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Numerical Simulation of Cell Nucleation in Polymer Foaming Using a Modified Classical Nucleation Theory

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In this paper, a modified heterogeneous nucleation theory which considers the nucleation that occurs at the nucleating agents with randomly distributed shapes is employed to simulate cell-nucleation of polymeric foaming. In order to avoid the error involved in the bubble pressure and surface tension approximations that are commonly used in cell-nucleation simulations, the approaches suggested in our previous study are employed to estimate the values of these parameters. To evaluate the validity of the modified nucleation theory, simulation results based on the theory are compared to the experimental results observed in a batch foaming process. It is interesting to note that the modified heterogeneous nucleation theory explains the experimental observation quantitatively when using the contact angle and the concentration threshold determined through an iterative approach. Although the validity of the choices of the contact angle and the concentration threshold has to be further investigated experimentally and theoretically, this paper has illustrated that the theory has provided qualitative directions to further improve the understanding of cellnucleation phenomena in polymeric foaming processes.