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Macro and nano behavior of salt water in pressure retarded osmosis membrane module

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HIGHLIGHTS

- The simulation model to analyze the salt water flow in the PRO module is proposed.
- The improvement of the membrane does not always improve the module performance.
- The concentration distribution is not uniform in the PRO membrane module.
- The interaction of the membrane surface affects the diffusion of the water.
- There is a correlation between the diffusion and the contact angles on the surface.

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ABSTRACT

There are two characteristics of the behaviors of salt water in PRO membrane module, macro flow in the membrane module and nano behavior in vicinity of the membrane surface. It is proposed to use the numerical simulations in macro and nano fluid behaviors. It is focused on the advection of the salt water in the hollow fiber membrane module and the diffusion of molecules in vicinity of the membrane surface. The macro flow and nano behavior of salt water are simulated with 3-dimensional advection diffusion equation and the molecular dynamics, respectively. It is pointed out for the macro behavior that the distorted flow exists in the membrane module, therefore the concentration distribution is not uniform in the module. So the improvement of the membrane does not always improve the module performance. The membrane performance is closely depended on the flow condition of salt water at high performance membrane. The nano simulations indicate that the interaction between salt water and membrane surfaces affects the diffusion coefficients of the water in the vicinity of surfaces. There is a strong correlation between the diffusion coefficients of water in the vicinity of the surface and the contact angles of water on the surface.

1. Introduction

There are a lot of conversion techniques of the sustainable energy that are solar, wind, biomass, and ocean energies. The salinity gradient energy that used the osmotic power is one of the new techniques [1–8]. The pressure retarded osmosis (PRO) which is suggested by S. Loeb [1] has attracted in the various clean energy generation methods [1]. But the PRO power generation does not carry out for low permeation performance that is caused by three problems; the concentration polarization in and on the membrane, the fouling on the membrane and the flow deviation of the salt water in the module. It is studies to reduce the fouling by antifouling surface [9–11]. In relation to the concentration polarization in and on the membrane, there are many studies for the membrane materials and geometries by using molecular simulation; polymer materials [12,13], carbon nanotube membranes [14–16] and nano-porous grapheme [17,18]. Nevertheless, there is no research that examines microscopically the concentration polarization on the membrane. It is important to make clear a phenomenon that the retained ions are concentrated on the membrane surface. The flow deviation of the salt water in the module is considered in the membrane module that is pointed out the performance of permeation becomes low at the membrane module. But the phenomena in the module do not make clear because a lot of membrane and the small gap space prevent to measure the flow characteristics.

In this paper, the two types of simulations for nano and macro scale behaviors of salt water, the molecule dynamics and advection–diffusion simulation are proposed. In the nano scale behaviors, when the movement of the water on the membrane surface is enhanced, the diffusion of the retained ions in the water will be increased and, consequently, the concentration polarization might be reduced. The interaction between salt water and membrane surface on the diffusion is discussed

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by the molecule simulation that has been used widely to obtain molecular and atomic-level information. To make clear the macro scale flow in the membrane module, the simulation model by using the advection–diffusion simulation that is used for 3-dimensional laminar flow is proposed. In the osmotic region, the salt water is prevented to flow and permeated the pure water that is consists of a lot of membranes and gaps. In this simulation, it is proposed that the domain is modeled with the uniform porous material with permeation of pure water and the flow resistance. This model makes the salt water flow in the module easy to simulate.

2. Macro behavior of salt water

2.1. Basic equations of salt water flow

The flow in the module is analyzed with the continuity and advection diffusion equations that are used to clear the macro behavior of the salt water and the concentration distribution.

$$\frac{\partial \rho}{\partial t} + \nabla(\rho U) = S_{MS} \tag{1}$$

$$\frac{\partial \rho U}{\partial t} + \nabla(\rho U \otimes U) = -\nabla P + \nabla \cdot \tau + S_M \tag{2}$$

where ρ is the density, U is flow velocity of salt water, P is pressure, S_{MS} is the mass source, τ is the stress tensor and S_M is momentum source. The mass source is set by the permeation flow rate that is governed by the difference between the osmotic pressure and the hydraulic pressure. It is estimated by the following equation.

$$J_w = A(\Delta\pi - \Delta P)a \tag{3}$$

where J_w is the permeation flow rate, A is the water permeability coefficient of the membrane, ΔP is hydraulic pressure difference between the salt water and fresh water ($\Delta P = P_s - P_f$),a is the area of the membrane, and $\Delta\pi$ is the osmotic pressure given by Van't Hoff equation.

$$\Delta\pi = 2CRT \tag{4}$$

where C is the molecule concentration, R is the gas constant, and T is the temperature.

The momentum source S_M is set as the momentum loss of the salt water when the salt water pass through among hollow fibers. This is expressed by the following equation.

$$S_{M,i} = -\frac{\mu}{K_{perm}} U_i - K_{loss}\frac{\rho}{2}|U|U_i \tag{5}$$

where μ is viscosity, K_{perm} is permeability, K_{loss} is resistance loss coefficient, U_i is velocity component at each direction, and $|U|$ is magnitude of salt water velocity.

Hollow fiber diameter affects to area of membrane area. The relation of the membrane area, hollow fiber diameter and number of hollow fibers are shown in Eqs. (6) and (7.

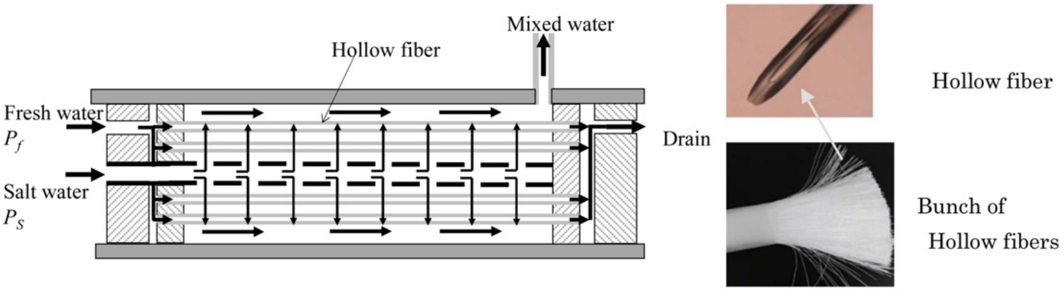
$$S = \pi d_o l N \tag{6}$$

$$N = \frac{D_e^2}{d_o^2} K \tag{7}$$

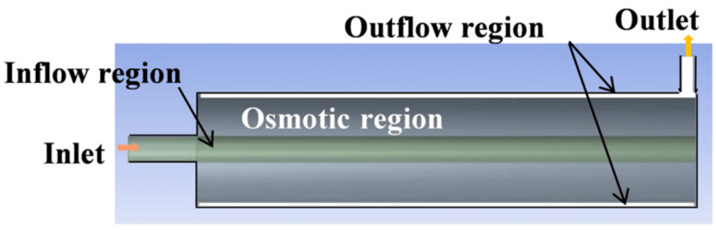
where d_0, l and N are outer diameter, length an number of hollow fiber, D_e is outer diameter of element, and K is occupancy of hollow fiber in module.

2.2. Simulation model of PRO module

Fig. 1 shows the schematics of the section geometry of the module. The main dimensions are listed in Table 1 for 10 in. module. The module diameter and length are 400 and 1392 mm, respectively. The inner and outer diameters of the hollow fiber are 137 and 53 μm, respectively. The nominal area of hollow fiber membrane is 1033 m^2 and the number of hollow fiber is 1,500,000. Fig. 1(a) is the schematics of the section geometry of the module. The salt water flows into the module from center of the left side. Salt water flows radial direction from the center pipe. The fresh water flows in from the left side of the hollow fiber. The salt water contacts with the fresh water with semi-permeable membrane. In this part, the permeation occurs from the fresh water to salt water. The bunch of the hollow fibers is shown in Fig. 1(b). Two hundred fibers



(a) Actual module (b) Hollow fiber and brunch



(c) Simulation module

Fig. 1. Schematics of hollow fiber module.