



Article A Facile Ultrapure Water Production Method for Electrolysis via Multilayered Photovoltaic/Membrane Distillation

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Abstract: Ultrapure water production is vital for sustainable green hydrogen production by electrolysis. The current industrial process to generate ultrapure water involves energy-intensive processes, such as reverse osmosis. This study demonstrates a facile method to produce ultrapure water from simulated seawater using a low capital cost and low-energy-consuming membrane distillation (MD) approach that is driven by the waste heat from photovoltaic (PV) panels. To optimize the PV-MD operation, modeling efforts to design a multilayered MD system were carried out. The results were used to guide the construction of several prototype devices using different materials. The best performing PV-MD device, containing evaporation and condensation regions made from steel sheets and polytetrafluoroethylene (PTFE) membranes, can produce high-purity water with conductivity less than 40 mS and flux higher than $100 \text{ g/m}^2 \text{ h}$, which is suitable for typical electrolyzer use.

Keywords: ultrapure water; photovoltaic; membrane distillation; electrolysis; hydrogen production

1. Introduction

Green hydrogen production via electrolysis offers new opportunities for energy storage in dynamic and intermittent power generation (solar and wind). This is because hydrogen can be used as a clean fuel to produce electricity with water being the only byproduct. This process makes hydrogen a desirable option for sustainable energy storage, as it is highly efficient and versatile, producing zero carbon emissions. Furthermore, utilizing hydrogen as a fuel can help mitigate the impacts of climate change. However, in the process of electrolysis, it is often desirable to use ultrapure water to ensure the efficient production of hydrogen. In other words, the water source for electrolysis should contain a very limited number of contaminants and metal ions (with low resistivity as low as 18 M Ω -cm [1]).

The current industrial approach to produce ultrapure water is mainly through the following processes: the source water is passed through activated water carbon filters and treated with a UV disinfection unit before it enters a reverse osmosis (RO) system to remove small contaminants (especially metal ions). RO is a pressure driven process that utilizes semi-permeable membranes to filter feed water [2] by rejecting contaminants/ions with sizes larger than 0.5 nm (i.e., the size of the hydrated Na⁺ ion cluster). Subsequently, RO-filtered water is passed through an ion exchanger to remove the residual ions. The role of activated carbon enables the physical adsorption of contaminants through chemical and physical interactions between the substrate surface (with active functional groups) and contaminants [3]. This process has a relatively low operational cost for production of prefiltered water [4]. However, the whole ultrapure water generation systems involving RO and/or ion exchanger are usually more capital intensive. Additionally, typical RO



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Copyright: © 2023 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). systems consume large amounts of energy and use about three times as much water as they produce [5]. Excluding the instillation cost, the ultrapure water costs USD $0.15/m^3$ to USD $0.50/m^3$ [6]. If the system installation and maintenance are included, the cost would be much higher.

In this study, we present a facile method to produce ultrapure water from simulated seawater based on the combined photovoltaic/membrane distillation device, where both capital and operational costs are low. Membrane distillation (MD) is a non-isothermal membrane separation process to purify water. Inside the MD system, there is a hydrophobic membrane that divides the feed and permeate streams. The driving force of MD is the partial pressure difference between the two streams, induced by the temperature difference. Bodell and Weyl have shown that this process is well suited for desalination and wastewater treatment [7,8]. There are several different MD configurations. Our focus was on the development of a flat-top air gap membrane distillation (AGMD) system, taking advantage of the waste heat created by the photovoltaic (PV) panels (Figure 1). In the AGMD setup, a hydrophobic membrane is used to separate the feed water and condensation channels. The feed water is in direct contact with the hydrophobic membrane and there is an air gap present on the other side of the membrane with a condensation plate. The purpose of the hydrophobic membrane is to allow the vapor to travel through but permitting the liquid feed water to pass through. The vapor traverses the membrane and the air gap until it reaches the cooling plate on the opposite side and condenses into water with high purity.



Figure 1. The integration of the PV-MD unit (with three-staged crossflow assemblies) with an electrolyzer to produce hydrogen fuel.

The partial vapor pressure difference across the membrane in MD requires an outside heat source. Recently, the Wang group has demonstrated the use of waste heat from solar panels as an energy source to purify water by MD operation [9–12]. This is because although solar panels can absorb a large amount of energy, the typical PV can only convert about 20% of solar energy into electricity [13], where the rest of the absorbed energy is converted to heat. This waste heat is a good energy source to be capitalized by a flat MD unit, attached beneath the PV panel, to produce ultrapure water that may be suitable for hydrogen production by electrolysis. The coupling of the PV-MD unit for green hydrogen production by electrolysis is illustrated in Figure 1, where the detailed study of this system will be described elsewhere. In the present study, we used a simulated seawater (conductivity of 58.5 mS) as a model source water to produce pure water with conductivity below 40 μ S as a benchmark target. The design of the multilayered MD unit was carried out with computer simulation first, where materials selection was carefully made to evaluate the performance of the constructed unit.

2. Materials and Methods

2.1. Simulation of PV-MD Design

The design of the flat multilayered MD device, attached to the back of a PV panel, was initiated by computer simulation using the COMSOL® software. In this simulation, several parameters were considered in the flat sheet design using an air gap membrane distillation (AGMD) configuration (Figure 2). The design of the one layer assembly consists of (1) a top (left) thermal conducting plate to transfer the heat from the back of PV panel or the heat from the bottom of the assembly, (2) a narrow gap for the feed water, (3) a thin hydrophobic porous membrane, (4) an air gap for moisture transfer, and (5) a condensation plate that condenses the vapor and transfer the latent heat to the next assembly. The bottom of each layer assembly is a channel with water flow that can take out the latent heat from the system. The system must be able to maintain heat throughout the device to ensure that the apparatus will work. The heat flux from the back of the solar panel enters the stainless-steel plate, where the radiation and convection cooling are taken into consideration. The heat is then transferred to the water channel. Moisture flux and evaporation take place on the surface (boundary) of the porous hydrophobic membrane. The evaporated vapor is condensed on the stainless-steel condensation plate, where the latent heat from condensation is transferred to the next stainless-steel sheet. This latent heat in a one-layer system is then removed by the cooling water channel. In the simulation carried out by COMSOL[®], each plate/membrane/gap was considered a domain, where the thermal and mass balances were considered within such a domain and on its boundaries. The conditions considered for each domain and its boundaries in a MD assembly layer are as follows (each domain was assumed to have a unified heat transfer condition).



Figure 2. The physics involved in the flat sheet MD design (only one assembly layer is illustrated here for simplicity).

2.2. Top Thermal Conducting Plate

The heat from the back of PV panel was considered as the input of heat flux from the boundary to the domain. For the rest of the layers, the heat flux was the latent heat from condensation of the last assembly. Radiation and convection were also considered for the top plate of the first assembly layer.

2.3. Feed Water (Evaporation) Channel

In this simulation, feed water (simulated seawater) was fed from one end of the assembly layer at a very low flow rate, where the water temperature was raised by the heat from the top thermal conducting plate of the assembly.

2.4. Hydrophobic Porous Membrane

Hydrophobic porous membrane is the most important domain to simulate. For simulation, the membrane is considered as a porous matrix containing a certain amount of moisture and water, with the initial humidity as ϕ_0 . Water is evaporated at the very surface of the membrane and forms a "moisture flux" to enter the porous membrane. In this membrane, as well as the air gap, the heat transfer (h_t) in the porous medium, moisture transfer (m_t) in the porous medium, and their coupling were considered.

2.5. Air Gap

The vapor (moisture air) generated from the porous membrane, driven by the partial vapor pressure, is transferred to the air gap to initiate the condensation process on the condensation plate (described later). The released latent heat from condensation can be considered as the heat flux input to the next layer. The condensed vapor formed the pure water stream, leading to the exit of the air gap along the condensation plate. In the simulation, the feed water flow rate was also taken into consideration. Since the design was aimed to maximize the use of the heat from the back of PV panel, a slow cooling water flow rate was desired. For practical matter, the final design involved the utilization of a water diversion/spacer inside the evaporation channel, where the Brinkman flow can be used to describe the flow. It is noted that the Brinkman flow is an extension of Darcy's flow (Darcy's flow deals with low-speed feeding through the porous medium, while Brinkman flow deals with a higher rate flows through the porous medium).

The moisture flux is an important parameter to consider in the membrane domain and its boundaries. The vapor generation on the membrane surface and its subsequent penetration into the membrane matrix were simulated by the vapor pressure from 100% relative humidity. The rate of the moisture flux (g_0) crossing the boundary of the membrane domain can be described by the following equation:

$$g_0 = C_{mf}(\psi_0 p_{sat}(T_0) - \psi_1 p_{sat}(T_1))$$
(1)

where T_0 and T_1 are the temperatures cross the membrane, respectively; ψ_0 and ψ_1 are the relative humidity of the two locations; $p_{sat}(T_0)$ and $p_{sat}(T_1)$ are the saturated pressure at temperature T_0 and T_1 , respectively; and C_{mf} is the coefficient of vapor generation, which will be discussed in detail below. Since the relative humidity on the feed water side always has $\psi_0 \equiv 1$, and $\psi_1 p_{sat}(T_1) = p_{v1}$, which represents the partial pressure of water vapor at location 1, Equation (1) can be simplified to

$$g_0 = C_{mf}(p_{sat}(T_0) - p_{v1})$$
(2)

where the partial vapor pressure p_{v1} is automatically provided in the COMSOL[®] moisture transfer simulation.

The coefficient C_{mf} is directly related to the membrane property. As illustrated in Figure 3, the actual mass transfer process in the MD process can be judged by the specific value of the Knudsen number, which is defined as

$$K_n = \frac{\lambda}{d} \tag{3}$$

where *d* is the pore size in diameter, and λ is the mean free path of water vapor as follows.

$$\lambda = \frac{K_B T}{P \sqrt{2} \pi \sigma^2} \tag{4}$$



Figure 3. Details of the porous membrane and the air gap in the assembly layer. 0 indicates the membrane side exposed to the evaporation channel that is in contact with the water, while 1 indicates the membrane side facing the air gap of condensation channel. δ indicates the membrane size measurement and d indicates the size of the pores in the membrane.

In Equation (4), *T*, *K*_{*B*}, and *P* are the average temperatures, the Boltzmann constants, and the absolute pressure in the membrane pores, respectively, and σ is the vapor collision diameter (2.641 × 10⁻¹⁰ m).

There are three cases in the vapor transportation process: (1) $K_n > 1$, the influence of the pore radius dominates due to the collision between the diffused molecules and the membrane pore wall (this process is called Knudson diffusion); (2) $K_n < 0.01$, the mass transfer resistance is primarily the collision among the diffused molecules; and (3) $0.01 < K_n < 1$, the mass transfer is combined with the molecular diffusion mechanism and Knudsen diffusion processes. The coefficients C_{mf} for the above three cases are

$$C_{mf} = \frac{2\varepsilon r}{3\tau\delta} \sqrt{\frac{8M}{\pi RT}} \quad K_n > 1$$
(5)

$$C_{mf} = \frac{\varepsilon}{\tau \delta} \frac{PD}{P_a} \frac{M}{RT} \qquad K_n < 0.01 \tag{6}$$

$$C_{mf} = \left[\frac{3\tau\delta}{2\varepsilon r}\sqrt{\frac{\pi RT}{8M}} + \frac{\tau\delta P_a}{\varepsilon PD}\frac{RT}{M}\right]^{-1} \quad 0.01 < K_n < 1 \tag{7}$$

where ε is the porosity of membrane, r is the average pore radius of the membrane, δ is the membrane thickness, τ is the membrane tortuosity, M is molar weight of water, R is the universal gas constant, T is the temperature, P_a is the absolute pressure of air in the membrane, D is the diffusion coefficient of water vapor, P is the total pressure in the membrane, and PD gives a value of $1.895 \times 10^{-5}T^{2.072}$. Since the thickness of the hydrophobic membrane used in the MD process is in the range of $0.1-0.5 \,\mu\text{m}$, the C_{mf} value is most likely to be in the range of Case 3. As a result, Equation (7) was used in the simulation. Figure 4 shows the calculated results of coefficient C_{mf} of a typical PTFE membrane in MD operation.



Figure 4. Vapor generation coefficient C_{mf} of the porous membrane at different temperatures.

Another important property of the membrane considered is the so called "leading entry pressure" (*LEP*), which is the minimum pressure that water can pass through the membrane. It is defined as

$$LEP_W = \frac{-2B\gamma_L \cos(\theta)}{\rho_{max}} \tag{8}$$

where LEP_W is the liquid entry pressure of pure water in pascals, *B* is a dimensionless geometrical factor that includes the irregularities of the pores (*B* = 1 for cylindrical pores), γ_L is the liquid surface tension in N/m, θ is the water contact angle of the membrane, and ρ_{max} is the maximal pore (non-closed) radius in meters. In the design and operation of the assembly system, the pressure asserted on the surface of the membrane should be kept below LEP_W , which is the limit for the feed water pressure.

2.6. Condensation Plate

The moisture transportation (m_t) was simulated in the air gap together with the membrane (porous matrix) domain until the moisture hit the surface of the condensation plate. This surface (boundary) is defined in the COMSOL[®] simulation as the "moist surface", which deals with the moisture condensation process. The latent heat released by condensation presents the heat flux to the next assembly layer.

2.7. Cooling Channel

After the condensation plate of the last assembly layer is the cooling water channel. This channel allows the ambient temperature water flow removes the remaining latent heat and establishes a stable temperature gradient across the layered assembly. This cooling water flow is considered as the heat sink, where its efficiency depends on the nature of the water flow rate, which will be discussed later.

2.8. Materials Selection

The 316 stainless-steel plates were used as the top thermal conducting and end condensation plates (Figure 2), where the plate dimensions were $200 \times 200 \text{ mm}^2$ in width and 1.2 mm in thickness. These stainless-steel plates provided good corrosion resistance and mechanical strength to the system. A water flow diversion cloth with epoxy coating (provided by HORNWOOD Inc., Lilesville, NC, USA) was employed to define the feed water channel. This cloth (0.47 mm thickness) is typically used in the purified water channel of the spiral-wound reverse-osmosis (RO) cartridge. The PTFE membrane (provided by YOUKEFA Inc., Wuzhong District, Suzhou, Jiangsu Province, China) possessed a thickness of about 50 micron and an average pore size of 0.45 micron was used. The spacer placed in the air gap was a 1.65 mm diamond shaped polypropylene net (purchase from Industrial Netting, Maple Grove, MN, USA) with a thickness of about 1.0 mm. The condensation plate was also a 316 stainless-steel sheet with 0.125 mm thickness. The chosen adhesives included Loctite 9430 (from McMaster-Carr Supply Company, Elmhurst, IL, USA), West System Epoxy 650 and West System Epoxy 655.

2.9. Assembly of the PV-MD System

The overall design of the multilayered MD system is depicted in Figure 5. As is shown, the heat is absorbed by the top thermal conducting plate, and this heat carries downward through the assembly layer. Each assembly layer can be considered as having two regions: the evaporation region and the condensation region. On the bottom of the final assembly layer is a water-cooling channel that utilizes the same feed water as the cooling source. The feed water runs through both the assembly layer(s) and the water-cooling channel.



Figure 5. Assembly of the MD system: (**A**) the evaporation region, which consists of a sheet of epoxy coated fine mesh (or the water diversion cloth) as the spacer, and (**B**) the condensation region, which consists of a polypropylene (PP) mesh as the spacer. Both regions are separated by a porous hydrophobic (PTFE) membrane. (**A**,**B**) share the same PTFE membrane and laminated to form a complete "layer" of the membrane distillation unit. A multilayered MD system contains up to 5 A/B layers.

When the feed water enters the evaporation region, the partial pressure difference enables the production of pure water vapor from the feed water. The partial pressure difference depends on the temperature difference between the evaporation and condensation regions. From the simulation results, the partial pressure difference is quite similar throughout the membrane in the different assembly layer. This evaporation traverses the membrane and condenses in the condensation channel of the assembly. The water passed through the evaporation region can be circulated back to the feed water source to minimize the total amount of the feed water. We note that with the use of seawater as the source water, reintroduction of the brine into the initial feedwater can increase the salinity, which must also be considered.

3. Results and Discussion

3.1. PV-MD System Simulation

Based on the configurations discussed in the Materials and Methods section, simulations using the two-layered, three-layered, four-layered, and five-layered assemblies were carried out. Simulations were carried out with increasing layer configurations to investigate how the increasing layers could impact the production rates of ultrapure water. This investigation allows for the determination of a system that could possess the maximum number of layers without affecting the MD cost-performance value. With over five layers in the system, the production rate was found to increase only marginally. The increase in layers would increase the production cost but does not notably enhance the performance. For simplicity of the simulation, only the case of the two-layered assembly is discussed here, which can be considered as the base unit consideration for all other layers.

3.1.1. Feed Water Flow Rate Consideration

To utilize the waste heat from the PV panel, the following feed water flow rates (relatively slow) were chosen, 3.5×10^{-7} m/s, 3.5×10^{-6} m/s, and 3.5×10^{-4} m/s, to investigate if the flow rate could affect the heating of the feeding water. These flow rates represent the typical range of the operational conditions in the MD device. The simulation results showed that the feed water flow can reach to a constant temperature after a few millimeters entrance to the channel, even at the "largest" chosen flow rate. The feed water temperature was chosen to be the ambient temperature at Doha International Airport on 1 June, 12:00 PM, which was also the same as the cooling water temperature. The simulation conditions and values are summarized in Table 1, where these parameters were used to simulate the results obtained below.

Table 1. Simulation conditions utilized in the COMSOL software for all simulation works.

Simulation Abbreviation	Input Value	Description
pv.alpha	0.85	PV absorption coefficient
pv.eta_ref	0.12	PV average efficiency at reference temperature
pv.beta_ref	0.0045 1/K	PV efficiency temperature slope
pv.q_s	300 W/m^2	PV solar energy flux in unit of (W/m^2)
pv.theta	0.38397	PV device tilt angle, 0 for vertical standing
md.L	0.15 m	MD device length
md.H_st	0.001 m	Height of evaporation/condensation stainless-steel plate
md.H_wa	0.001 m	Height of evaporation layer (water)
md.H_va	0.001 m	Height of vapor layer
md.H_me	$1 imes 10^{-4}~{ m m}$	Thickness of the membrane
md.delta	$7.5 imes10^{-5}~{ m m}$	PTFE membrane thickness
P_water_header	9806.4 N/m ³	1 m water header pressure
md.H_ga	$5 imes 10^{-4}~{ m m}$	Condensation seal gap
md.H_ga1	0 m	Condensation seal gap 1
kai_s	0.01138	Molar fraction of NaCl in sea water
p_abs	$1.01 imes 10^5$ Pa	Absolute pressure in the membrane pore
sigma	$2.641\times 10^{-10}~\text{m}$	Water vapor collision diameter
M_wa	0.018015 kg/mol	Molar weight of water
t_factor	1	Tune factor
t_alpha	0.4	Tune factor
u1	0.05 m/s	Cooling water speed

3.1.2. Relative Humidity Consideration

Figure 6 shows the relative humidity distributions in the air gap as well as in the porous membrane of the two-layered system. In the chosen design, small blocks on the left represent the opening of the air gap, where the condensed water exits. From the simulation,

it is seen that the relative humidity reached 100% on the surface of the condensation plate (as shown by the color map in Figure 6). Investigating the relative humidity within the air gap region can allow us to predict if the water vapor is present in the air gap, as well as to understand if the water vapor can condense on the condensation layer. The simulation results indicate that the air gap region of the system had a high humidity, showing the presence of water vapor. The humidity measurements at the surface of the condensation plate exhibited a value about one, which indicated that the water vapor condensed on the surface of the condensation plate. The dashed line indicates the cutting line through the device that allows for the investigation of the arc length. Arc length is the length coordinates along the cutting line (dashed line) that were used in the simulation study. Using this cross-section or cut line allows for the investigation of the temperature loss, as well as vapor pressure differences in the condensation layer of the device.





Figure 6. Relative humidity of the permeation channel.

3.1.3. Temperature Distribution across the Assembly Layer

Figure 7 shows the temperature distribution across the central line of the two-layered assembly. Each region of the two-layered system was divided into sections within the image. The region labeled III represents the region of the air gap, which experienced a sharp temperature drop. In the feed water gap, there was also a slight temperature drop between the heating plate and membrane surface.



Figure 7. The temperature distribution across the central cut line of the two assembly layers in Figure 6. The arc length is length along the dash line in Figure 6.

3.1.4. Vapor Pressure across the Assembly Layer

Figure 8 shows the calculated saturate vapor pressure and the real partial vapor pressure, based on the relative humidity, as a function of distance in the air gap. It is seen that the differences of the saturated pressure and partial vapor pressure at the location of membrane were almost the same for the two air gaps. According to Equation (2), this differentiation is a part of the driven force for the moisture flux generation and transportation; however, the coefficient of moisture generation C_{mf} decreased almost linearly as the temperature decreased; as is shown in the Figure 4, this result in the production of condensed water will decrease linearly as the number of group of layers increase. The simulation shows that the production efficiency will be greatly reduced if the number of group of layers is in excess of five. The vapor pressure after the membrane exhibited a large difference when compared to the vapor pressure at the condensation plate. With each assembly layer, the pressure differences were relatively similar to one another. Figure 8 indicates that there were no data present from the arc length measurements between 0.003 m and 0.005 m. This was because there was a steel sheet and the evaporation channel present in the assembly. There can be no partial pressure differences across the steel plate, and there was also no vapor transfer or in the evaporation channel as the feed water was present.





Figure 8. The saturated vapor pressure vs. partial vapor pressure (real) in the air gap. The arc length is the length along the dash line in Figure 6.

3.1.5. Calculated Condensation Rate

In the simulation results, one can directly evaluate the condensation rate on the condensation plate. The results are shown in Table 2. These results were determined by utilizing the conditions outlined in Table 1. This condensation plates in this table represent the layer in the apparatus, where the condensation plate on the air gap side of the unit marks the end of a layer. While investigating the different layers, the simulation results indicate that the device can produce ultrapure water at each layer. While there was a slight decrease in the condensation rate from layer to layer, the PV-MD device with a multilayer assembly was capable of producing ultrapure water at increased production rates (i.e., production rate increases with the number of layers in the PV/MD unit).

Table 2. Condensation rate at each condensation plate.

Condensation Plate	Condensation Rate (g/m ² h)
#1 layer	727.9
#2 layer	706.2

3.2. Reuse of Latent Heat

One of the important features of this layered assembly design is to reuse the latent heat from the condensation of the first layer as the heat flux to heat the feed water in the next layer and so on. It is important to exam the input of the energy to the feeding channel for each assembly layer. Table 3 shows the total energy flux at the boundary of feeding channels. The layer number in Table 3 is the same as the layer number in Table 2.

Table 3. The total energy flux to the feeding channels.

Feeding Channel	Total Energy Flux (W/m ²)
#1 layer	613.02
#2 layer	597.20

The differences in energy flux between the first and second feeding channels were small but noticeable. However, five-layer simulation results showed that the difference for the sequential layers was less than the difference between layer 1 and layer 2. From the two-layer simulation, it was determined that the energy flux was present from one layer to the next. The energy (heat) that was released from the condensing water (ultrapure) on the condensation plate was transferred to the following layer. This transferred energy indicated that heat was present in the next layer, and this induced the vapor pressure differences that allowed for the water vapor to form in the air gap of the proceeding layer. When this simulation was extended to a five-layer system, this was also found to be true. The total energy fluxes in the five-layer system from the top layer to bottom layer were 508.47 W/m^2 , 485.99 W/m^2 , 468.33 W/m^2 , 455.02 W/m^2 , and 445.79 W/m^2 , respectively. While there was diminishing energy flux measurements as the layer went farther from the top plate, there was still sufficient energy transferred to allow for water production. The fifth layer energy was transferred to the water-cooling channel, which allowed for the cooling of the system.

3.3. Cooling Methods and Comparison

It is very important to have a cooling mechanism to dispatch the remaining latent heat. The simulation shows that effectiveness of cooling will have a direct effect on the production of condensation. There are two methods to provide the cooling, one is by heat transfer (heat sink) through air flow and the other is by water flow to cool down the device. The advantage of the first method is that it has no moving parts. However, the cooling effects are highly dependent to the speed of the air flow. The chosen configuration of the heat sink approach using air flow is shown in Figure 9, and the wind (air flow) speed as a function of the condensation rate (i.e., the pure water production rate) is shown in Figure 10.

Figure 11 shows the dependence of the condensation rate on the water flow speed by our simulation. From this figure, it is seen that the cooling effect was more effective through water flow cooling than the air flow cooling. As a result, the water-cooling mechanism was adopted in our device demonstration. In Figure 11, it is seen that a stable condensation rate should be achieved as long as the cooling water flow speed is larger than 0.005 m/s, which was used as a benchmark value in our system demonstration.



Configuration of Air Cooling Assembly

Figure 9. Configuration of the air-cooling mechanism.



Figure 10. The effect of air flow (wind) speed using the configuration in Figure 9 on the condensation rate of the MD system.



Figure 11. Water-cooling effects on the condensation rate of the MD system.

3.4. Demonstration of the PV-MD System Based on the Simulation Results

Based on the simulation results, we constructed several PV-MD units using different materials, wherein the performance of each unit was evaluated. The simulation results allowed us to design the physical parameters of the unit; however, the materials selection played an important role in the system performance. The test of the PV-MD system started off with a two-layered assembly. This system was used to identify the engineering issues based on the selection of different materials.

Test of the Two-Layered Assembly

Prior to the development of the five-layered unit, small two-layered systems $(200 \times 200 \text{ mm}^2)$ using different materials were developed (using stainless-steel plates as the top thermal conducting and end condensation plates, PTFE membrane, polypropylene in the air gap, and Loctite 9430 as a sealant) to evaluate the performance based on the simulation results. The rate of freshwater production as well as the corresponding conductivity were determined. The initial study was carried out using tap water as the feedwater. A small mechanical pump was used to pipe the feedwater into both the MD system and the water-cooling channel. A heating pad connected in series was placed on the top plate of the system to produce a range of heat to investigate the effect of temperature on the conductivity and production rate of the clean water. The initial conductivity of the tap water was 132.3 mS, where the conductivity of the purified water can be lower than 30 mS depending on the temperature. The overall performance was similar to the simulation results. With this performance using tap water, synthetic saltwater was used to test the MD unit.

With saltwater as the feed water, we expected that the production rate of pure water would drop as compared to tap water. This is because there were slight differences in the vapor pressure between the two. The synthetic salt water was created by dissolving NaCl into the tap water and possessed a concentration of 35 g per liter, which led to a conductivity of about 58.5 mS. This water was introduced into the MD system and the water-cooling channel as the test of the tap water. Depending on the voltage applied to the heating pad, the rate of production and conductivity of the purified water varied.

Figure 12 illustrates the pure water production rate as a function of heating pad power for a two-layered MD unit in two separate runs (T1—first run; T2—second run). It was seen that the pure water production rate (water permeability) increased with the increase in heating pad power (120 volts to 180 volts) in the first run. However, in the second run, the water production rate was found to increase quite significantly, although the trend of water permeability increases with the heating power was much more enhanced. The close examination of the system indicated that there was a minor leak, where the task of selecting a proper sealant to assemble the system had become an essential task. There are few possibilities that would cause the system to leak. For example, the epoxy or sealant cannot properly handle the thermal expansion of the different materials, resulting in the failure of sealing around the entry and exit of the feed water. Since this was the initial work, the sealant was not investigated exhaustively. We believe that the thermal expansion caused by heating of the device could form minor cracks between the sealant and the contacting materials, which could explain the minor leak that observed. This conclusion is also consistent with the conductivity results.

The permeate conductivity from the two-layered MD unit using simulated sea water as the feed water (58.5 mS) as a function of heating pad power is illustrated in Figure 13. In the first run, the conductivity of the purified water was found to decrease with the heating power. All the permeate conductivity values were below 235 mS, which was similar to the DI water system that we used. However, these values are slightly higher than the desired conductivity level (the benchmark value was set as 40 μ S) for electrolyzer. However, in the second run, the permeate conductivity was found to increase quite notably, supporting the hypothesis of a minor leak in the system. However, the general trend of the permeate conductivity decreases with heating power was confirmed.



Figure 12. Production rate of pure water from a two-layered MD unit (stainless-steel thermal conducting and condensation plates, PTFE membrane, and polypropylene in the air gap) as a function of heating pad power in two separate runs (T1—first run; T2—second run).



Figure 13. Permeate conductivity of the two-layered MD unit as a function of heating pad power in two separate runs (T1—first run; T2—second run).

3.5. Engineering Improvement

As discussed above, the initial two-layered MD system could produce pure water with conductivity similar to that of DI water from simulated seawater. However, this conductivity was relatively high. Additionally, the system suffered a leaking problem. To resolve the latter problem, two different types of epoxy (West System G/Flex 650 and 655 epoxies) were used to replace the initially tested sealant (Loctite 9430) as possible engineering solutions. We hypothesize that Loctite 9430 could not hold the maintain the system integrity and handle the different thermal expansion coefficients of the different material. Figures 14 and 15 illustrate the permeability and conductivity of the purified water at different heating power from a two-layered MD system using 650 epoxy and 655 epoxy as sealants (square: 650 epoxy, circle: 655 epoxy) at the different runs. The evaluations were carried out using the operating conditions that can mimic the field conditions (i.e., temperature profiles).



Figure 14. Water permeability comparison using West System G/Flex 650 epoxy (square) and 655 epoxy (circle) as sealants in the two-layered MD system (the number indicates the different run).



Figure 15. Permeate conductivity comparison using West System G/Flex 650 epoxy (square) and 655 epoxy (circle) as sealants in the two-layered MD system (the number indicates the different run).

From the figures above, it was seen that the two-layered system performance using West System epoxy as a sealant was greatly improved. All the results indicated that the permeability increased, and the conductivity decreased with the heating power (or the applied MD surface temperature). It was found that the system using 655 epoxy exhibited better performance than that using 650 epoxy (we note that the system with 650 epoxy exhibited a high conductivity at run 2, probably because of a very minor leak; however, the system healed itself with the thermal expansion of the material chosen). From this study, the use of the West System 655 epoxy is clearly a better choice to construct an integrated and robust multilayered MD system to produce ultrapure water with conductivity below the benchmark value of 40 mS. However, this system was further improved by carefully selecting a material to replace the steel plate in contact with water to lower the risk of contaminating the water in the MD system.

Replacing the Contacting Steel Plate to Reduce Water Contamination

In the above two-layered system, a steel plate was in direct contact with water, which may provide a source for water contamination. To eliminate this possibility, a thin PET film was used to replace the steel sheet in the layer, where the PET film acted as the direct

condensation plate allowing the heat transfer to the next layer. To test this system, the real seawater was used as the feed water (the conductivity was around 68–70 mS). This improved system was found to exhibit impressive permeation rate and permeate conductivity. The permeate conductivity of the improved two-layered system never went above 40 mS while maintaining a high permeation rate. With the higher heat plate power, the permeate conductivity was around 12 mS. These are highly desirable values for ultrapure water production that are suitable for electrolysis to produce green hydrogen.

3.6. PV-MD System Optimization

In the two-layered PV-MD device, the latent heat released during the vapor condensation process in the first MD layer could be effectively used as the energy source for the next MD layer. The experimental results are generally consistent with the simulation results using the same operational conditions. The conductivity of the purified water using the properly chosen materials (PET film as the condensation plate, and West System 655 epoxy as a sealant) was consistently low and very suitable for electrolysis. Currently, our lab is building a MD system with a high number of layers (up to five layers) and larger dimensions ($500 \times 500 \text{ mm}^2$) using the best materials identified. The results of this system and its integration with the PV panels and an electrolyzer will be discussed elsewhere.

3.7. Perspective of PV/MD Integration for Electrolysis

Green hydrogen production by electrolysis has become an intense research area for future energy storage because of its environmental cleanness and local sustainability. The U.S. Department of Energy has recently launched a campaign known as the Hydrogen Shot [14], which is an ambitious program to reduce the cost of clean hydrogen by 80% to USD 1 per 1 kg of hydrogen gas in 1 decade (the 1:1:1 goal). This goal can only be reached if one can reduce production costs in every aspect of the operation, including the low-cost ultrapure water production from a broad spectrum of source water, including seawater. If the quality of the water quality is poor in electrolysis, the efficiency of hydrogen will be low. This is because electrolysis is an electrochemical process (the process is often known as water splitting), which can create many undesirable products if the feed water is not pure [15,16].

4. Conclusions

Our comprehensive study of multilayered PV-MD system, involving simulation, physical construction, and testing of the device, indicates that it is a facile pathway to produce ultrapure water from simulated and real seawater. The conductivity of the purified water is lower than 40 mS, which is suitable for electrolysis to efficiently produce hydrogen gas. The PV-MD design is a promising solution that harnesses the waste heat from typical solar panel for membrane distillation operation, which offers a sustainable approach to produce ultrapure water from a wide range of source water. In the future work of this project, the integration of this PV/MD unit, with the best designed configuration and materials selection, with a 5 kW electrolyzer, will be demonstrated in a future study. Future work will also include the examination of using other materials and automatic techniques to fabrication the PV-MD device, aiming to enhance the device's performance and quality control.

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