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Theoretical Design of Reverse Osmosis Membranes by Investigating the Microscopic Mobilities of the Molecular Chains

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Summary

To control membrane fouling on a reverse osmosis membrane for seawater desalination, molecular modeling on the interface between a membrane surface and foulant molecules is essential. In this study, molecular dynamics (MD) simulations were conducted to gain an insight into the microscopic interactions of organic foulants and those of the surrounding water molecules in the vicinity of three types of repeating units of low-fouling zwitterionic material: sulfobetaine, carboxybetaine, and phosphobetaine. As a simplified foulant molecule, isopropyl alcohol (IPA) was adopted, and the ternary mixture systems consisting of zwitterionic moieties, IPA molecules, and water molecules, were used as simulation cells. After the MD runs at 298 K, radial distribution functions (RDFs) of water molecules and IPA molecules around the ionic groups of the repeating units were calculated to evaluate the interactions between the solvent molecules and the zwitterionic moieties. As a result, the RDF peaks of water molecules around the anionic oxygen atoms are markedly higher than those of IPA molecules. The peaks of water molecules around the cationic nitrogen atoms are also higher than those of IPA molecules. These results indicate that the water molecules selectively coordinate around the ionic groups of the zwitterionic moieties. To evaluate the selectivities more quantitatively, coordination numbers of the two types of solvent molecules were calculated by using the RDF curves. Consequently, the numbers of water molecules around the anionic oxygen atoms were 1.9–2.5 times larger than those of IPA molecules, suggesting that the higher selectivities of water over organic foulant is one of the origins of antifouling properties of polyzwitterions.