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Molecular dynamics simulations in membrane-based water treatment processes: A systematic overview

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ABSTRACT

A thorough investigation of membranes as well as their transport and material properties is a key to understanding the governing principles and unresolved issues of membrane processes. Through molecular dynamics (MD) simulations, static and dynamic properties of membrane separation systems may be investigated on a molecular level. By reviewing over 70 articles, this paper aims to highlight the usefulness of applying molecular dynamics in membranes (MDM) in order to broaden our knowledge of membrane-based water treatment processes. Here, the theoretical foundations of classical MD are described together with the results that are obtainable from MDM simulations. By compiling results from published works, we emphasize the ability of MD to determine membrane transport and material properties from simulations. The authors conclude by suggesting the further use of MDM for prospective research areas pertaining to membrane-based water treatment processes.

Contents

1. Introduction

Due to the growing concerns about the availability of water, researchers are currently searching for more efficient ways of obtaining clean and safe drinking water and maintaining the quality of freshwater sources, without causing further environment and energy issues. As a solution to these challenges, membrane-based water treatment processes have become relevant in recent decades because of their ability to improve water

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treatment effectiveness and productivity. In addition, membrane processes are easy to operate and scale up for industrial applications [1] and are able to deliver high energy efficiency.

There are many types of membrane technology commonly used for water treatment these days. They may be categorized based on their driving forces: pressure difference (microfiltration (MF), ultrafiltration (UF), nanofiltration (NF), reverse osmosis (RO)), concentration difference (forward osmosis (FO)), electric potential difference (electrodialysis (ED), electrodeionization (EDI)), and temperature difference (membrane distillation). Because of the increasing usage of membrane technology in water treatment processes, improving our understanding of synthetic membranes and separation mechanisms has become all the more necessary. One way to achieve this objective is to employ the computational technique known as molecular dynamics (MD).

MD uses step-by-step computer simulations to numerically solve the Newtonian equations of motion. It investigates physical phenomena and movement in systems on a molecular level, usually in nanometer scale, by calculating equilibrium and dynamic properties that are typically difficult to measure using simple analytical or experimental methods [2]. For these reasons, MD is gaining popularity in the field of membrane science whose processes are rooted on the molecular movements of its components. The succeeding sections shall show the application of molecular dynamics in membranes (MDM) for various research areas related to membrane-based water treatment.

To capitalize on the advantages of membrane processes, it is important for the users of the technology to gain a deeper understanding of the principles behind membrane operations. According to She et al. [3], understanding the concepts behind MF and NF requires the effective characterization of membrane materials and processes; this holds true not only for MF and NF but also for all membrane-based processes in general. By using MDM, we can achieve two feats that will help us improve our understanding of membrane processes: (1) determination of the quantities that will describe the movement of particles *on* and *through* membranes, and, (2) characterization of the membrane material properties.

In this paper, the authors would like to encourage further use of MDM as a tool for observing and explaining phenomena in membrane-based water treatment processes. The potential contributions of MDM in understanding membrane processes are validated in this paper by first presenting a brief background about classical MD (Section 2) and an outline of the static and dynamic properties MD can calculate (Section 3). Then, published studies that have used MD simulations for water treatment or related areas are shown (Section 4) and possible applications of MDM in prospective membrane research areas are suggested (Section 5). By promoting MDM in this paper, the authors expect that MDM can contribute new and valuable knowledge to the field of membranes and membrane-based water treatment processes.

2. Molecular dynamics: Principles and methods

Compared to other computer simulation methods, classical MD simulations have advantages since, by using time averages, they can calculate quantities related to the dynamics of a system such as transport coefficients, time-dependent fluctuations, and responses to system changes, rheological properties and spectra [4,5]. MD calculates these quantities by combining concepts from mathematics, chemistry, physics, and computer science so as to shed light on more practical sciences such as material science, biology, environmental science, and nanotechnology.

2.1. Theoretical background

The concept of classical molecular dynamics is founded on Newtonian mechanics. According to Newton's second law of motion, the relationship between mass (m), acceleration (a), and force (F) exerted on particle i follows Eq. (1). This Newtonian force may also be expressed as the gradient of potential energy (U), shown in Eq. (2), where F_i, indicates the force on particle i caused by $N-1$ other molecules, and r and t represent the distance between the particles and time, respectively.

$$F_i = m_i a_i = m_i \frac{d^2 r_i}{dt^2} \tag{1}$$

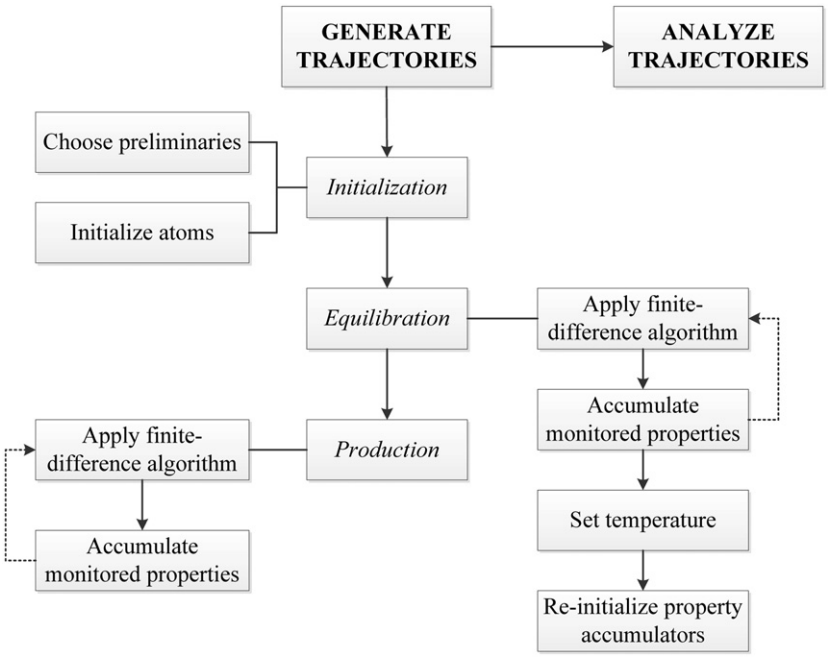

Fig. 1. Steps involved in molecular dynamics simulations. Dotted lines indicate recursive steps. Adapted from Haile [8].