

Factors determining ion rejection and one-step freeze desalination

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Freeze desalination is an emerging, membrane-free desalination method that utilizes the ion rejection phenomenon during the freezing of seawater, where salt ions tend to be rejected by ice. However, it requires the ion rejection rate to be higher than 98.2% to generate drinking water; i.e., at least 98.2% of the salt ions remain in the liquid phase. This poses a challenge for one-step seawater freezing due to the trapping of salt ions in ice. In this work, we first reveal that the ion rejection phenomenon is governed by the competition between two factors: ice growth and ion diffusion, which can be described by two characteristic timescales, τ_{ice} and τ_{ion} , respectively. To enhance the ion rejection rate, the ratio $\tau_{\text{ice}}/\tau_{\text{ion}}$ should be increased. Based on this criterion, we propose a freeze desalination method by freezing flowing seawater, where τ_{ion} is reduced due to the enhancement of the ion diffusivity caused by flow shear, to obtain potable water through a single cycle of seawater freezing with the ion rejection rate exceeding 98.2%. With additional temperature control, the productivity of drinking water can be further improved. The proposed freeze desalination method shows great potential for commercialization.

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I. INTRODUCTION

Water scarcity has been a serious issue faced by many regions and countries. Globally, about one-third of the world's population lacks access to safe drinking water [1]. Although 70% of the Earth's surface is covered by water, 97% of it is seawater, which is not suitable for direct human consumption. The tremendous volume of seawater on Earth, however, makes seawater desalination a potential solution to mitigate or resolve the worldwide water scarcity. Currently, the most widely used desalination methods include thermal distillation [2–4] and osmosis-based membrane methods [5–8]. In thermal distillation, seawater is evaporated and then condensed to produce potable water. This method is simple but energy-intensive due to the high latent heat required for water distillation (2256.7 kJ/kg) [9]. For osmosis-based membrane methods, reverse osmosis (RO) is the most popular desalination technique [10]. Compared with thermal distillation, RO methods have a relatively low energy consumption. However, a critical challenge for RO systems is membrane fouling, which reduces both the permeation flux and the desalination efficiency [11–14]. The cleaning or replacement of the membrane increases the overall cost of this method [15].

Recently, a seawater desalination technique, freeze desalination, has gained great attention, which consumes only 1/7 of the energy in distillation methods due to the low latent heat

of freezing (333.5 kJ/kg) and is superior to RO methods in terms of maintenance cost because it is free of membranes. Freeze desalination takes advantage of the ion rejection phenomenon that occurs during the freezing of seawater [16]; i.e., as seawater freezes, salt ions (mainly Na^+ and Cl^-) are apt to be expelled by ice crystals and remain in the liquid phase. Consequently, the ice formed from seawater is less salty than the original seawater. The ion removal rate is described by the ion rejection rate, which is the percentage of ions in the aqueous phase. If a high ion rejection rate (>98.2%) could be reached, the ion concentration in the ice can meet the drinking water standards [17]. This will make freeze desalination an appealing method that may outperform the traditional desalination techniques and has the potential to dominate the seawater desalination market.

Unfortunately, ion rejection is a dynamic process. The growth of ice crystals and the thermal motion of salt ions may cause ion trapping in the ice, which reduces the ion rejection rate. Although progress has been made in the past decade in understanding ice formation in seawater and salt exclusion kinetics [16,18–21] since the first attempt in seawater desalination through freezing in 1859 [22], the highest ion rejection rate achieved through one-time seawater freezing is only around 60% [23,24], which is far below the drinking water standard (98.2%) set by the World Health Organization (WHO) [17]. To improve the ion rejection rate, various strategies have been implemented. An ion rejection rate of 90% has been reported by minimizing the formation of brine pockets, which occur during the freezing of seawater and contain high-salinity solutions [24,25]. Ion rejection rates exceeding 98.2% can certainly be achieved through multiple freezing cycles, where ice is formed, melted, and then frozen to further remove salt ions. However, this method typically requires four to five freezing cycles in order to obtain drinking water, making it less favorable in practice [26,27]. Strategies incorporated with

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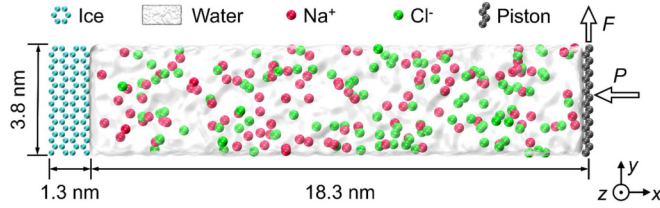


FIG. 1. Molecular dynamics simulation system. The ice slab at the left end serves as the cold surface for triggering ice formation. The piston at the right end is used to control the pressure of the system. Water molecules are shown as transparent clouds. Na^+ and Cl^- are denoted as red and green spheres, respectively.

seawater prefiltering and ice washing processes could enhance salt removal and improve the ion rejection rate [28]. Unfortunately, these additional efforts make them less competitive compared with membrane-based methods. To compete with traditional methods, one-step freeze desalination approaches that can achieve ion rejection rates meeting drinking water standards are highly desired, which, however, have not yet been realized.

In this work, we propose a one-step freeze desalination method to obtain potable water, based on the understanding of the underlying physics of ion rejection kinetics. Through molecular dynamics (MD) simulations, we first reveal that the ion rejection phenomenon is determined by the competition between two processes: the growth of ice and the diffusion of ions, which can be described by two characteristic timescales, τ_{ice} and τ_{ion} , respectively. To improve the ion rejection rate, the ratio $\tau_{\text{ice}}/\tau_{\text{ion}}$ needs to be raised, which can be achieved by reducing the ice growth rate and/or enhancing the ion diffusivity. Based on this criterion, we propose a method to enhance the ion rejection rate by freezing flowing seawater. In this strategy, both the ice growth rate and ion diffusivity can be regulated. Optimal configurations can achieve high ion rejection rates, ensuring the production of potable water through one-step freezing of seawater. Experiments using both artificial and natural seawater have been conducted to validate this approach, which shows great potential for commercialization.

II. UNDERSTANDING ION REJECTION KINETICS THROUGH MOLECULAR DYNAMICS SIMULATIONS

We first conduct MD simulations to understand the kinetics of ion rejection processes. The MD system contains a hexagonal ice slab, which acts as a solid surface to trigger ice nucleation, an aqueous sodium chloride (NaCl) solution with a salt concentration of 0.6 M (same as natural seawater), and a piston that is used to maintain the system pressure at 1 atm, as shown in Fig. 1. The width of the simulation box in the z direction is 4.0 nm. The shearing force F acting on the piston in the y direction is varied from 0 to 6.16×10^{-11} N. Nonequilibrium MD simulations are conducted using the lammps package [29]. The ice is simulated in the NVT ensemble, with the temperature ranging from 261 to 269 K. The NaCl solution is performed in the NVE ensemble. Molecular interactions for the ice, water, and ions are described by the mW-ion model, which has been widely used for ice nucleation [30–33]. Interactions involving piston atoms

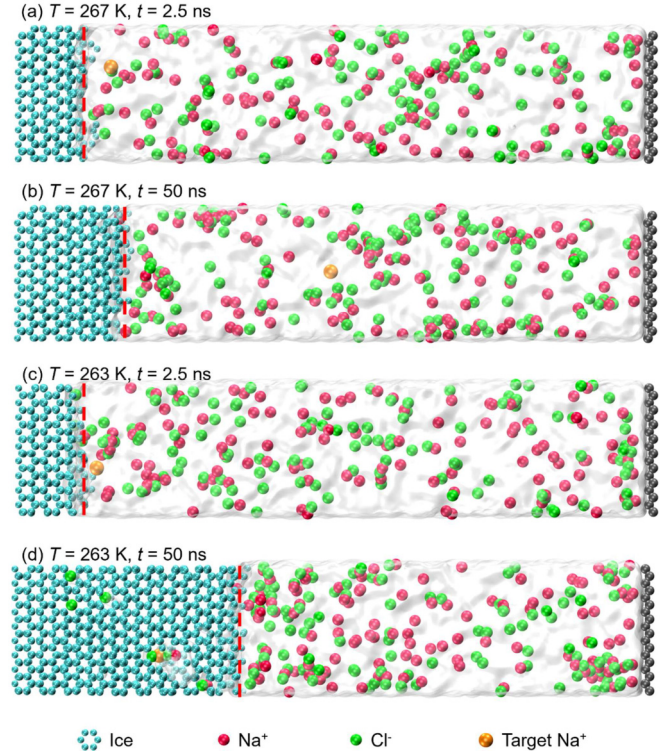


FIG. 2. Snapshots of ice formation at different temperatures: (a) $T = 267$ K and $t = 2.5$ ns, (b) $T = 267$ K and $t = 50$ ns, (c) $T = 263$ K and $t = 2.5$ ns, and (d) $T = 263$ K and $t = 50$ ns. Target Na^+ is denoted as orange spheres. The red dashed lines indicate the ice-water interfaces.

are computed using the Lennard-Jones (LJ) 12-6 potential, $U(r) = 4\epsilon[(\sigma/r)^{12} - (\sigma/r)^6]$, where the binding energy ϵ and collision diameter σ are set as 0.3 kcal/mol and 3.2 Å, respectively.

Figures 2(a) and 2(b) show two snapshots of the ice formation process at $T = 267$ K. At $t = 2.5$ ns, an Na^+ at the ice-water interface is targeted, as indicated by the big orange sphere. As the ice grows, this Na^+ keeps diffusing in the liquid phase and migrates faster than the growth of the ice in the x direction, as illustrated in Fig. 2(b) at $t = 50$ ns. For another case at $T = 263$ K, a target Na^+ also diffuses around the ice-water interface (orange sphere in Fig. 2(c) at $t = 2.5$ ns) but is trapped in the ice later, as illustrated in Fig. 2(d) at $t = 50$ ns. In Figs. 2(c) and 2(d), the ice growth rate is higher than that in Figs. 2(a) and 2(b) and exceeds the diffusion of the Na^+ , leading to the trapping of ions in the ice (Videos S1 and S2 [34] show the dynamics of target Na^+ in the two cases in Fig. 2).

Figure 2 indicates that an ion rejection process is primarily determined by two effects: the diffusion of ions and the growth of ice. If ions diffuse fast compared to the growth of the ice, they have sufficient time to migrate into the liquid phase due to relatively strong ion-water interactions [16], which increases the ion rejection rate [Figs. 2(a) and 2(b)]. Conversely, if the ice grows fast relative to the diffusion of ions, ions may become trapped in the ice, reducing the ion rejection rate, as shown in Figs. 2(c) and 2(d). Therefore, the competition between the diffusion of ions and the growth of ice governs

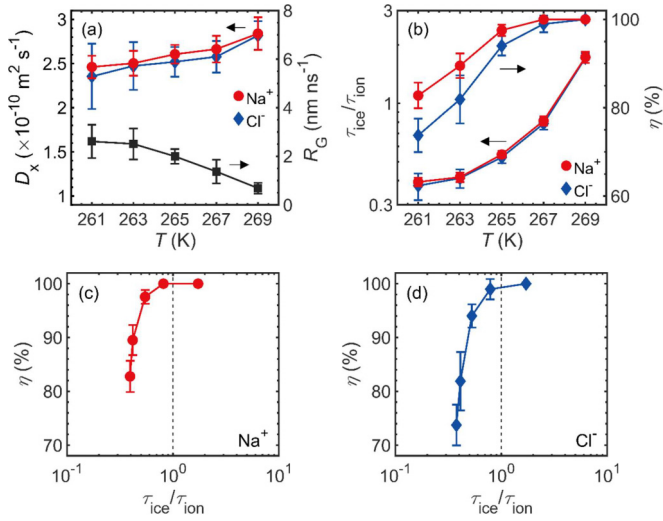


FIG. 3. Seawater freezing kinetics. (a) Diffusion coefficient D_x of Na^+ and Cl^- and ice growth rate R_G , as a function of temperature. (b) τ_{ice}/τ_{ion} and ion rejection rate η vs temperature. (c), (d) Effects of τ_{ice}/τ_{ion} on η for Na^+ and Cl^- , respectively.

the ion rejection rate. These two effects can be characterized by two timescales: τ_{ion} and τ_{ice} . The former represents the time needed for an ion to diffuse across the interfacial region, while the latter is related to the time required for the ice to grow through the interfacial region. If the length of the interfacial region in the ice growth direction is denoted as L , which is the length equivalent to two ice layers and determined as 0.23 nm through MD simulations [16,35], $\tau_{ion} \sim L^2/D_{ion}$ with D_{ion} being the diffusion coefficient of ions, and $\tau_{ice} \sim L/R_G$, where R_G is the ice growth rate. To achieve a high ion rejection rate, the criterion $\tau_{ion} < \tau_{ice}$ needs to be met. In this scenario, the ion rejection rate is expected to increase as the ratio τ_{ice}/τ_{ion} rises.

To confirm this criterion, the ion rejection rate η , ice growth rate R_G , which is the length of ice in the x direction per unit time, and the diffusion coefficient of ions are calculated for ice formation processes under various temperatures T . The CHILL+ algorithm is used to detect ice crystals [36,37] and identify the ice-solution interface. The number of ions in the ice is used to compute the ion rejection rate, which is obtained as [16]

$$\eta = \left(1 - \frac{C_I}{C_L}\right) \times 100\%, \quad (1)$$

where C_I and C_L are the number densities of ions in the ice and the initial solution, respectively. The diffusion coefficient of ions in the x direction, D_x , is calculated using the mean square displacement of ions through the Einstein relation,

$$D_x = \lim_{t \rightarrow \infty} \frac{\langle [x(t) - x(0)]^2 \rangle}{2t}, \quad (2)$$

where t is time and x is the position coordinate in the x direction.

Figure 3(a) plots D_x and R_G as T is varied. It is seen that D_x increases with increasing T for both Na^+ and Cl^- , which is consistent with the classic transport theories [38]. In contrast, R_G decreases as T is increased. This agrees well

with previous work [16,32]. Figure 3(b) depicts τ_{ice}/τ_{ion} and the ion rejection rate η as a function of T . It is seen that τ_{ice}/τ_{ion} increases when T is raised, and η also increases with increasing T . Figures 3(c) and 3(d) show η versus τ_{ice}/τ_{ion} for Na^+ and Cl^- , respectively. It is seen that η increases with increasing τ_{ice}/τ_{ion} when $\tau_{ice}/\tau_{ion} < 1.0$ and reaches $\sim 100\%$ for $\tau_{ice}/\tau_{ion} > 1.0$, which confirms that τ_{ice}/τ_{ion} qualitatively governs the ion rejection rate.

The ratio τ_{ice}/τ_{ion} serves as a guideline for enhancing the ion rejection rate. Any factor that can reduce τ_{ion} and/or increase τ_{ice} to raise τ_{ice}/τ_{ion} will enhance the ion rejection rate. In other words, a method that can improve the ion diffusion or lower the ice growth rate will have a high ion rejection rate. Practically, however, low ice growth rates are not preferred because it reduces the productivity of potable water. Therefore, the best strategy is to enhance the diffusion of ions.

Under this criterion and inspired by previous work [39–41], we propose to improve the ion rejection rate by enhancing ion diffusion using external shear, which can be achieved by freezing flowing seawater. In MD simulations, this can be realized by applying an external force F on the right piston (see Fig. 1). When the piston moves upward, a shear flow is generated. The velocity gradient in the solution is termed shear rate $\dot{\gamma}$. Figure S1 in the Supplemental Material [42] shows the velocity profiles and $\dot{\gamma}$ under various F . Figures 4(a) and 4(b) plot the ion rejection rate η as a function of $\dot{\gamma}$. It is seen that η increases with increasing $\dot{\gamma}$ at a given temperature for both Na^+ and Cl^- . This is because the diffusion of Na^+ and Cl^- is enhanced by the shear [Fig. 4(c)]. Moreover, the ice growth rate R_G is reduced by the shear (Fig. S2), which also helps enhance η . The temperature effects on η in Fig. 4 are the same as those in Fig. 3.

III. EXPERIMENTS

Experiments were also conducted to confirm the proposed method. The experimental setup is illustrated in Fig. 5, where seawater flowed over an inclined cold surface. Ice was formed on the cold surface. The flow rate of seawater, $\dot{m}$, inclined angle of the cold surface, θ , temperatures of the cold surface, T_s , and seawater temperature T_w could be varied. Details of experiments are described in the Supplemental Material [42]. Both artificial seawater and natural seawater were tested. The shear rate $\dot{\gamma}$ was varied by changing $\dot{m}$ and θ . According to the classic fluid mechanics, $\dot{\gamma} \propto \sqrt[3]{\sin^2 \theta} \times \dot{m}^{1/3}$ if a stick boundary condition is assumed [43]. Furthermore, the temperatures of the cold surface and seawater were also altered as they affect both the ice growth rate and ion diffusion.

Figures 6(a) and 6(b) show η as $\dot{m}$ and θ are varied ($\dot{\gamma}$ is also provided) for artificial seawater. In Fig. 6(a), it is seen that η increases with increasing $\dot{m}$ or $\dot{\gamma}$. It reached the drinking water level when $\dot{m} > 600$ g/min. This is because the shear enhanced the diffusion of salt ions, which reduced τ_{ion} and consequently raised τ_{ice}/τ_{ion} . Figure 6(b) plots η as a function of θ and $\dot{\gamma}$. It shows that η is enhanced when θ or $\dot{\gamma}$ is increased and became higher than 98.2% for sufficiently large θ and $\dot{\gamma}$. The results in Figs. 6(a) and 6(b) qualitatively confirm the criterion for enhancing the ion rejection rate and show that one-step freeze desalination can be achieved.

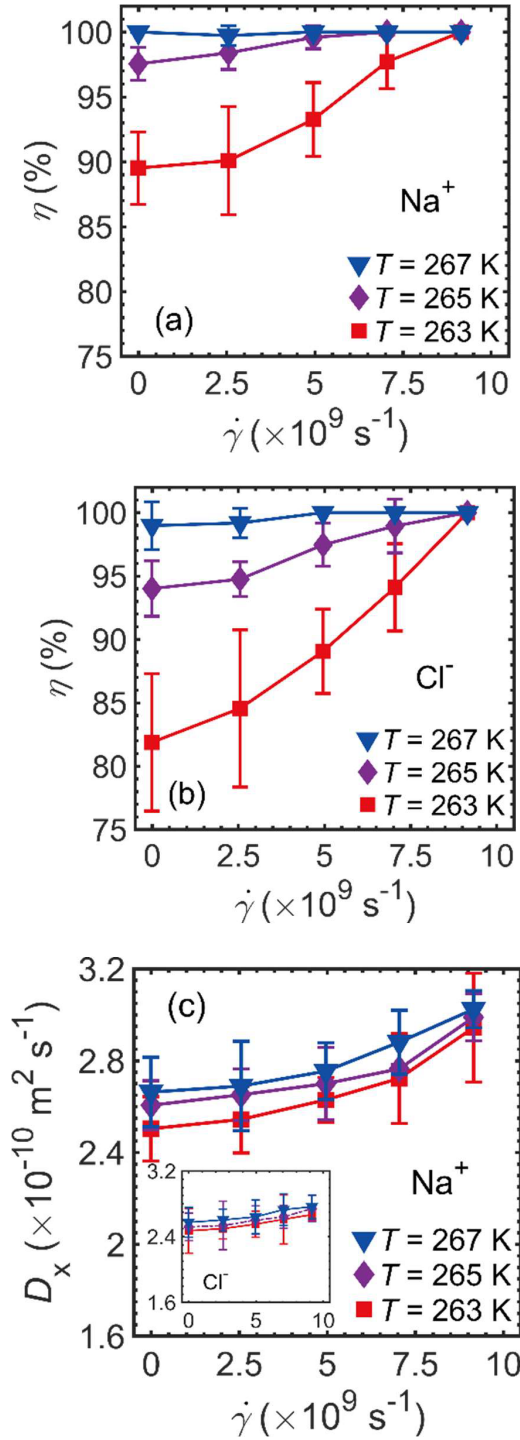


FIG. 4. Ion rejection rate η and diffusion coefficient of ions under shear. (a), (b) η as a function of shear rate $\dot{\gamma}$ for Na^+ and Cl^- . (c) Diffusion coefficient of Na^+ as $\dot{\gamma}$ is varied. The inset shows the diffusion coefficient of Cl^- .

It is worth mentioning that temperature plays an important role in ion rejection as it affects both the diffusion of ions and the ice growth rate. A high temperature usually lowers the ice growth rate [16] and boosts the ion diffusivity [38], and consequently increases $\tau_{\text{ice}}/\tau_{\text{ion}}$. Figure 6(c) shows η as a function of the surface temperature T_s . It is seen that η

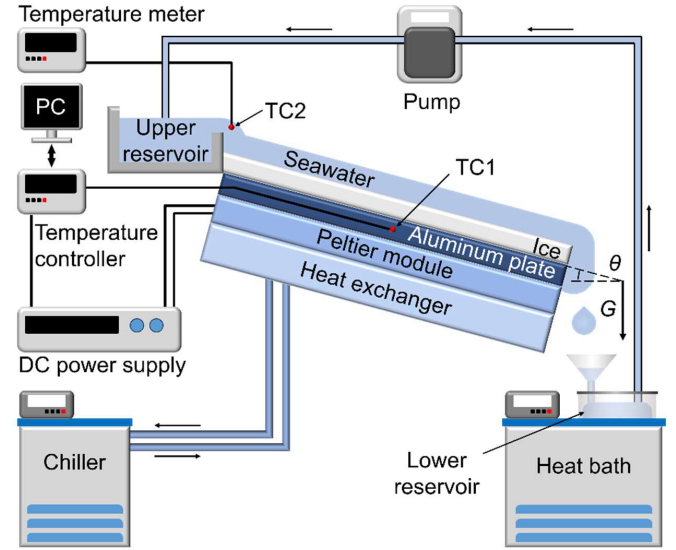


FIG. 5. Schematic of experimental setup. The inclined aluminum plate serves as the cold surface for ice formation. Its temperature is monitored by a thermocouple TC1 and controlled by the Peltier module underneath. Seawater flows over the aluminum plate from the upper reservoir, where the temperature is measured by thermocouple TC2. Unfrozen seawater is collected in the lower reservoir and then pumped back into the upper reservoir.

increased from 87% to 99% as T_s was raised from 261 to 267.5 K. It was above the drinking water level for $T_s \geq 267$ K. The enhanced ion rejection rate was caused by the reduced ice growth rates as T_s was increased, as shown in Fig. 6(d). Practically, a low ice growth rate is not favored because it affects the desalination productivity. To maintain a relatively high ice growth rate, the surface temperature T_s was linearly decreased with time at a certain rate $\dot{T}_s$ (K/h), during the ice formation process. The time evolutions of T_s are shown in Fig. S3 in the Supplemental Material [42] for various $\dot{T}_s$. Figures 6(e) and 6(f) depict η and the ice growth rates, respectively, as a function of $\dot{T}_s$ under various seawater temperatures T_w . It is seen that η remains above the drinking water level with relatively high ice growth rates for $T_w = 283$ K. Parameters for the experiments in Fig. 6 are listed in Table S1 in the Supplemental Material [42].

Natural seawater was used to examine the performance of the proposed freeze desalination method. Experiments were conducted at $\dot{m} = 100$ g/min, $\theta = 10^\circ$, and $\dot{T}_s = -2$ K/h, with $T_w = 283$ K. The concentrations of six major ions, i.e., sodium (Na^+), magnesium (Mg^{2+}), calcium (Ca^{2+}), potassium (K^+), chloride (Cl^-), and sulfate (SO_4^{2-}), were analyzed. Figures 7(a) and 7(b) show η and the concentrations of these ions, respectively. It is seen that η exceeded 99% for all the ions. The concentrations of Na^+ , Mg^{2+} , Ca^{2+} , K^+ , Cl^- , and SO_4^{2-} after the desalination were 59.0 ± 11.4 , 9.1 ± 2.5 , 6.2 ± 0.8 , 3.0 ± 0.7 , 132.3 ± 47.3 , and 26.5 ± 5.1 mg/l, respectively, meeting WHO drinking water standards.

Furthermore, the energy consumption is roughly analyzed. If thermal insulation of the system can be maintained, the energy consumption of the proposed method is estimated as

$$E_{\text{tot}} = E_{\text{freezing}} + E_{\text{pump}} = E_L/\text{COP} + E_{\text{pump}}, \quad (3)$$

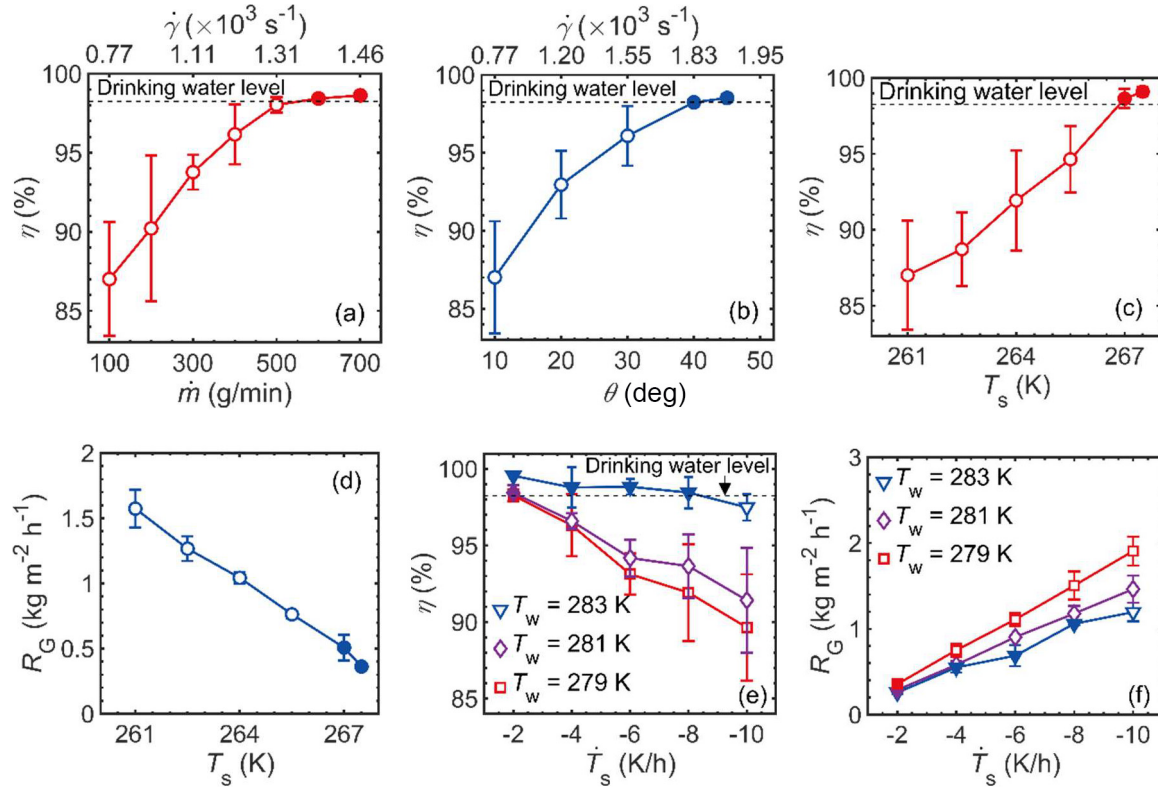


FIG. 6. Results of freeze desalination experiments. Ion rejection rate η as a function of seawater mass flow rate $\dot{m}$ (a), inclined angle of the cold surface, θ (b), and surface temperature T_s (c). (d) R_G vs T_s . (e) η as a function of $\dot{T}_s$. (f) R_G vs $\dot{T}_s$.

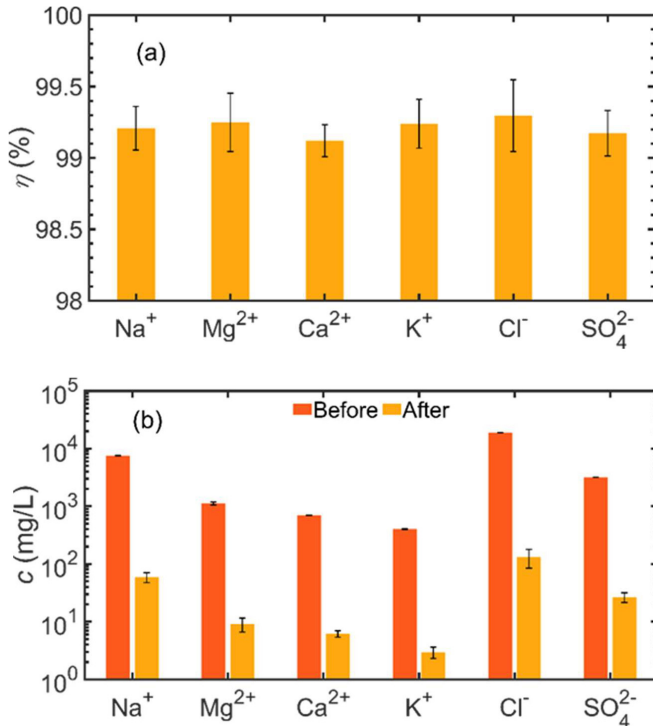


FIG. 7. Freeze desalination performance with natural seawater. (a) Ion rejection rate η for Na^+ , Mg^{2+} , Ca^{2+} , K^+ , Cl^- , and SO_4^{2-} . (b) Concentrations c of ions before and after freeze desalination.

where E_{tot} is the total specific energy consumption, i.e., energy consumption per unit mass, and E_{freezing} and E_{pump} are the specific energy consumption for ice formation and seawater circulation, respectively. E_{freezing} depends on the latent heat of freezing, E_L , which is 333.5 kJ/kg. The coefficient of performance of the cooling system is estimated to be 10. E_{pump} can be obtained using the power (17 W) and efficiency (70%) of the pump. Based on these data, E_{tot} is approximately 9.26 kWh/ton (or 9.26 kWh/m³), demonstrating superior energy efficiency compared to freeze desalination methods involving multiple freezing steps and/or postprocessing (15–130 kWh/m³) [44,45].

Finally, it is important to note that the ice formed on the cold surface needs to be removed when it reaches a certain thickness, as the ice hinders heat transfer and makes the ice formation ineffective once it becomes sufficiently thick. Fortunately, the removal of ice is straightforward and does not take much time. Additionally, we refer to this method as a one-step strategy, meaning that potable water can be obtained through a single cycle of seawater freezing.

IV. CONCLUSIONS

In summary, we have probed the primary factors determining the ion rejection rate during the freezing of seawater and revealed that the competition of two characteristic timescales τ_{ion} and τ_{ice} governs the ion rejection rate. The ratio $\tau_{\text{ice}}/\tau_{\text{ion}}$

can be used as an index for improving the ion rejection rate. Based on this mechanism, we have proposed a desalination strategy to enhance the ion rejection rate by freezing flowing seawater. Both MD simulations and experiments have demonstrated that the ion rejection rate could be improved by enhancing the ion diffusivity through shear and controlling the ice growth rate via adjusting the temperatures of seawater and the cold surface. Under optimal conditions, one-step freeze desalination to obtain drinking water was achieved for both artificial and natural seawater.

ACKNOWLEDGMENTS

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DATA AVAILABILITY

Some of the data that support the findings of this article are openly available [34]. The data are available upon reasonable request from the authors but are not publicly available.

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