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Molecular Dynamics Simulation Study of Sulfonated Polybenzimidazole Polymers as Promising Forward Osmosis Membranes

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Abstract : With increased levels of clean and affordable water scarcity crises in many countries, wastewater treatment has been chosen as a viable method to produce freshwater for various consumptions. Even though reverse osmosis dominates the wastewater treatment market, forward osmosis (FO) processes have significant advantages, such as potentially using a renewable and low-grade energy source and improving water quality. FO is an osmotically driven membrane process that uses a high concentrated draw solution and a relatively low concentrated feed solution across a semi-permeable membrane. Among many novel FO membranes that have been introduced over the past decades, polybenzimidazole (PBI) membranes, a class of aromatic heterocyclic-based polymers, have shown high thermal and chemical stability because of their unique chemical structure. However, the studies reviewed indicate that the hydrophilicity of PBI membranes is comparatively low. Hence, there is an urgent need to develop novel FO membranes with modified PBI polymers to promote hydrophilicity. A few studies have been undertaken to improve the PBI hydrophilicity by fabricating mixed matrix polymeric membranes and surface modification. Thereby, in this study, two different sulfonated polybenzimidazole (SPBI) polymers with the same backbone but different functional groups, namely arylsulfonate PBI (PBI-AS) and propylsulfonate PBI (PBI-PS), are introduced as FO membranes and studied via the molecular dynamics (MD) simulation method. The FO simulation box consists of three distinct regions: a saltwater region, a membrane region, and a pure-water region. The pure-water region is situated at the upper part of the simulation box, while the saltwater region, which contains an aqueous salt solution of Na+ and Cl− ions along with water molecules, occupies the lower part of the simulation box. Specifically, the saltwater region includes 710 water molecules and 24 Na+ and 24 Cl− ions, resulting in a combined concentration of 10 weight percent (wt%). The pure-water region comprises 788 water molecules. Both the saltwater and pure-water regions have a density of 1.0 g/cm^3. The membrane region, positioned between the saltwater and pure-water regions, is constructed from three types of polymers: PBI, PBI-AS, and PBI-PS, each consisting of three polymer chains with 30 monomers per chain. The structural and thermophysical properties of the polymers, water molecules, and Na+ and Cl− ions were analyzed using the COMPASS forcefield. All simulations were conducted using the BIOVIA Materials Studio 2020 software. By monitoring the variation in the number of water molecules over the simulation time within the saltwater region, the water permeability of the polymer membranes was calculated and subsequently compared. The results indicated that SPBI polymers exhibited higher water permeability compared to PBI polymers. This enhanced permeability can be attributed to the structural and compositional differences between SPBI and PBI polymers, which likely facilitate more efficient water transport through the membrane. Consequently, the adoption of SPBI polymers in the FO process is anticipated to result in significantly improved performance. This improvement could lead to higher water flux rates, better salt rejection, and overall more efficient use of resources in desalination and water purification applications.

Keywords : forward osmosis, molecular dynamics simulation, sulfonated polybenzimidazole, water permeability
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