Development of a macro-scale CFD-PBE model for the Polyurethane foaming process

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Polyurethane (PU) foams are widely used in a variety of applications such as soft cushioning foam, thermal insulation material, car dashboard and many other applications. Because of the wide usage and good mechanical and thermal properties of the PU foams, there exists a steady increase in its commercial interest. Thus, the transition of the modeling methods from the empirical-based models to the numerical ones receives a lot of attentions, recently.

This class of material forms from the exothermic reaction of isocyanate groups with active hydrogen atoms (e.g. alcohol, amines, and water). The reaction comprises two steps of development, including the gelling reaction (i.e., hydroxyl group + isocyanate) and the blowing reaction (i.e., water + isocyanate). Additives such as blowing agents and surfactant can also be incorporated to adjust the reaction rate and the mechanical properties of the final product. The second reaction (i.e., the blowing reaction) produces carbon dioxide gas which triggers the foaming process. Furthermore, the characteristics of the final product depend on the size of the gas bubbles. The foaming process begins with mixing of the two components and proceeds with the generation of small gas nuclei with a stirrer or whipping air. The diffusion of gas from the blowing reaction into the liquid phase results in the continuous grow of bubbles leading to the bubble coalescence and breakup. The final morphology of the foam is determined by the size distribution of the gas bubbles [1]. A typical foaming process is shown in Figure 1.



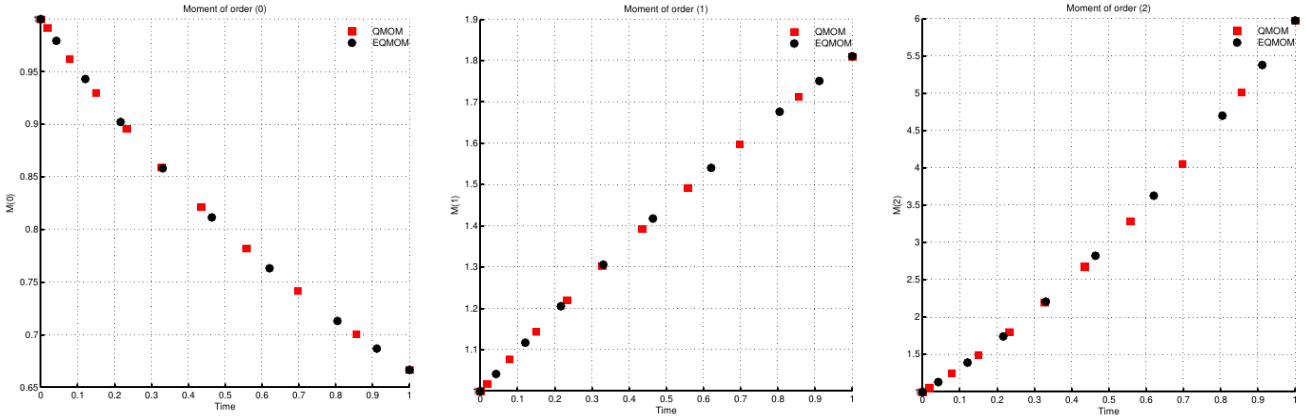
Figure 1. Foaming process: including mixing the components, stirring for nucleation, bubble growth and coalescence and final foam, adopted from BASF Polyurethanes [2].

As mentioned above the final bubble size distribution within the foam can significantly alter the properties of the PU foams. Therefore, the main objective is to formulate a macro-scale computational model for the foaming process capable of predicting the evolution of the bubble size distribution during

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Computational Fluid Dynamics (CFD) is utilized to simulate the behavior of the polymer mixture. This complex multiphase systems is considered to be constituted by two immiscible fluids. One phase is air, which fills the majority of the computational domain at time zero. As the time progresses the expansion of the PU foam, treated as a pseudo-continuous phase, replaces the air phase and the interface between the two phases is captured by using Volume of Fluid (VOF). It is also worth pointing out that the varying properties of the PU foam/mixture, such as the density and viscosity of the foam, are modeled using sub-models that will be developed within the project via multiscale modeling. Both OpenFOAM and Fluent CFD solvers are compared for solving the governing equations.

In addition, a population balance equation is incorporated in the CFD framework to assess how the size distribution of the disperse gas bubbles in the PU foam varies in time and space. Appropriate source terms are included in the population balance equation (PBE) to take into account the influence of the continuous and discontinuous phenomena such as bubble nucleation and coalescence. The Quadrature-Based Method of Moment (QBMM) is used to solve the PBE. In this method the number density function, representing the expected number of bubbles with certain size, is approximated with simple basis functions [3], and the evolution of the system is done by tracking some moments of the bubble size distribution. The time efficiency and accuracy of this approach is demonstrated by Marchisio et al. [4-5]. In the current work, two kernel density functions, Dirac delta functions (QMOM) and log-normal distributions (EQMOM) are compared to approximate the PBE solution. An example of results for a case of a PU foam undergoing bubble growth (due to gelling and blowing) and bubble coalescence is shown in Figure 2. In this figure the evolution of the first moments of the bubble size distribution (normalized by their initial value) as a function of time is illustrated for two different methods, i.e., QMOM and EQMOM. As can be seen both methods provide identical solutions. In this case study the moment of order zero, representing the total number density of the bubbles in the foam, decreases due to coalescence, whereas the moment of order one, representing the total bubble gas volume fraction in the foam increases, due to the growth rate. Higher-order moments (related to the skewness and kurtosis of the distribution) also show reasonable evolutions.



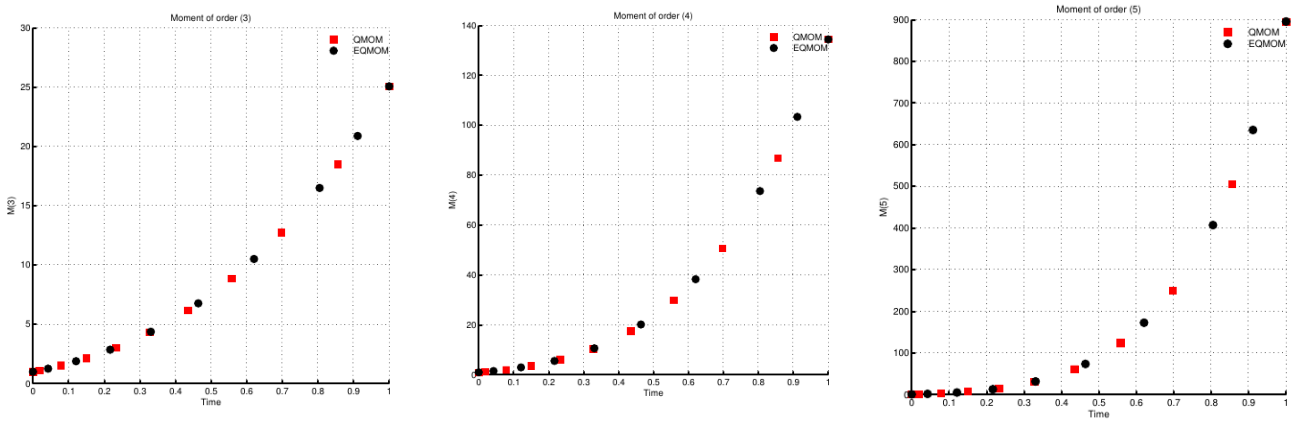


Figure 2. Evolution of the first six normalized moments with respect to the dimensionless time.

Results will focus on the preliminary steps of the work, namely the verification of the implementation of the two different approaches for solving the population balance equation, QMOM and EQMOM into OpenFOAM and the comparison of model predictions with experimental data.

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