Abstract

Phase change phenomenon has always been an area of interest considering the accompanying nonlinearity and its interesting outcomes. Present work aims at studying various aspects of nonsolvent induced phase inversion during preparation of polymeric membranes.

Thermodynamics of phase inversion was modelled using Flory Huggins theory of polymer solutions and the study of phase inversion kinetics was carried out by measuring solvent concentration in the precipitation bath. These two studies were used to quantify the thermodynamic and kinetic parameters, interplay of which determines the final morphology of the membrane matrix. The comparative study was used to predict the membrane morphology and was validated using extensive membrane characterization.

The thermodynamic and kinetic study, as explained above, was attempted for simple ternary system with polyvinylidene fluoride as polymer and its interactions with four different solvents were explored. Binary interactions among various components were correlated with the widely differing morphologies exhibited by the membranes. This was further extended to study the thermodynamics of membrane system with mixed solvents. A model was proposed to represent solvent leaching with simultaneous evaporation for volatile solvents.

Moving one step ahead, thermodynamic model was developed for quaternary polymeric blend system for locating the complete phase diagram (binodal curve, spinodal curve and critical point). The model was validated using cloud point data and the membrane properties available in literature.
Finally, a multi-component model was developed to study the thermodynamics of polymeric membrane systems with more than one additive. This model was applied to locate the binodal curves with varying additive concentration for systems containing complex organic or inorganic additives (polyaniline, polypyrrole and bentonite) along with other membrane forming components. The interplay of thermodynamic and kinetic parameters resulted into membranes with interesting properties. The novel characteristics exhibited by these membranes such as pH responsive properties were studied in details and explanatory mechanisms were proposed. The solubility parameters of the organic additives were calculated using group contribution method, whereas the same for bentonite was determined by modeling its solubility sphere using its interaction with various solvents.

This work presents a complete solution for modeling the thermodynamics of phase inversion for any polymeric membrane system and can be used as a tool to study the properties of novel compositions or for intermediate compositions eliminating the need for performing a large number of experiments.

Keywords: *Thermodynamic modeling, kinetic study, polymeric membrane, phase inversion, solubility parameter, binodal, spinodal, pH responsive membranes, polymer blend, permeability hysteresis.*