Dissipative particle dynamics simulations of polyethersufone membrane via nonsolvent induced phase separation

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Nonsolvent induced phase separation (NIPS), in which a polymer collapses from solution into a thin film upon exposure to another phase, represent the most widely adopted method to fabricate porous polymeric membranes. The performance associated with the membrane microstructure mainly depends on the complicated mechanism of the NIPS process. The level of understanding of the connection between complex process variables and final membrane structure remains surprisingly empirical. This gap in knowledge necessitates a substantial amount of trial-and-error experimental work to discover and define the "process window" for a particular membrane product, increasing R&D costs and limiting innovation. We have established a novel dissipative particle dynamics (DPD) model to investigate the membrane pore structure formation via NIPS. The model has mapped the polyether sulfone/methyl-2-pyrrolidinone/water (PES/NMP/water) system, incorporating millions of particles. The effects of polymer concentration and polymer molecular weight on membrane pore structures were investigated. Both qualitative and quantitative results are compared to manufactured membrane structures. The analysis in this study provides a better understanding on the formation mechanism of the membrane pore structure via NIPS and proves that the simulation tool developed will enable significant speed-up in membrane development.