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Effect of channel thickness on the particle diffusion and permeability of carbon nanotubes a membrane in reverse electrodialysis process using molecular dynamics simulation

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Abstract

Adopting innovative technology and solutions is critical for ensuring clean water. Several methods may be used to remove salts from water. They may be divided into two categories: membranes and heat. Reverse electrodialysis, which uses a membrane, is an efficient way of separating substances. Prior research investigated system-level factors, but the nanoscale mechanisms that drive ion and water penetration across membranes were poorly understood. This study closed a research gap by investigating the influence of carbon nanotube membrane thickness on particle mobility and fluid dynamics in reverse electrodialysis systems. The research is contributed to the enhancement of energy conversion efficiency and membrane performance in reverse electrodialysis systems by offering a comprehensive understanding of the influence of channel thickness on particle transport and selectivity through the carbon nanotube membrane. Molecular dynamics simulations using the LAMMPS software package are conducted to examine the effect of carbon nanotube thickness variation (1-layer vs 2-layer) on fluid flow, ionic current, hydrogen bonding, and fluid density. To the findings, increasing the thickness of a carbon nanotube from one layer to two layers decreases the fluid flow rate to 203.79 atoms/ns and the current from 5.31 e/ns to 5.15 e/ns. Additionally, the number of broken hydrogen bonds decreases from 116 to 105, indicating decreased permeability and increased stability of the hydrogen-bonding network. In addition to offering useful information for the construction of more effective and selective membranes in renewable energy applications, these results provided a molecular understanding of how carbon nanotube thickness affected reverse electrodialysis effectiveness.

Introduction

The global water demand is on the rise as a result of the increasing water consumption by individuals and businesses. Nevertheless, our water supply is rapidly diminishing [1]. To guarantee that the populace has access to pure water, it is imperative to implement innovative technologies and solutions [2]. There are numerous methods for the removal of soluble ions from water. Membranes and heat are the two primary categories into which these methods can be categorized. The methods employed to remove dissolved substances from water determine the separation. Membrane methods are a group of techniques that are of great significance because they facilitate the remediation of water and effluent through a variety of methods. The consistent efforts to enhance the utilization of electricity were motivated by its affordability and convenience of accessibility [3]. In membrane methods, specific membranes permit the passage of certain ions but prevent the passage of water molecules. Membrane technologies can be classified into two categories: technology under pressure and technology under electric potential. Electrodeionization (EDI), Reverse electrodialysis (RED), and Electrodialysis (ED) are the three primary technologies included in electropotential membrane methodologies. The advantages of the RED method have resulted in its increasing popularity and significance. RED is capable of treating water that contains significant concentrations of unsaturated sodium without the use of chemical additives. This is achieved by directing the passage of water. The RED process has the advantage of not necessitating acid treatments or anti-fouling agents when saline water is employed [4]. This procedure presents a substantial challenge due to the discrepancy between the increase in ion movement and the voltage in the EDR membrane, except for a specific current density range. However, it leads to the water dissolving into H+ and –OH ions, which enhances its functionality. This circumstance has rendered the system inoperable. This method has a wide range of applications. Its effects include the reinforcement of saline water, the enhancement of mineral levels in water similar to furnaces, the purification, and recycling of polluted water from industrial locations, the increase in mineral content in food, and the removal of beneficial substances from liquids used in metal cleansing [5]. With the increasing emphasis on advanced materials in enhancing membrane performance, nanomaterials, such as carbon nanotubes (CNTs) attracted significant interest due to their unique physical properties. CNTs exhibit remarkable strength and exceptional heat conductivity [6]. The carbon composition of nanotubes is the reason for their exceptional strength. Carbon's economic value and low weight have motivated scientists to conduct a comprehensive examination of its atoms and electrons [7]. The utilization of CNTs facilitates the development of miniature electronic devices, including sensors, filters, and batteries. Additionally, they can retain power and be employed in devices that respond to light [8]. These tubes are widely used in chemical reactions, electrical systems, and machinery due to their extensive surface area [9]. CNTs can demonstrate selective permeability toward specific ions, such as cations or anions, as a result of their distinctive surface properties and structure. This selective ion transport can strengthen the membrane's capacity to effectively utilize the salinity gradient between the two solutions, resulting in an increase in energy conversion efficiency in the RED process [10]. The cylindrical structure of CNTs can facilitate the transportation of ions and water molecules across the membrane by ensuring high permeability. In the RED system, this high permeability can result in an increase in the total flux of ions through the membrane, which in turn leads to an improvement in energy output and power density [11]. CNTs exhibit exceptional mechanical properties, including flexibility and high tensile strength. The mechanical stability of the membrane can be enhanced by incorporating CNTs into it, which ensures its integrity and efficacy during the RED process, particularly under high-pressure or high-flow conditions [12]. The selective transport of cations and anions through the CNT channels is crucial because it determines the membrane's capacity to harness the salinity gradient between two solutions to produce renewable electricity. The total energy conversion efficiency of the RED process can be improved if the membrane demonstrates selective permeability toward specific ions [13]. By examining the impact of channel thickness on particle diffusion and permeability, the study offers a deeper understanding of the CNTs' selective ion transport properties. Ultimately, the efficacy and efficiency of the RED system for blue energy generation can be enhanced by utilizing this information to optimize the membrane design and fabrication to maximize the selectivity toward cations and anions. In addition to membrane design considerations, previous research utilized numerical and analytical models to examine the underlying transport phenomena and performance restrictions in RED systems. The movement in ED and RED when coping with imperfect membranes was illustrated by Tedesco et al. [14] in a simplified 2D model. The selectivity and electrical conductivity of ion exchange membranes can be assessed to ascertain their efficacy. This typically led to a 20% decrease in power density in RED. Moya [15] investigated the impact of concentration polarization on the maximal power output in a system that employed an ion exchange membrane and RED. Utilizing the internal resistance as determined by the brief circuit current is the most efficient approach to optimizing the power output of a RED stack. This was more effective when the membrane was thinner, the flow rate is higher, and the concentration of fixed-charge in the membrane is lower.

Additional knowledge of membrane behavior and ion transport efficiency in energy and desalination applications was gained via practical and simulation-based research in addition to theoretical modeling. Molecular dynamics (MD) simulations were used to test different membrane materials and architectures, and techniques like electrolysis and reverse osmosis were used to remove ions from liquids. Cation exchange membranes were frequently employed to distinguish compartments in microbial fuel cells. Their function was to facilitate the passage of Na^+ ions, and their exceptional conductivity was a result of negatively charged sulfonate groups. ED utilized these robust acid polymer membranes, which contained numerous sulfonic acid groups [16]. RED utilized ion exchange membranes to extract energy from the salinity difference between two water currents. Spacers were employed in conjunction with cation exchange membranes and anion exchange membranes to facilitate the flow of saline and river water. The salinity gradient was converted into electricity in the stack by the collaboration of electrodes and an electrolyte solution [17]. Li et al. [18] explored how CNT channel roughness impacts ion diffusion and permeability in reverse electrodialysis. They found that armchair-edged CNTs maximized electric current, while roughness enhanced fluid-duct interactions, reduced particle mobility, and increased broken hydrogen bonds. Li et al. [19]investigated the effects of gold nanoparticle addition and CNT edge structure on paraffin-based phase change materials, finding that gold nanoparticles enhanced thermal conductivity and energy storage, while armchair-edged CNTs maximized electric current due to strong atomic interactions. ABM Ali et al. [20] investigated the water transport through CNT under electric current, focusing on how varying ion atomic ratios affect system behavior. They found that increasing ion concentration boosted electric current and ionic mobility, while also raising the number of broken hydrogen bonds and slightly reducing maximum density, thereby influencing water flow dynamics. After these preliminary investigations, additional research was directed toward the examination of the precise applications of ion-selective membranes and nanomaterials in the purification of water and the elimination of pollutants under a variety of operational conditions. EDR systems were the subject of research by scientists to generate renewable and environmentally friendly electricity. Their research entailed the examination of salinity disparity between river water and seawater. The examination of research that was conducted enabled us to observe the progression of this process [21]. Chagami et al. [22] investigated the impact of pH levels and voltage on the separation of copper ions from water. The findings indicate that the rate at which copper ions were extracted from water increased as the pH increased and the voltage decreased. Khataee et al. [23] investigated using silicon carbide nanotubes as a filter to eliminate nitrate ions from water. The results indicate that SiC nanotubes that were tested were capable of effectively eliminating nitrate ions from water. Georgescu et al. [24] evaluated the efficacy of sulfur dioxide elimination from a contaminated electric current through electricity by analyzing the effects of voltage and electrode size changes. The research shows that the effective elimination of sulfur dioxide necessitated the incorporation of ammonia into the system. Moisture can be introduced into the air to enhance the efficiency of sulfur dioxide removal from a gas, and the gas must be cooled before entering the system. Yip et al. [25] focused on the energy efficiency and durability of RED and delayed pressure osmosis. Pressure-delayed osmosis was more efficient in generating energy from a variety of salt concentrations, as indicated by this study. Conversely, RED necessitated superior-quality membranes to achieve comparable performance. Chen et al. [26] identified a method that streamlines the process of obtaining potable water from saline water by integrating ED and RED. This work was unique in its ability to produce energy autonomously, without the need for external energy inputs or additional devices. Ultimately, this process converted saline water into potable water without the need for additional energy. Gong et al. [27] conducted a study on the absorption of heavy metal ions in water solution and the fabrication of multipurpose nanocomposites. The results indicate that the adsorbent under investigation exhibited a high removal efficiency for metal ions and a high tolerance to low pH.

Prior research on ED and RED systems focused on optimizing ion exchange membranes by assessing characteristics, such as thickness, ion transport, and system resistance. Using simplified models, such as Nernst-Planck-Donnan equations, these investigations demonstrated that membrane charge, flow rate, and fixed-charge concentration all had a substantial influence on performance. Effective membranes were required to overcome polarization losses and inadequate ion selectivity in RED. Furthermore, prior investigations showed that CNT-based specimens outperformed the RED method [[28], [29], [30]]. Despite the useful information provided by these reports, an important gap remained in our understanding of the role of nanoscale structural characteristics, particularly the thickness of CNT-based channels, in determining fluid behavior, ion distribution, and membrane stability in RED systems. Most molecular simulations in this area represented CNTs as perfect single-walled materials, with little research into how multilayered CNT configurations affected atomic-level interactions and transport processes. Because mechanical tensile strength, fluid permeability, and ion selectivity were all factors of nanotube shape, the absence of CNT wall thickness represented a substantial information gap. To investigate the issue, the current work compared the fluid and ion behavior in an environment resembling RED as a function of CNT thickness in 1-layer and 2-layer CNT channels. Using MD simulations, we investigated the effect of structural adaptation on physical stability, water molecule permeability, hydrogen bonding, and electric current production. The distinctive aspect of this study was its atomistic-scale approach to linking membrane thickness with system performance, which provided a fresh viewpoint on improving CNT-based membranes for RED applications. The correlation was critical for building mechanically robust, high-efficiency nanoengineered membranes with selective ion transport. These membranes had the potential to significantly increase the performance and durability of RED systems, which were emerging as a viable technique for generating electricity from salt gradients in areas where energy famine and water scarcity occurred. The results informed the rational design of next-generation membranes for water treatment, desalination, and renewable energy applications.

Section snippets

Simulation details

This study aimed to investigate how CNTs affect water flow in nanochannels. The simulation box was constructed as a nanochannel 260Å in length in the x-direction and 60Å in y and z-directions to facilitate one-way fluid flow and to accommodate room for realistic boundary interactions. Adjacent to the simulation container were two water containers. Each box was 60Å broad and contained 10,000 water molecules. This configuration caused the system to simulate pressure-driven flow conditions and …

Results

The thickness of the nanotube used in the simulated atomic structure influenced the fluid flow inside the channel and the electric current generated in the sample. To examine this problem, the quantity of CNT walls was regarded as equivalent to 1 atomic wall and 2 atomic walls. The atomic structure in the simulated samples was subjected to an ideal external force of 0.001 eV/Å post-balancing, and the electric current in the sample was quantified. The findings from this segment of study …

Conclusion

The researchers carried out computer simulations to examine the movement of water through a nanotube under the application of electricity. This research focused on examining how a channel's thickness affected particles' movement and passage through CNTs in RED. The primary structure revealed essential information at the beginning of the simulations.

- T stabilized to 300 K at 10 ns of simulation, indicating system equilibrium. …
- Besides, the kinetic energy leveled off at 0.0374 eV, confirming that …

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CRediT authorship contribution statement

Shuai Sun: Writing – review & editing, Conceptualization, Data curation, Formal analysis, Supervision, Investigation, Writing – original draft, Writing – review & editing. **Ali Basem:** Writing – review & editing, Conceptualization, Data curation, Formal analysis, Supervision, Investigation, Writing – original draft, Writing – review & editing. **Narinderjit Singh Sawaran Singh:** Writing – review & editing, Conceptualization, Data curation, Formal analysis, Supervision, Investigation, Writing – …

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper. …

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Recommended articles

References (44)

A. Cipollina *et al.*
Reverse electrodialysis: applications

V.N. Popov
Carbon nanotubes: properties and application
Mater. Sci. Eng. R. Rep. (2004)

Y. Wang *et al.*
Recent progress on carbon based desalination membranes and carbon nanomaterial incorporated non-polyamide desalination membranes
J. Environ. Chem. Eng. (2021)

M. Tedesco *et al.*
Nernst-Planck transport theory for (reverse) electrodialysis: I. Effect of co-ion transport through the membranes
J. Membr. Sci. (2016)

A. Moya
A numerical comparison of optimal load and internal resistances in ion-exchange membrane systems under reverse electrodialysis conditions
Desalination (2016)

K. Scott
Microbial fuel cells: transformation of wastes into clean energy

Y. Li *et al.*
Effect of channel roughness on the particle diffusion and permeability of carbon nanotubes in reverse electrodialysis process applying molecular dynamics simulation
J. Mol. Graph. Model. (2025)

X. Li *et al.*

The impact of channel edge type on the particle diffusion and permeability of carbon nanotubes as a membrane in reverse electrodialysis process using molecular dynamics simulation
Int. Commun. Heat Mass Transf. (2025)

A.B. Ali *et al.*
Effect of atomic ratio of ions on the particle diffusion and permeability of carbon nanotubes in reverse electrodialysis process using molecular dynamics simulation
Case Stud. Chem. Environ. Eng. (2025)

A. Khataee *et al.*
Separation of nitrate ion from water using silicon carbide nanotubes as a membrane: insights from molecular dynamics simulation
Comput. Mater. Sci. (2016)

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