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# Theoretical Design of Novel Aquaporin Like Reverse Osmosis Membrane to Realize High Water Flux and Salt Rejection

Hiromitsu Takaba

School of Advanced Engineering, Kogakuin University

Summary

For reverse osmosis membranes used for seawater desalination, membranes with high water permeability and salt rejection are required even at low pressure. Therefore, it is desired to develop a reverse osmosis membrane based on a novel transport mechanism to overcome conventional membrane performance. In this study, we focused on the mechanism of water permeation in water channels of biological membranes such as aquaporin, and theoretical design of reverse osmotic membrane based on novel transport mechanism was carried out by molecular dynamics (MD). Aquaporin has a water channel, showing a high-speed transport of water molecules realized by forming a continuous hydrogen bonding with amino acid residues in the pore wall. Such a transport mechanism would be different from the conventional reverse osmosis membrane based on polymer sorption / diffusion mecahnism, and if it can be realized even with artificial membranes using a pressure difference as a driving force, it will lead to the development of a novel reverse osmosis membrane. In this study, theoretical evaluation of water flux in a one-dimensional pore model modeling aquaporin water channel. Fluctuating wall – MD was used for modeling of permeation under a constant pressure difference by keeping the pressure of two liquid phases across the membrane constant. Single-walled carbon nanotube-like pores were used as a simplified pore model of aquaporin water channel. Charged atoms were arranged in the pore wall to form a hydrogen bonding with permeating water molecules. From the MD results, it is clarified that water molecule shows a single file diffusion with highly controlled molecular orientation by forming hydrogen bondings with charged atoms in the pore wall. The difference in the permeation behavior of water molecules influences the flux, and by arranging charges in a double helix in the pore wall, observed water flux was much higher than that reported in aquaporin of $10^8$ molecule / s. It was also revealed that the flux increases in proportion to the applied pressure. It would be concluded that a reverse osmosis membrane based on a novel mechanism with controlling molecular orientation in the pores has a potential to show a extremely high permeation flux comapredto the conventional ones.