A Combined Stochastic and Deterministic Simulation of the Polymer Foaming Process: Asymptotic Solution for the Initial Stages of Bubble Growth

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Thermoplastic foams are often created by the nucleation and growth of bubbles containing a blowing agent inside a polymer melt. The blowing agent is an inert gas such as carbon dioxide that has been dissolved at high pressure in the polymer. Expansion of the mixture through a die leads to a rapid pressure drop and the subsequent nucleation and growth of bubbles. The properties of the resulting polymer foam, such as its strength to weight ratio, depend sensitively on the structure of the foam, including the number density and size distribution of bubbles. Hence the design of processes to produce foams with desired properties requires models that accurately predict foam structural properties.

Final foam structure depends on the interaction between two factors: rate of nucleation of bubbles and rate of bubble growth. Bubble nucleation rates are functions only of local state properties since the characteristic length scale of the critical nucleus is much smaller than other length scales in the foaming process. Once the bubble is nucleated, however, it begins to grow and affects both the growth of other bubbles and the nucleation of subsequent bubbles. During bubble growth, the blowing agent from the surrounding polymer melt diffuses into the bubble establishing a concentration profile inside the polymer. As a result there is a lowering of the local supersaturation of the blowing agent in the polymer melt in the region close to the bubble. This in turn reduces the growth rate for nearby bubbles and locally suppresses subsequent nucleation of bubbles.

Due to the discrepancy in the characteristic length scales for nucleation and growth of bubbles, polymer foaming models use analytic solutions of the equations governing growth of a single bubble to provide initial conditions for the bubble dynamics.[1-3] We recently found that the existing asymptotic solution for the blowing agent concentration around a growing bubble [1] does not satisfy a mass balance. As a result, models based on these results [2,3] indicate too large an influence volume around each bubble.

In the oral presentation of this work, we present improved asymptotic results for the dynamics of bubble growth at low Peclet number. The solution gives both an inner and an outer solution, for the regions close to the bubble and far away from the bubble, respectively. Close to the bubble, the solution is consistent with previous asymptotic and numerical results.[1,2] Far from the bubble a singular expansion is required. A composite solution for the concentration profile is obtained via asymptotic matching. The composite solution satisfies the overall mass balance of the blowing agent around the bubble. Details of the solution are to be published elsewhere.[4]

The improved asymptotic results provide the initial bubble conditions for a combined stochastic/deterministic simulation of polymer foaming under development in our research group.[4]

[1] M. A. Shafi and R. W. Flumerfelt, Initial Bubble Growth in Polymer Foam Processes, *Chem. Eng. Sci.* **52**, 627 (1997).
[2] M. A. Shafi, K. Joshi, R. W. Flumerfelt, Bubble size distributions in freely expanded polymer foams, *Chem. Eng. Sci.* **52**, 635 (1997).
[3] K. Joshi, J. G. Lee, M. A. Shafi and R. W. Flumerfelt, Prediction of Cellular Structure in Free Expansion of Viscoelastic Media, *J. of Appl. Polym. Sci.*, **67**, 1353 (1998).
[4] S. Punnathanam and R. B. McClurg, In Preparation (2004).