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Molecular dynamics simulation of seawater reverse osmosis desalination using carbon nanotube membranes

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ABSTRACT

Reverse osmosis (RO) desalination of 35,000 ppm seawater consisting of sodium and chlorine ions with water was simulated using molecular dynamics. In this study, RO simulations were performed at different pressures using carbon nanotube (CNT) membranes having varying pore diameters (8–14 Å). Results showed that a CNT membrane allowed high water fluxes because of the presence of a low energy barrier for water–carbon interactions, with continuous and ordered water chains observed inside the CNTs. The investigations into the ion rejection capability of CNT membranes revealed that (6, 6) CNTs could provide high rejection rates (>95%). The rejection of ions was mainly due to the presence of a high energy barrier caused by removing the hydrating water molecules necessary for ions to pass through the narrow CNT pore. The desalination performance of (6, 6) CNT membranes and conventional polymeric membranes was then compared. It was found that CNT membranes have a higher normalized flux and comparable ion rejection, indicating their feasibility for effective seawater desalination. Overall, this study demonstrated the usefulness of molecular dynamics in investigating membrane processes and its potential role in improving desalination performance.

Keywords: Molecular dynamics; Reverse osmosis; Desalination; Water treatment; Carbon nanotube

1. Introduction

Seawater desalination has been highly regarded as one solution to the growing problem of water stress. Among technologies now being used to purify seawater, reverse osmosis (RO) is a popular choice because of its high efficiency and lesser energy consumption and cost compared to thermal techniques [1]. However, despite continuous research and development, seawater reverse osmosis (SWRO) processes using current polyamide membranes still have limitations in terms of both water production and resistance to fouling.

Because of the increasing availability of computers having a high computational power, new types of SWRO membranes based on graphite and nanomaterials, which can improve desalination, are being studied using molecular dynamics simulations. For example, RO through boron nitride nanotubes and carbon nanotubes (CNTs) was simulated, and the performance of both nanotubes exceeded that of a polymeric

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