

396b Modeling and Simulation of Nonsolvent Vapor-Induced Phase Separation

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A model is developed for the nonsolvent vapor-induced phase separation process (VIPS). The model incorporates coupled heat and mass transfer, ternary diffusion and a moving boundary at the polymer solution/air interface. Predictions are shown for mass transfer paths, composition profiles, film temperature, and thickness for evaporation of solvent from a binary polymer/solvent system under an atmosphere containing the nonsolvent vapor. Four systems used for simulations are cellulose acetate/acetone/water, poly(vinylidene fluoride)(PVDF)/dimethylformamide(DMF)/water, polysulfone(PS)/N-methyl-2-pyrrolidone(NMP)/water, and poly(etherimide)(PEI)/NMP/water. By superposing mass transfer paths onto the ternary phase diagram, a number of detailed morphological features can be predicted. The effects of different controlling parameters including relative humidity, solvent volatility, air velocity, evaporation temperature, initial film thickness, and polymer concentration are investigated. A critical humidity is needed to induce phase separation in VIPS and it is closely related to the nature of the homogeneous region of the ternary phase diagram. The role of diffusion formalism on the morphological predictions is also illustrated to show the accuracy of the multicomponent diffusion theory.