Semi−Aromatic Polyamide−Based Membrane in Forward Osmosis: Molecular Insights

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Despite the increased interest in forward osmosis (FO) in recent years, the technology's advancement in commercial and industrial applications has been hampered by the absence of suitable FO membranes, which demands the exploration of new membranes targeted for some specific uses. Polyamide (PA) thin−film composite (TFC) membranes with high performance are in high demand. However, enabling PA TFC membranes to overcome the perm−selectivity trade-off is still challenging. A fundamental understanding of semi−aromatic PA (SAPA) in the FO process at the molecular scale is crucial to improving their performance capabilities, leading to significant societal and industrial benefits. Here, an atomistic model was built with an equilibrated mixture of hydrolysed trimesoyl chloride and piperazine monomers to address this issue. Nonequilibrium molecular dynamic simulations are used for investigating the membrane model structure and transport characteristics of water and two different solutes, NaCl and Na_2SO_4, through the SAPA FO membrane. Results reveal that the hydrophilic functional groups (−COOH) of the membrane facilitate the transport of water molecules, increasing the water transport across the free volume of the membrane network due to the interactions between the water molecules and the membrane atoms. The SAPA membrane exhibits a high-water flux without sacrificing the rejection of Na_2SO_4 (> 99%). The pathways of monovalent solute ions (Na^+ and Cl^-) follow the same fashion as water molecules; in contrast, divalent solute molecules (Na_2SO_4) are trapped due to high units of −COOH groups in the membrane. The performance of the SAPA membrane in this work reveals the potential of PA TFC membranes in the textile industry for wastewater treatment.

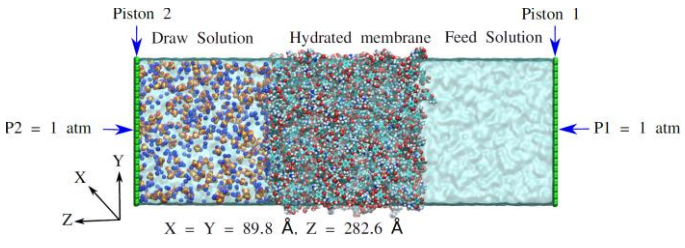

Fig.1 FO simulation system

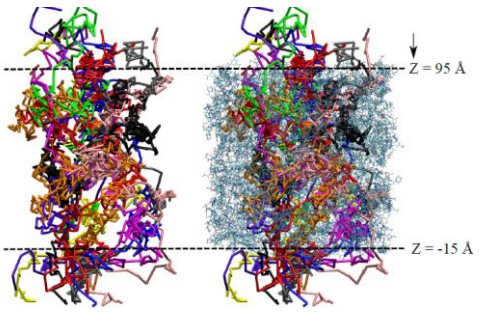

Fig.2 Pathways of water molecules