



# Multi-scale modelling of expanding polyurethane foams: Coupling macro- and bubble-scales



Pavel Ferkl<sup>a</sup>, Mohsen Karimi<sup>b</sup>, Daniele L. Marchisio<sup>b</sup>, Juraj Kosek<sup>a,\*</sup>

<sup>a</sup> Department of Chemical Engineering, University of Chemistry and Technology, Prague, Czech Republic

<sup>b</sup> Department of Applied Science and Technology, Institute of Chemical Engineering, Politecnico di Torino, Italy

## HIGHLIGHTS

- A new multi-scale framework for the simulation of polyurethane foam is presented.
- Two modelling scales, bubble- and macro-scales, are linked using MoDeNa framework.
- The bubble-scale model computes the bubble growth rate for individual bubbles.
- The macro-scale model solves a PBE for prediction of bubble size distribution.
- Validations showed the successfulness of the proposed modelling framework.

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## ABSTRACT

In this work, we apply a general multi-scale methodology to the simulation of reacting and expanding polyurethane (PU) foams. The approach starts from the baseline macro-scale model of Karimi and Marchisio (2015), which describes the foam as a continuum and applies the population balance equation (PBE) to determine the evolution of the bubble size distribution (BSD) during the foaming process. The main novelty of this work is the replacement of the simplistic bubble growth rate model used previously, with the detailed bubble-scale model, which resolves the mass, momentum and energy boundary layers around the bubble. A second important novelty concerns the way in which the macro- and the bubble-scale models are coupled, namely on-the-fly and by using the MoDeNa interface. The performance of the final multi-scale model is evaluated by analysing the predictions for foam density, temperature and BSD on 11 different test cases. Comparison for these test cases demonstrates a significant improvement in the ability of the model to describe the PU foaming process.

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## 1. Introduction

Its world wide market size and its wide range of applications, from the auto-mobile industries, to the construction and household appliances, indicate the importance of polyurethane (PU) foams. From the manufacturer standpoint, a-priori knowledge of the properties of the final product leads to the ease of process design, optimization and transferability. Besides the economical benefits, this reduces the sensitivity of the PU production to human faults and human dependencies. In other words, a fully predictive and viable modelling framework is required to determine the foam characteristics.

However, the foaming process itself is a complicated physical phenomenon. It involves chemical reactions of different

components that determine the evolution of the bubble/cell size distribution (BSD) due to the bubble growth and coalescence. Furthermore, material properties such as the foam density and the viscosity, as well as the thermal conductivity, are directly affected during this process (Gibson and Ashby, 1997). The aforementioned complexity makes the modelling techniques to be more biased toward empirical approaches. For example, different groups described in the past the main reactions and physical phenomena involved during the foaming process (i.e., gelling and blowing reactions, evaporation of the blowing agent) by using an empirical approach (Baser and Khakhar, 1994a,b, Gupta and Khakhar, 1999) and validated predictions with experimental measurements of foam temperature and density. Among the different approaches employed (Princen and Kiss, 1986; Qin et al., 2007) there are few instances where Computational Fluid Dynamics (CFD) is utilized for the modelling and simulation of PU foams. As a case in point, Seo et al. introduced an explicit high resolution method for capturing the foam interface for mold filling applications (Seo et al.,

\* Corresponding author.

E-mail address: [Juraj.Kosek@vscht.cz](mailto:Juraj.Kosek@vscht.cz) (J. Kosek).

2003; Seo and Youn, 2005). They were able to reproduce experimental profile describing the decrease of foam density, while the foam viscosity was modelled by using the Castro–Macosko model (Castro and Macosko, 1982). Several research groups then improved the CFD model using Volume-of-Fluid (VOF) method (Bikard et al., 2007; Geier et al., 2009; Winkler, 2009; Samkhaniani et al., 2013). They included extra equations for the kinetics of the reactions and empirically derived formulations for the foam properties, such as thermal conductivity. It should be indicated that none of the above-mentioned models did take into account the occurrence of bubble growth and the evolution of the BSD.

The bubble growth in PU foams was also considered separately, neglecting the macro-scale. Harikrishnan and Khakhar (2009) used a simple mass transfer model with the mass transfer coefficient as a model parameter. Kim and Youn (2000) used a similar bubble-shell model, as in this work, to predict the evolution of bubble radius in PU foams. However, none of these works considered the BSD.

Recently, Karimi and Marchisio (2015) introduced a macro-scale baseline model that describes the reactive-expanding PU foam as a continuum, by solving a population balance equation (PBE) to track the evolution of the BSD. In this modelling strategy, the polymerization reactions in conjunction with the presence of physical and chemical blowing agents were considered and predictions were validated against the literature data. The macro-scale baseline model, developed for future CFD applications, but verified and validated for the moment on simple zero-dimensional test cases, made however a very simple assumption on bubble growth: the process was modelled as diffusion-controlled, resulting in a constant multiplied by the concentration gradient around the bubble.

The aim of this work is to overcome this limitation by coupling the macro-scale model for the PU foam with a detailed bubble-scale model for the growth rate. The detailed bubble-scale model considers the interaction between molecular diffusion and chemical reactions by resolving the mass, momentum and energy boundary layers around the bubble and is coupled with the macro-scale model with the use of an ad hoc interface library: the MoDeNa interface (MoDeNa-EUProject, 2015). This efficient coupling of the two scales allows us to simulate the macro-scale foam evolution, without missing the important bubble-scale details, with reasonable computational costs. Comparison of the multi-scale model predictions with experimental data on 11 different test cases shows a significant improvement, with respect to the simpler stand-alone macro-scale baseline model, paving the way for the final extension of the approach to real three-dimensional CFD simulations.

## 2. Governing equations

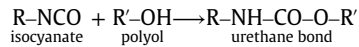
The mathematical model presented in this work constitutes from several parts. At the top level, we have a macro-scale model, which uses the PBE to track the evolution of the BSD. The bubble growth rate needed by the PBE is, in turn, obtained from the bubble-scale model, which describes the detailed growth of individual bubbles. The overall model is complemented by the kinetic model, which is used by both the macro-scale and the bubble-scale models. In what follows the different parts will be described, together with the strategy used to interface them.

### 2.1. Kinetic model

PU foams are created from the mixture of initial reactants, i.e., isocyanates, polyols and water with surfactant and catalyst. The overall reaction rate depends on the functionality, type and

amount of used compounds. It is still a standard practice to simplify the complex polymerization scheme to just two global reactions to limit the number of kinetic parameters that should be determined.

The reaction between isocyanates and polyols, during which the urethane bonds are formed, is called the gelling reaction. Schematically, it can be written as:



The reaction between two isocyanate groups and water molecule creates an urea bond and a molecule of carbon dioxide. This is called the blowing reaction and it can be written as:



The kinetics of these simplified reactions can be expressed in terms of the conversion of polyol groups  $X_p$ :

$$\frac{dX_p}{dt} = A_p \exp\left(-\frac{E_p}{R_g T}\right) (1 - X_p)(c_{c,0} - 2c_{w,0}X_w - c_{p,0}X_p) \quad (1)$$

and conversion of water molecules  $X_w$ :

$$\frac{dX_w}{dt} = A_w \exp\left(-\frac{E_w}{R_g T}\right) (1 - X_w) \quad (2)$$

where  $t$  is the time,  $A_p$  and  $A_w$  are the pre-exponential factors,  $E_p$  and  $E_w$  are the activation energies,  $R_g$  is the gas constant,  $T$  is the temperature and  $c_{c,0}$ ,  $c_{p,0}$  and  $c_{w,0}$  are the initial concentrations of isocyanate groups, polyol groups and water, respectively. In these equations the foam is treated with a zero-dimensional approach, assuming negligible property gradients, however their extension to three-dimensional approaches is straightforward.

If the foam is considered to be internally and externally adiabatic the enthalpy balance can be written as follows:

$$\frac{dT}{dt} = \frac{(-\Delta H_p)c_{p,0}}{\rho_{\text{tm}} c_{p,f}} \frac{dX_p}{dt} + \frac{(-\Delta H_w)c_{w,0}}{\rho_{\text{tm}} c_{p,f}} \frac{dX_w}{dt} + \sum_{\alpha=1}^N \frac{(-\Delta H_{v,\alpha})dw_\alpha}{c_{p,f}} \frac{dw_\alpha}{dt} \quad (3)$$

where  $\Delta H_p$  and  $\Delta H_w$  are the reaction enthalpies of the gelling and blowing reactions, respectively,  $\rho_{\text{tm}}$  is the density of the liquid mixture undergoing polymerization,  $c_{p,f}$  is the thermal capacity of the foam,  $\Delta H_{v,\alpha}$  is the heat of evaporation for the  $\alpha$ th blowing agent and  $w_\alpha$  is the mass fraction for the  $\alpha$ th blowing agent in the gas phase with respect to the foam. The adiabatic condition is justified by the facts that foams have low thermal conductivity and that the internal structure of the foam is formed relatively quickly when the temperature is still quite low. The temperature continues to increase during the polymer curing. However, the foam density remains practically constant after the gel point is reached.

Eqs. (1)–(3) represent a system of ordinary differential equations. This system is subjected to the following initial conditions

$$X_p|_{t=0} = 0, \quad (4)$$

$$X_w|_{t=0} = 0, \quad (5)$$

$$T|_{t=0} = T_0, \quad (6)$$

where  $T_0$  is the initial temperature.

### 2.2. Bubble-scale model

The bubble-scale model simulates the growth of a single bubble surrounded by a shell of reaction mixture (see Fig. 1). There are several simplifications associated with this model: (i) the model

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