Numerical simulation for nonsolvent-induced phase separation by ternary phase field theory

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Abstract

Polymeric membranes are essential materials for industrious applications such as wastewater treatment, seawater desalination, or support for bioreactors. The separation capacity of these membranes is determined mainly by their microstructure. The most popular and economical approach to design those membrane microstructures is non-solvent induced phase separation (NIPS), also known as wet-phase inversion. During this process, the exchange of non-solvent and solvent between a bath and a polymer film induced the film to separate into two phases. Even though rich experimental studies have been done on NIPS, the desired morphology is typically found by multiple experimental tests on process parameters, which is ineffective for material design. In this study, we simulate the NIPS process of the target system: Water/DMF/PVDF by phase field model, a well-known mesoscopic computational framework for predicting spinodal decomposition. In the model, the Flory-Huggins free energy with concentration-dependent mobility is used to model the mass transfer process. Furthermore, random force following the fluctuation−dissipation theorem (FDT) [1] is included in the governing equation to consider thermal fluctuation. We also consider a bath-film system [2] used in experiments and industrious processes to make the model closer to the application scenario. The system's governing equations are solved by an advanced implicit pseudo-spectral method to obtain maximum numerical stability and accuracy. The final simulation would be validated with experimental results by suitable statistical tools such as structure factor, characteristic length, porosity, and morphology. We expect the simulation results can advance the discovery of the dynamics in NIPS.

Keywords: Nonsolvent-induced phase separation, Flory-Huggins, Fluctuation-Dissipation, Cahn-Hilliard, Pseudo-Spectral, Structure Factor

Reference

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