No. 2312

Evaluation of Microscopic Interactions for Three Types of Components for the Materials Design of Reverse Osmosis Membranes

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Summary

Reverse osmosis membranes have been used as a process for desalinating seawater, and efforts to reduce membrane fouling are essential to enhance the process efficiency. Ionic components, biopolymers such as proteins and polysaccharides, and various organic compounds have been pointed out as diffusing solids/particles (foulants) that cause membrane fouling. Thus, it is essential to analyze the microscopic interactions between the three components: membrane surface, foulants which diffuse near the surface, and numerous water molecules surrounding the foulants.

Our group has investigated the mechanisms of the fouling behavior of polymeric materials, by using molecular dynamics (MD) simulations. In particular, we have focused on the relationship between surface properties, such as hydrophilicities and charge densities, and fouling behavior. For example, betaine polymers, which have zwitterionic groups and exhibit excellent antifouling properties, have been put to practical use as biomaterials. Nonionic poly(2-methoxyethyl acrylate) (PMEA) has also been used as a biomaterial. Although the PMEA surface is not more hydrophilic than the poly(2-hydroxyethyl methacrylate) (PHEMA) surface, PMEA surface exhibits much more excellent antifouling properties than PHEMA surface, indicating that the approach to form a barrier of water molecules by coating the membrane surface with hydrophilic agents is not absolutely effective.

In this study, we set the two main objectives. The first is the analysis of the correlation between the constituent charged groups in the side chains of betaine polymers and the antifouling properties, by using MD simulations. A theoretical approach to investigate the mechanisms of antifouling properties of betaine polymers was proposed. The second is the development of a methodology to evaluate the hydrophilicity/hydrophobicity of nonionic polymeric materials, by using MD simulations. In particular, a simplified approach to assess the hydrophilicity of poly(*N*-isopropylacrylamide), which is a representative temperature-responsive material, was proposed.