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ABSTRACT

A new dissipative particle dynamics (DPD) simulation methodology adopting a mass transfer algorithm was established to investigate the membrane formation process via nonsolvent induced phase separation (NIPS). The effect of the interphase mass transfer between the casting solution and the nonsolvent bath on the membrane formation process and the membrane morphology was elaborately analyzed. Factors including the solvent–nonsolvent interaction, the polymer concentration and the nonsolvent temperature were considered. The results showed that as the solvent-nonsolvent interaction got better, the mass transfer was intensified which contributed to an intense phase separation. Thereby asymmetric membrane structure with a thick dense surface layer and a porous sub-layer would be formed. With the nonsolvent temperature raising, the relatively symmetric structure with small pores was obtained due to the declined polymer aggregation rate and the increased phase separation rate caused by the accelerated mass transfer. As the polymer concentration increased, the flexibility of the system reduced. Thereby the phase separation slowed down, resulting in highly asymmetric structure with a thicker and denser surface layer and a more porous sub-layer. The analysis of the phase separation in this study benefits to a better understanding on the mechanism of the membrane structure via NIPS.