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ABSTRACT

We study the impact of the induced pressure fields on the water flow and salt rejection in nanopores produced in MoS₂ membranes. We observe that the water permeability and the salt rejection are not impacted by the distance between the pores. This result contradicts the continuous fluid mechanics calculations in microfilters, which indicates the existence of hydrodynamic interactions between adjacent pores that increase the water mobility. Our results suggest that at this nanoscale, the hydrodynamic interactions do not affect the water mobility through nanopores.

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I. INTRODUCTION

Water scarcity is one of the major challenges of our time. Changing climate patterns responsible for disturbing the hydrological cycle combined with growing water demand are shifting the water security toward high-risk levels.¹ In the face of the problem, seawater desalination technology has gained attention. Over the past decades, improvements in the sector have allowed a considerable reduction of power needed to desalinate seawater due to advances in membrane technology and energy recovery equipment.^{2,3}

High-performance membranes, which can exhibit superior selectivity and a high water flow rate, are key to the next-generation desalination technology.^{3,4} Meanwhile, computational models have been used to better understand the desalination process at the nanoscale. In this context, molecular dynamics simulations are a powerful theoretical approach to study the physics behind nanofluidic systems since they allow for probing the microscopic behavior of a collection of atoms while performing timescale feasible simulations,^{5,6} giving rise to new nanostructured membrane materials designed to improve the desalination process.

One suited simulation branch to better understand the desalination process is to mimic the reverse osmosis desalination system at the nanoscale.^{8–20} This technique enters in the scope of Non-Equilibrium Molecular Dynamics (NEMD). In addition, its

procedure has been used to get insights into designing new membrane materials for desalination. Recently, a number of studies have suggested molybdenum disulfide (MoS₂) as a promising nanoporous membrane not only due to its water permeability but also for its salt selectivity.^{16,17,21–26}

The transport properties of water confined in nanopores are very different from the bulk water and are not properly described by the continuum hydrodynamics.²⁷ The continuum hypothesis is one of the fundamental assumptions of fluid mechanics, which is successful in describing the macroscopic behavior of fluid flow, and states that fluid properties, such as pressure, density, and velocity, are well defined at infinitesimally small points and vary continuously from one point to another.²⁸ However, in narrow nanopores (< 2 nm of diameter), the water flow is layered and a non-quadratic velocity profile emerges from it.²⁹ For such small molecular size pores, the hydrodynamics approach fails. Then, it is more useful to discuss the fluid transport using permeability and the flow rate rather than viscosity and the slip length; for example, see Ref. 28.

The continuous fluid mechanics calculations in microfilters assume the existence of hydrodynamic interactions between adjacent pores. The interaction arises from the pressure field induced by the next pore, which, in turn, makes the single pore water flow solution not sufficiently precise to expand its conclusions to the microfilter flow system.³⁰ The influence of the pore number and

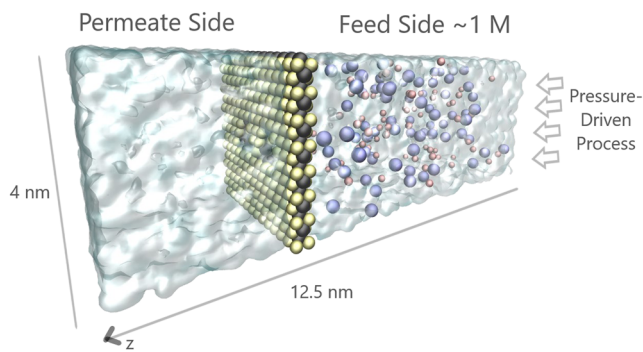


FIG. 1. The illustration of a typical NEMD desalination system at the nanoscale. The saltwater (right side) is separated from the pure water (left side) by a MoS_2 nanoporous membrane. Pressure-driven transport can be simulated by imitating the reverse osmosis process. The image is created using the Visual Molecular Dynamics (VMD) software.⁷

its distance plays an important role in the overall water flux in the classical hydrodynamic picture. Ignoring these pore-pore “interactions,” the simulations conducted so far in the scope of molecular dynamics desalination systems assume that the water flux results

scale linearly with the nanopore number³¹ in an “ideal gas” modeling of the system.

In this work, we test if the assumption that the distance between identical pores does not affect the transport properties of water in a nanopore membrane is valid. We employ NEMD simulations to investigate the behavior of liquids in the nanoscale.³² We obtain the nanopore number and its proximity implications in water flux and salt rejection. We use six different MoS_2 membrane (crystal structure of 2H) designs with different nanopore numbers and different nanopore distances (Fig. 2). These membranes were designed in order to maintain the nanopore chemistry and geometry the same in each case. Hence, the only difference in water flow would be due to hydrodynamic interactions. The remainder of this paper goes as follows: In Sec. II, the computation details are presented, and the results are commented in Sec. III. The conclusions follow Sec. IV.

II. COMPUTATIONAL DETAILS

Our system is designed as two reservoirs: one with water and salt molecules, the feed side, and another with only pure water, the permeate side. The two reservoirs are separated by a membrane, as illustrated in Fig. 1. The system is limited in the z -direction by

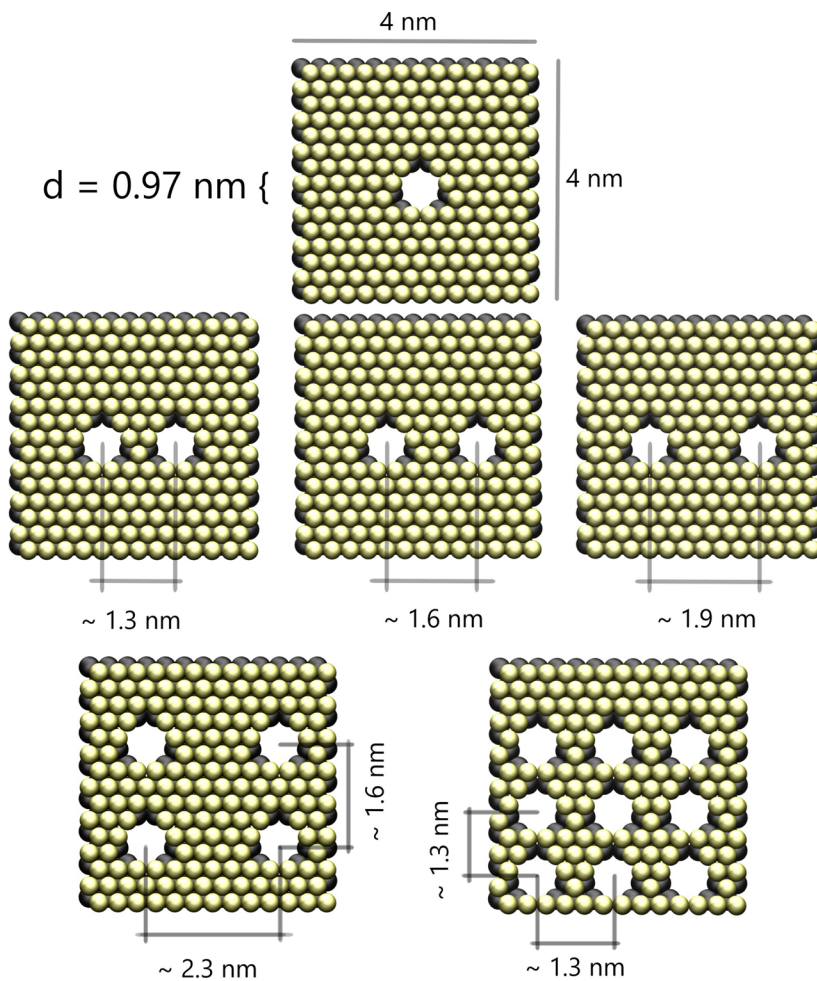


FIG. 2. The MoS_2 nanoporous membranes studied in this work. All the membranes are square shaped ($4 \times 4 \text{ nm}^2$).

graphene barriers, which, in turn, can serve as pistons to control the fluid pressure during the desalination process. We analyze six systems with a pore diameter of 0.97 nm: one single pore at the center of the membrane; three pairs of pores separated by 1.3, 1.6, and 1.9 nm; four pores; and nine pores, as illustrated in Fig. 2.

The system is initialized with 1550 water molecules at the permeate side and 170 ions mixed with 4930 water molecules at the feed side, resulting in a solution of 1 mol/l concentration. The MoS₂ membrane has a dimension of 4 × 4 nm², and it is held fixed in space. We work with high pressure gradients for statistical purposes, allowing us to generate a large number of events in a time interval of 10 ns. MoS₂ has nanopores with 0.97 nm diameter (defined as the center to center distance of atoms), which is the minimum size that does not show the ion blockage effect.¹⁸

The simulations were performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS).³⁷ The particles interact with each other via Lennard-Jones (LJ) and Coulomb potentials. The parameters used in this work are summarized in Table I. The Tip4p/ε water and NaCl/ε models were selected because they provide the correct value of bulk water³⁴ and water-NaCl³³ dielectric constants important for our analysis.

The simulations were performed as follows: First, the nanopore was kept closed and the two reservoirs were isolated. We performed simulations during 0.5 ns in the NVE ensemble. Next, simulations were conducted in the NPT ensemble during 1 ns at 300 K and 1 bar at each reservoir. Then, the simulation was further equilibrated for 2 ns at 300 K in the NVT ensemble to achieve the water equilibrium density of 1 g/cm³. Finally, the nanopore was opened by removing the desired atoms from the MoS₂ sheet and the different pressures were applied at each reservoir for 10 ns. The feed pressures used in this work were from 100, 500, 1000, 2500, 5000 to 10 000 bars.

The water flux throughout the membrane is computed by the membrane specific permeability,³¹ namely,

$$A_m = \frac{\phi}{(P - \Pi)}, \quad (1)$$

which incorporates information about the nanopore density and the membrane resistance to water flow (the pressure needed to induce certain flow). In this expression, ϕ is the water flux, P is the applied pressure, and Π is the osmotic pressure and has dimensions of L m⁻² h⁻¹ bar or LMH/bar.

TABLE I. The Lennard-Jones parameters and atomic charges employed in the simulations.

	σ_{LJ} (Å)	ϵ_{LJ} (kcal/mol)	Charge (e)
Na ³³	2.52	0.0346	0.885
Cl ³³	3.85	0.3824	-0.885
O-Tip4p/ε ³⁴	3.165	0.1848	-1.054
H-Tip4p/ε ³⁴	0.0	0.0	0.5270
Mo ³⁵	4.20	0.0135	0.6
S ³⁵	3.13	0.4612	-0.3
C ³⁶	3.40	0.0860	0.0

III. RESULTS

In order to test if the water flow through nanopores in MoS₂ membranes obeys the hydrodynamic behavior, we compare the flow of a single pore, two pores at three distances, four pores, and nine pores. Classical hydrodynamics predicts that for pores close enough, the behavior is not the same as observed in a single pore.³⁰ First, we analyze the membrane permeability. Figure 3 illustrates the membrane permeability as a function of pressure for six cases: isolated pore; two pores separated by 1.3, 1.6, and 1.9 nm; four pores; and nine pores. The graph shows that the membrane permeability is a linear function of the pressure gradient. Using Eq. (1), we obtained the specific permeability as illustrated in Table II.

Next, we study the behavior of salt in the analyzed configurations. In reverse osmosis, an efficient system is expected to show a salt rejection higher than 99%.² Figure 4 shows that the MoS₂ nanoporous membrane with 0.97 nm of diameter exhibits an excellent salt rejection capability, achieving 100% of rejection per pore working in pressures below 1000 bars. The graph also shows that the salt rejection per nanopore not only is the same for one or more pores but also does not depend on the distance between the pores.

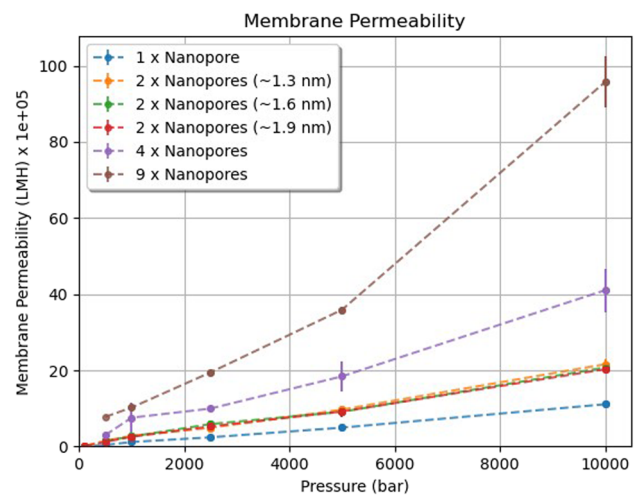


FIG. 3. The membrane permeability as a function of pressure for each membrane design. The error bars are the deviation from the mean value (error bars smaller than the points are not shown).

TABLE II. The membrane specific permeabilities (A_m) obtained as a function of nanopore density and distance. The numbers inside the parentheses are the membrane specific permeability's standard deviations evaluated in this work.

Nanopore density (10 ¹² cm ⁻²)	A_m (LMH/bar)	Distance (nm)
1 × nanopore—6.25	101.7 (25.2)	
2 × nanopores—12.5	242.9 (55.8)	1.3
2 × nanopores—12.5	241.6 (54.7)	1.6
2 × nanopores—12.5	223.6 (38.1)	1.9
4 × nanopores—25.0	436.0 (87.1)	2.3 × 1.6
9 × nanopores—56.25	934.2 (323)	1.3 × 1.3

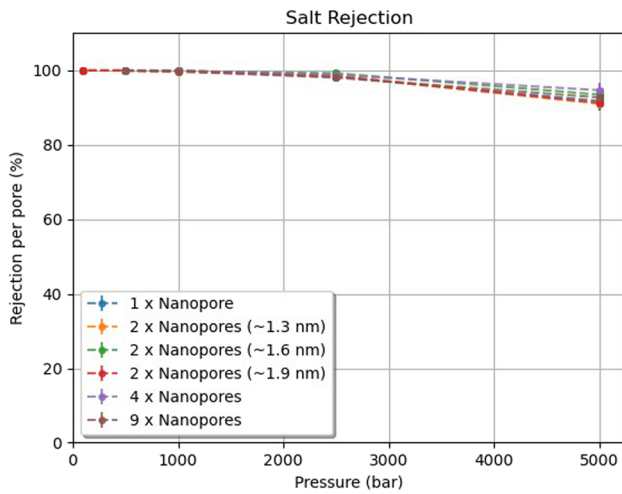


FIG. 4. The salt rejection per nanopore as a function of pressure. The error bars are the deviation from the mean value. For small pressure gradients (<100 bars), near those from the realistic process operation in reverse osmosis systems,¹⁹ the salt rejection is 100% for such MoS₂ nanopore size.

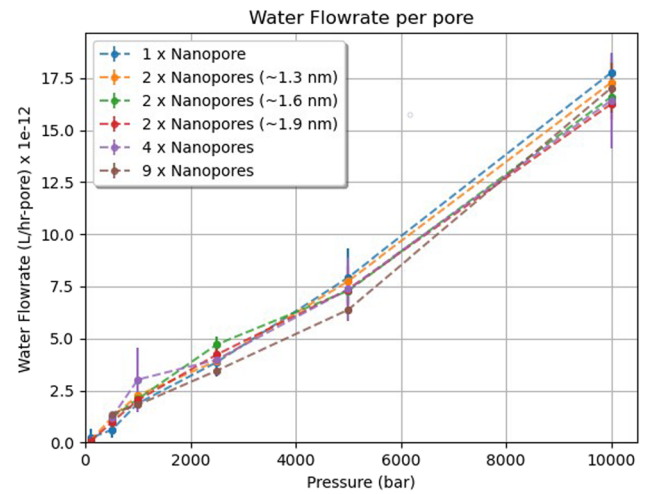


FIG. 6. Water flow rate per pore as a function of applied pressure.

Another important aspect of the reverse osmosis process is the concentration polarization (CP) phenomena, which is responsible to reduce the water flux due to increased local osmotic pressure near the membrane, namely, the accumulation of salt near the membrane surface. Although the CP implications are higher for high water flow rates in reverse osmosis systems, this effect is observed within dozens of μm from the membrane surface.³⁸ Our nanoscale simulation box is very small to capture this effect, as we can see from the constancy of the salt concentration along the z-direction shown in Fig. 5.

Then, we studied the water flow rate per pore. The permeability per pore is the same in all cases; as the pores approach, no decrease in permeability is observed, as we can see from Fig. 6.

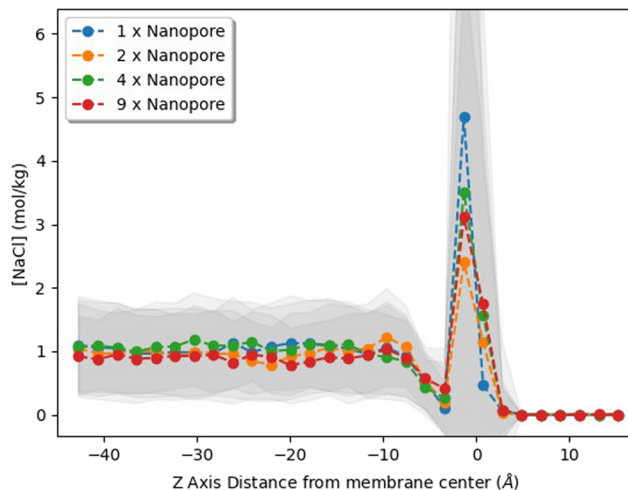


FIG. 5. The salt concentration along the simulation box in the z-direction from the membrane center. The shadows represent the concentration standard deviation during the running process.

In Fig. 7, the membrane specific permeability as a function of membrane porosity is shown. The area of the so-called 0.97 nm diameter pore corresponds to 0.66 nm². Here, we added a new nanopore design for hydrodynamic resistance comparison: a single nanopore with 1.33 nm of diameter corresponding to an area of

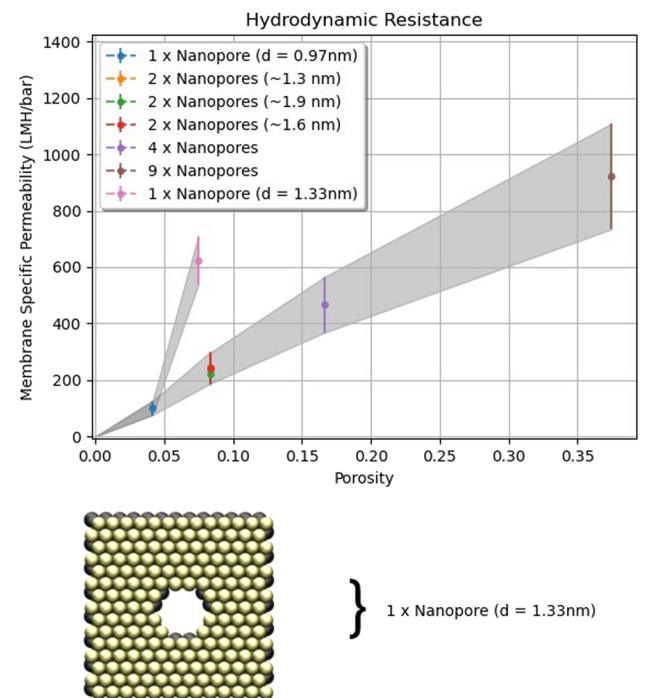


FIG. 7. Hydrodynamic resistance as membrane specific permeability vs membrane porosity. Beyond the set of nanopores with 0.97 nm of diameter investigated in this work, here we show a comparison with a single nanopore with 1.33 nm of diameter in order to illustrate the difference in hydrodynamic resistance.

1.19 nm². The pore area was obtained by computing the accessible area to water molecules considering the size of the atoms on the edge of the pore as the van der Waals radii of sulfur and molybdenum. We found that in this scale, the membrane specific permeability increases linearly, within the error bars, with membrane porosity for the 0.97 nm diameter systems.

These results reinforce the fact that the hydrodynamic interactions between adjacent pores do not play a significant role in this scale. Besides that, the large nanopore, named [1 × nanopore ($d = 1.33$ nm)], represents another set of hydrodynamic resistance, as shown in Fig. 7. It is worth to mention that the 1.33 nm diameter nanopore shows a higher water flow rate for the same porosity at the cost of lower salt rejection performance. As mentioned before, the whole set of 0.97 nm nanopores has 100% of salt rejection for small pressure gradients (<1000 bars, as shown in Fig. 4), while the 1.33 nm diameter nanopore shows 97% of salt rejection at the same pressure. This is the trade-off between selectivity and permeability that we have to deal with.

Then, in order to investigate if the membrane permeability is independent of the number of pores by a compensation of effects, we tested that what happens with the mobility of water through the membrane in the four cases: the one single pore vs the three pairs of pores separated by 1.3, 1.6, and 1.9 nm. Water flux, Q , is a function of the water density inside the pore channel, ρ ; the velocity, v ; and the pore area, A , namely,

$$Q = \rho \cdot v \cdot A. \quad (2)$$

The area A of the pores is a geometric parameter that, in turn, is maintained constant in our simulations. The density, ρ , and the axial velocity, v , are the remaining control parameters, and they are related to the pore chemistry.^{5,16,17} The pore chemistry depends on the particle interactions and their distribution around the pore. We know from previous studies that the charge distribution affects the overall water flux.^{39–41} In our simulations, we chose an arrangement of atoms, as illustrated in Fig. 2, to maintain the proportion constant between hydrophobic and hydrophilic sites in the pore. As a consequence of this choice, the charge distribution is the same in each one of the four cases and the pores are charge neutral. In summary, the nanopore chemistry and geometry are the same in all simulations. By doing that, we expect that any change in the water flux as a function of the nanopore number or distance would be due to hydrodynamic interactions between the pores, which, in turn, would be reflected in the water flux or water density around the pores.³⁰

Figure 6 shows the water flow rate per pore in the six cases. The graph indicates that there is no dependence of the flow on the nanopore number or on the distance between the pores. This result indicates that the classical hydrodynamic predictions fail in the systems we analyzed. The classical hydrodynamic equations assume the fluid distribution to be continuum, which is not the case. In order to confirm that the dynamics of water is localized and not continuum, we investigate the water density inside and around the pore. Oxygen distribution of water is illustrated in Fig. 8. Region 1 is defined as the water present between $8 > z > 3$ Å, where z is the distance from the membrane center (Mo atoms), and the positive numbers correspond to the permeate side. Region 2 corresponds to $3 > z > 1.56$ Å, and Region 3 is the water located at $1.56 > z > -1.56$ Å (the nanopore region).

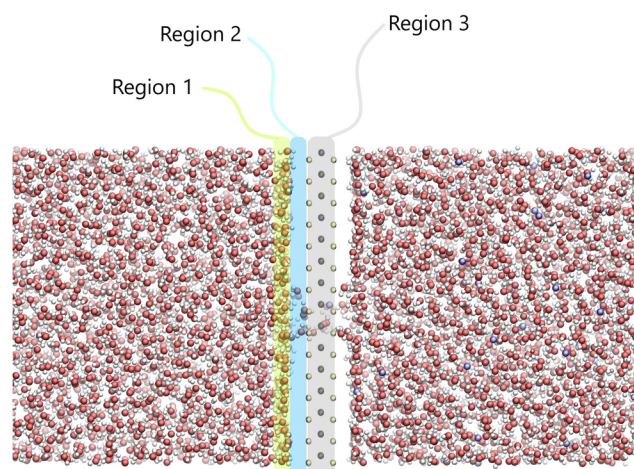


FIG. 8. Oxygen distribution of water in the two sides of the membranes. The three different regions, namely, Region 1, Region 2, and Region 3, are indicated by yellow, blue, and gray, respectively.

The oxygen color map illustrated in Region 3 of Fig. 9 shows how the water moves through the single and double nanopores. The three maps in this Region 3 show that the water molecule transport inside the pore occurs near the Mo atoms at the pore surface and the water does not pass throughout the pore center. The layered water structure, described by density oscillations in the radial direction, arises, and it is a signature of the implications of nanoconfinement. Region 2 of Figure 9 shows that water molecules enter the nanopore attracted mostly by the Mo sites.¹⁶ In addition, the first two water layers from the membrane surface shown in Region 1 of Fig. 9 indicate that even in this layer outside the pore, molecules prefer to stay between S sites, which is the region in which the Mo–water electrostatic interaction is less screened by the S atoms.

The oxygen density map from Region 1 of Fig. 9 in the single nanopore case (left column) shows that the first two water layers are modified locally by the presence of the nanopore. However, its extension is not larger than the nanopore size of 0.97 nm diameter, which suggests that the nanopore presence does not have a large effect on the water structure near the membrane but just local implications near the nanopore region.

Comparing with the two neighboring nanopores case, no deviation in the density map due to the presence of the second nanopore is observed. This conclusion extends to the last case when the two nanopores have the larger separation. To quantify if any implications in the water density exist due to the proximity of nanopores, we obtained the water density as a function of the radial distance from each nanopore center, as defined in Fig. 10. The radial water density was calculated binning the region inside the nanopore in circular shapes, counting the water molecules there, and dividing by its cylindrical volume.

As we can see from Fig. 11, there is no difference in the water density inside the nanopore due to the presence of a second one. Figure 11 shows that if any induced pressure field extends from one nanopore to the other one, it is not sufficient to produce a change in the water density inside the nanopore and its surroundings.

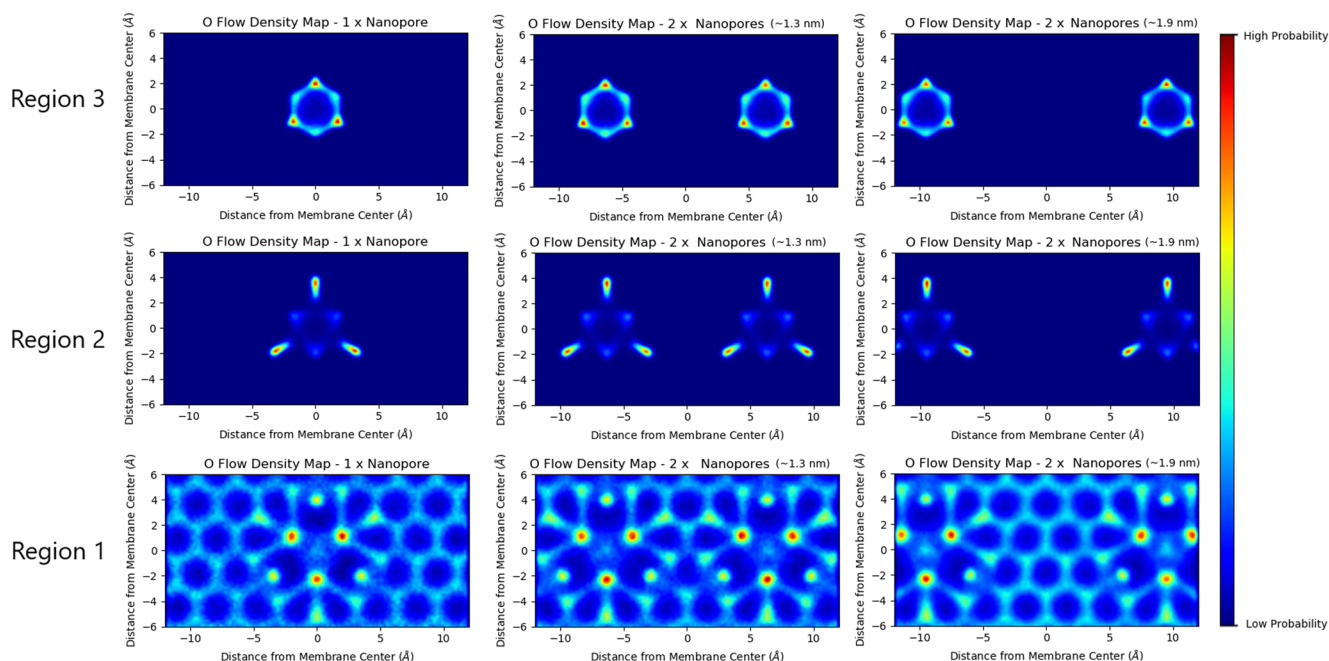


FIG. 9. Oxygen color map with red indicating high density, light blue indicating low density, and dark blue indicating the absence of water.

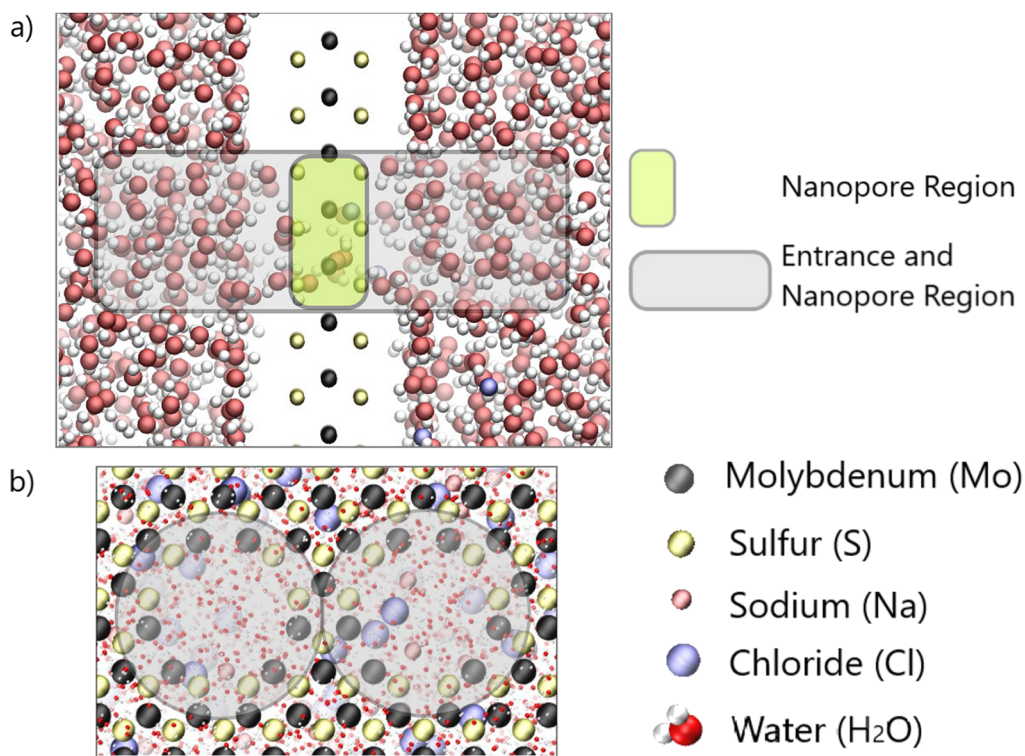


FIG. 10. (a) The definitions of the nanopore region and entrance region for the water density analysis. (b) The front view of the cylindrical regions of analysis.

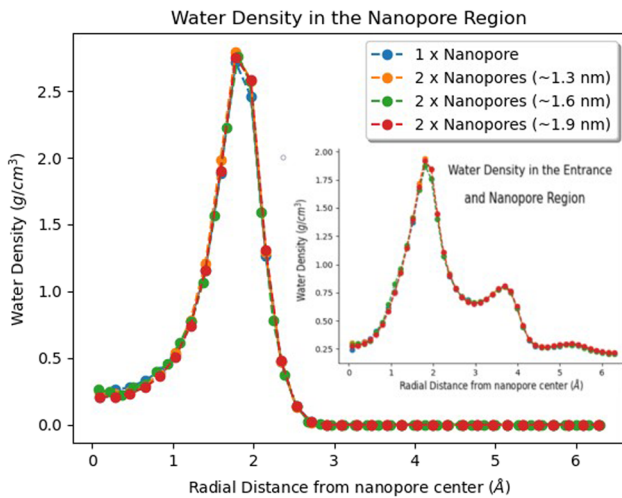


FIG. 11. The water density as a function of radial distance from each nanopore center in the nanopore region. Inset: the water density as a function of radial distance from each nanopore center in the entrance and nanopore region.

In addition, the water density is related to the Potential of Mean Force (PMF) through the following expression:^{17,25,42}

$$PMF(z) = -k_b T \ln[\rho(z)/\rho_0], \quad (3)$$

where $\rho(z)$ is the local density, ρ_0 is the bulk density, T is the temperature, and k_b is the Boltzmann constant. Equation (3) is usually computed in equilibrium states. However, we extrapolated the calculations to the steady-state flow once it refers to states near equilibrium, and our goal is to catch dynamic features.

The free energy barrier ΔG can be established from Fig. 12, and it is related to the probability of water molecules being able to

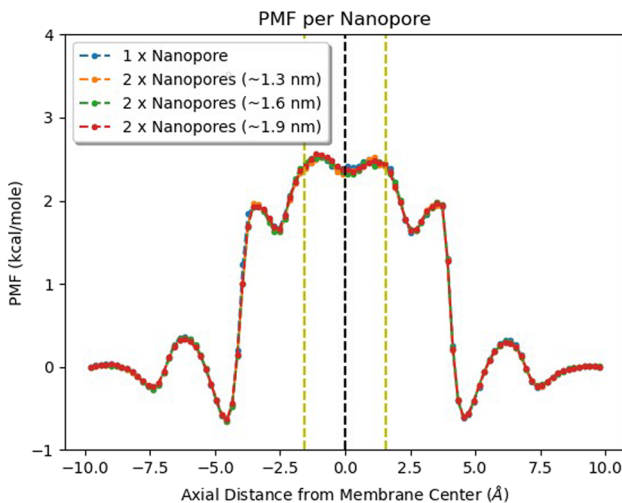


FIG. 12. The water PMF per nanopore as a function of axial distance from the membrane. The dashed lines represent the sulfur layer (yellow line) and the molybdenum layer (black line).

overcome the nanopore energy barrier $P \sim \exp(\Delta G/k_b T)$. As it can be seen, the PMF per nanopore is the same for each membrane. The hydrodynamic effects were not visible in this scale maybe due to the polar nature (atomic charges) of the MoS₂ membrane, which induces its structure in the first water layer.²⁶

IV. CONCLUSIONS

Different from the classical fluid mechanics calculations in microfilters,³⁰ the fluid flow through neighboring nanopores in MoS₂ membranes does not show in our NEMD simulations any significant hydrodynamic interactions between adjacent pores. The water flow strongly depends on the intermolecular force of the membrane, which is governed by the layered structure of the liquid in the nanopore region, and as a consequence, the collective effect of the hydrodynamic interaction between pores is suppressed. Nevertheless, we shed light on the assumption that the water flux would scale linearly with the nanopore density regardless of its distance. Of course, here the MoS₂ atoms were held fixed in space, and more careful simulations are needed to understand the relation between nanopore distance and material stability. Based on the results of Cohen-Tanugi and Grossman,¹⁹ although higher pressure gradient leads to greater membrane deformation, the implications of that are not significant to the flow of water across the graphene nanopores. Since the MoS₂ monolayer has effective Young's modulus⁴³ of $180 \pm 60 \text{ N m}^{-1}$ while graphene⁴³ has 335 N m^{-1} , we expect that the main conclusions of our work would not be affected if flexibility would be taken into account. As previous studies confirmed, the MoS₂ nanoporous membranes are promising candidates for the next-generation membrane material, allowing water to be filtered at high permeate rates while maintaining high salt rejection rates for sufficiently narrow pores.

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DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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