble growth rate [4], wall thickness profile evolution [5], and prediction of conductive and radiative properties [3]. Finally, at the scale of the whole foam, we have models for foam expansion [6] and heat transfer [3].

The coupling is implemented using a MoDeNa framework [7]. It introduces concept of surrogate models for the detailed lower scale models. Surrogate models are simple algebraic functions with free parameters that are automatically fitted by the framework using the results of the detailed model so that surrogate model supplies fast, yet accurate approximation of the detailed model. Surrogate models are evaluated instead of detailed lower scale models in multi-scale simulation, thus significantly reducing computational time.

The final output of the model is foam morphology and its heat insulation properties represented by the equivalent conductivity, which embodies the ability of the foam to transfer heat by conduction and radiation.

Moreover, the model also provides a lot of valuable information about the evolution of reactants concentrations and foam morphology, i.e., foam density, cell size distribution, and average wall thickness.

3. Results and discussion

Application properties of PU foams can be tuned in several ways. One of the most important parameters is the amount of blowing agent. It influences the size of bubbles, foam density and indirectly also reaction kinetics and evolution of temperature, because it consumes reaction heat for evaporation. Thus, foam formulations with different amounts of physical blowing agent typically lead to foams with different morphologies and heat insulation properties (see Figure 1). Larger amounts of pentane lead to foams with lower foam density and larger cell size. However, the equivalent conductivity remains almost constant for initial pentane concentration in the range [700, 1000] mol m^{-3}, because reduced conductive heat transfer caused by lower foam density is compensated by increased radiative heat transfer caused by larger cell size.

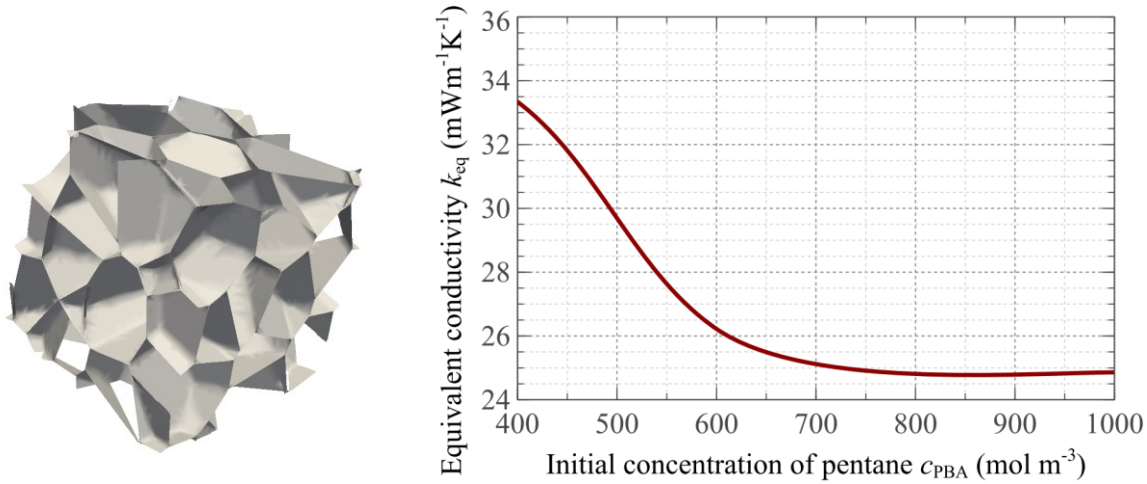

Figure 1. Reconstructed morphology using calculated foam density and cell size distribution on the left. Dependence of equivalent conductivity on initial concentration of pentane for physically blown PU foam on the right.

4. Conclusions

A multi-scale framework for the simulation of polyurethane foam morphology and its heat insulation properties is presented in this work. The multi-scale model is built from the bottom up using state-of-the-art mathematical models for the simulation of reaction kinetics, properties of individual phases, foam expansion and heat transfer phenomena. Thanks to the efficient scale coupling the model can be used to predict the foam density, cell size distribution, wall thickness, and equivalent conductivity of polyurethane foams.

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Keywords
Polymer Foams; Morphology evolution; Multi-scale modeling; Heat transfer