

EFFECT OF WATER INTERACTIONS ON POLYVINYLAMINE AT DIFFERENT PH FOR MEMBRANE GAS SEPARATION

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Polyvinylamine (PVAm) is a linear polyelectrolyte type of polymer which is water-soluble with highest contents of primary amine. It has been attractive in different fields such as: biomedical applications [1], encapsulation [2], oil recovery [3], and primarily it has extensively been used as a fixed-site-carrier polyvinylamine membrane for carbon dioxide separation and capture. A thin selective layer on polysulfone support for CO₂ Separation membranes[4, 5] has been successfully used in composite flat sheet and hollow fiber membranes. The amine group plays the role as the carrier of the gas, increasing the transport performance of the membrane by chemical and physical forces. PVAm composite membrane in dry condition will separate according to solution-diffusion mechanism only. It was however documented by Kim et al. in 2004 [4] that by allowing the membrane to be exposed gas with high relative humidity, the separation performance increased exponentially[4-6]. Through these efforts, it is needed to develop a greater understanding of the relationships between the structure and the interfacial properties of PVAm – water surface. The degree of hydrophilicity manipulation of a given surface necessarily requires understanding the micro-scale principles that, in turn, control the macro-scale surface wetting behavior. See Fig. 1.

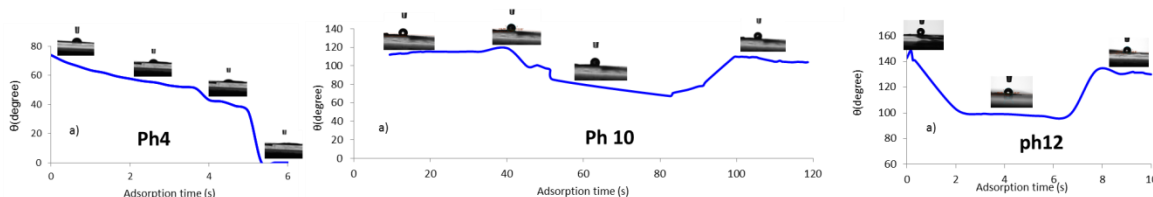


Fig. 1 Effect of PVAm surface of adsorption time on water contact angles at different pH (4, 10, 12)

Approaches based on atomistic molecular simulations should, in principle, yield vital insights on these interactions and constitute ideal tools to estimate the related technological parameter values. In the current project, these PVAm-water interactions were studied at the nanoscale level, both by experimental and molecular modeling. The molecular dynamic simulations contribute to an understanding of the inter-intramolecular interactions and give the possibility to estimate the related technological parameter values, which is assumed to be of great interest to the membrane community.

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