Study of the Efficiency of Nanostructures for Water Desalination

From Macroscale to Atomistic Approach

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Abstract

In order to evaluate how membrane permeability affects the performance in desalination, in this work the reverse osmosis desalination system was simulated by using a macroscale flow model and the potential is quantified in terms of improvements in membrane permeability. We find that increasing the membrane permeability by one order of magnitude would allow for 15% (SWRO - seawater) and 24% (BWRO - brackish water) less energy or 60% (SWRO) and 68% (BWRO) fewer pressure vessels with a given capacity. Besides that, the ultrafast water transport in nanoconfinement environmental such as carbon nanotubes, graphene and molybdenum disulfide nanopores hold the greatest potential to cause a reduction in desalination operating costs. In addition, the water flux throgouth a nanoporous membrane based on a 2D material was evaluated using molecular dynamics approach.

Introduction

By 2025, 1.8 billion people will be living in countries or regions with absolute water scarcity. Water scarcity emerges from a combination of hydrological variability and high human use. Besides that, the problem tends to grow quickly due to global warming and uncertainty related to hydrological future cycle.

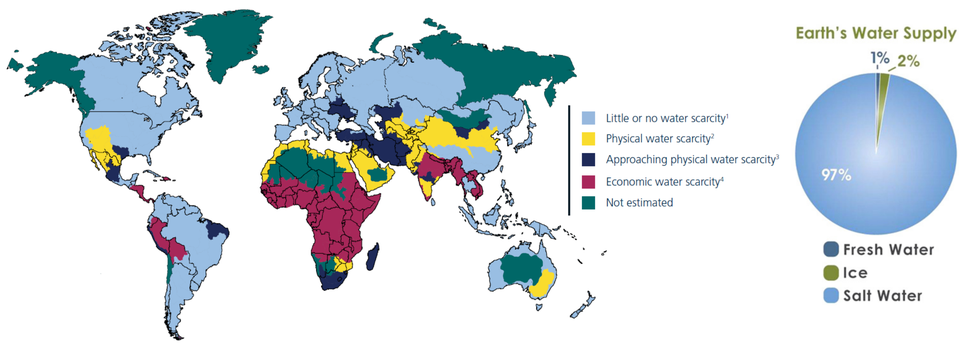

Figure 1: Global crisis [1].

In the face of growing water scarcity, it is critical to understand the potential of saltwater desalination as a long-term water supply option. The Reverse Osmosis system is the best available option in terms of energy consumption.

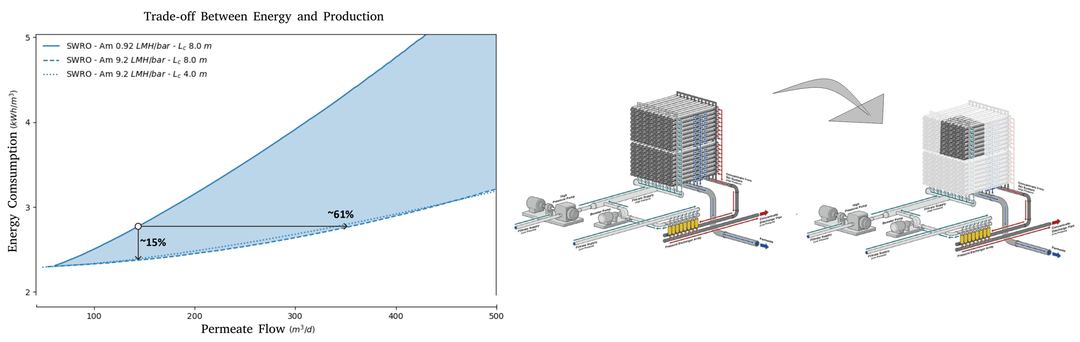

Figure 2: Trade-off between energy and vassels savings with an increase in one order the membrane permeability. Ilustration adapted from [2].

Our previous study based on a macroscale simulation developed by Cohen-Tanugi et al. [3] shows that an increase in one order of membrane permeability opens the possibility to desalinate water with 61 % less pressure vessels with a given capacity. To better understand the desalination process and its dependence on membrane nanopore density it is necessary to study the water flow at the nanoscale.

Materials and Methods

In the present work we simulate via molecular dynamics the efficiency of molybdenum disulfide (MoS_2) nanopore for water desalination. The LAMMPS package was used.

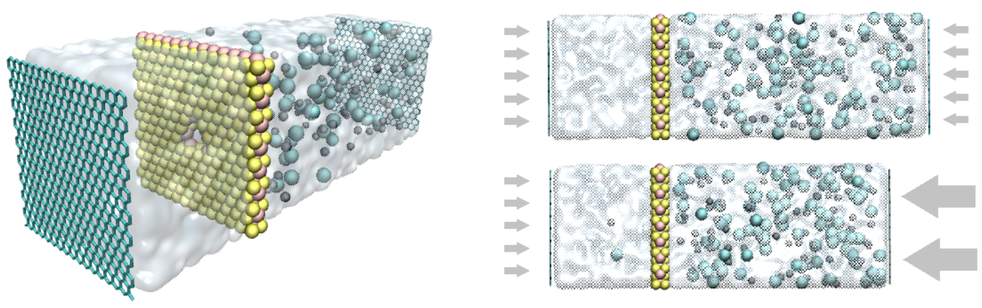

Figure 3: Desalination membrane based on MoS_2 nanopores.

The water box was placed between two graphene sheets acting as a rigid piston to exert external pressure. All of the species interact with each other by an Lennard-Jones potential and a Coulombic one. The MoS_2 sheet dived the water box in two. One of the sides contain 1 mol/L of salt (NaCl). The simulations were equilibrated in constant number of particles, pressure and temperature (NPT) ensemble for 1 ns at 1 atm and 300 K. After reached the equilibrium density, 2 ns simulation in NVT ensemble were performed to further equilibrate the system. Finally, the nanopore with 35 $\mathring{A}^2$ was opened and a range of external pressure was applied on the feed side for 10 ns controled by the graphene sheets. The TIP4P-ε [4] was used as water model and NaCl-ε [5] as salt model. For the MoS_2, the parametrization of a reactive many-body potential was used [6].

Results

The key component of a good membrane is the balance between high permeability and high salt rejection. The water flux is related to the membrane specific permeability through the following expression: $A_m = \phi/(P - \Pi)$, in which A_m is the membrane specific permeability, ϕ is the water flux, P is the applied pressure and Π is the osmotic pressure.

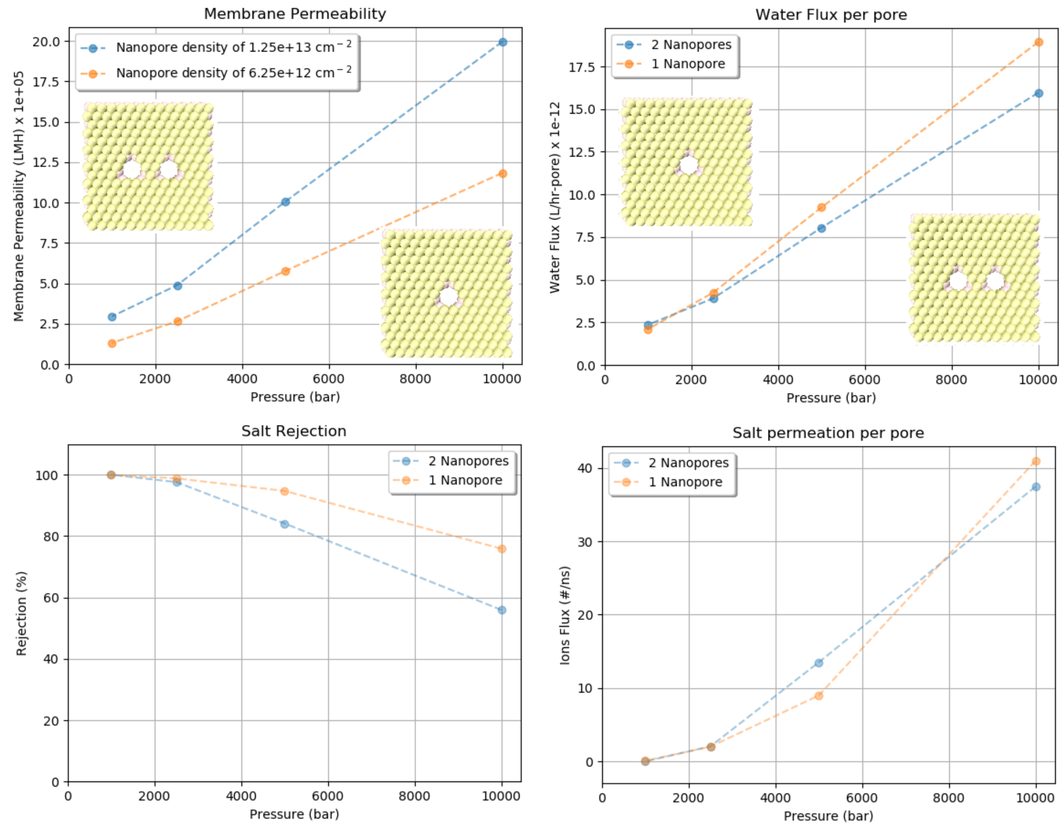

Figure 4: Water flux and salt rejection for different applied pressures and number of nanopores.

The membrane performance exhibits a high water flux and a high salt rejection rate at low pressure.

Parameter	Value	Units
Permeability-Commercial Membrane [7]	0.92 - 1.0	LMH/bar
Permeability-MoS_2 Membrane - $6.25 \times 10^{12}\ cm^{-2}$	119.3 (11.7)	LMH/bar
Permeability-MoS_2 Membrane - $1.25 \times 10^{13}\ cm^{-2}$	225.8 (51.9)	LMH/bar
Salt Rejection-Commercial Membrane [7]	99.70 - 99.86	%
Salt Rejection-MoS_2 Membrane	99.95 (0.17)	%

Table 1: Membrane parameters comparison.

In order to better understand the flow dynamics through the membrane, the image below ilustrates the eletrostatic potential map and the probability density of finding an oxygen inside the nanopore.

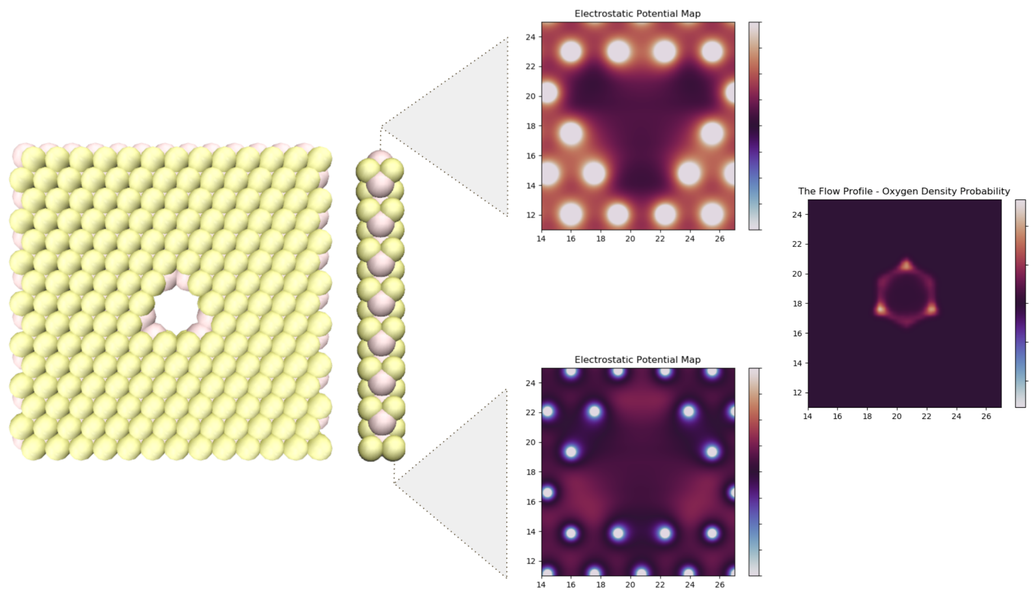

Figure 5: The Eletrostatic Potential Map and the Oxygen Probability Density.

Conclusions

- The MoS_2 nanoporous membrane exhibit water permeability two orders of magnitude greater than the commercial ones at the same rejection rate.
- The water flux scales linarly with the density of nanopores at low pressures.
- The water flow profile is strongly related to the nanopore charge distribution.

References

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Acknowledgements

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