Molecular Dynamics Simulation of Brine Droplet Freezing: Fundamental Understanding of SWRO Brine Treatment

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Introduction

SWRO systems encounter a pressing challenge: the disposal of hypersaline concentrated brine generated during the desalination process. This brine, containing high levels of salts and other contaminants, poses significant environmental and economic concerns. The discharge of brine into oceans and other water bodies can lead to ecological imbalances, harming marine life and coastal ecosystems. Moreover, the large volumes of brine produced by SWRO plants necessitate cost-effective and sustainable treatment strategies to mitigate environmental impacts and adhere to regulatory standards.

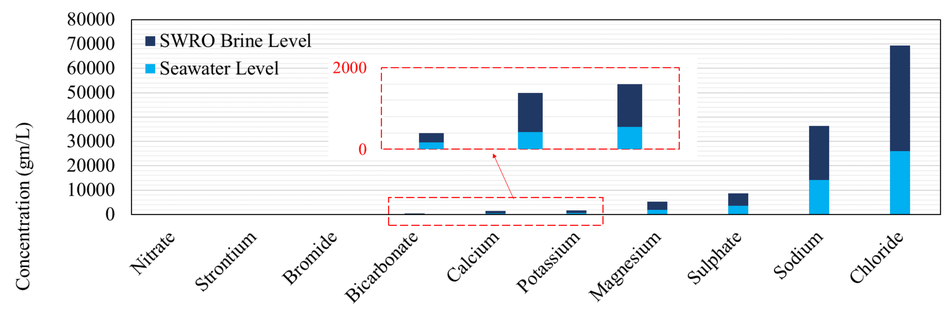

Figure: SWRO brine composition

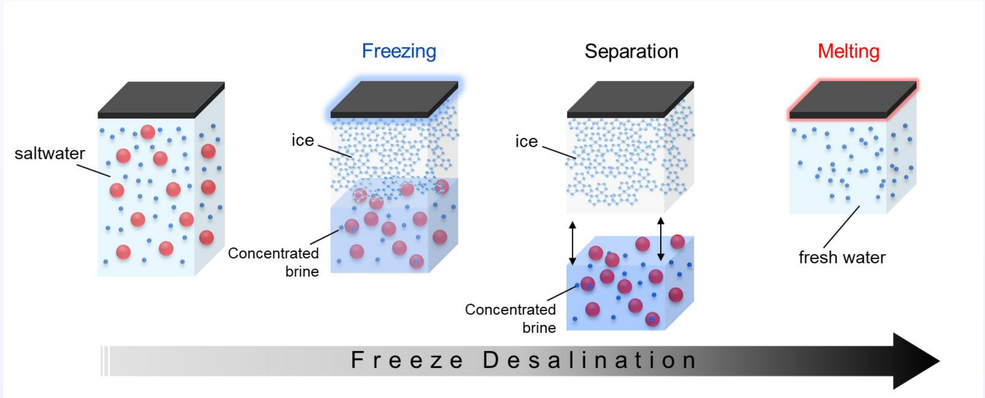

Figure: Freeze desalination process

To address these SWRO brine problems, we embark on a molecular dynamics (MD) simulation study focused on the freezing behavior of brine droplets. Freeze Desalination (FD) represents a potential solution for brine treatment as it enables the separation of water from dissolved salts and impurities. By gaining a fundamental understanding of brine droplet freezing, we aim to contribute to the development of efficient and environmentally friendly brine treatment technologies.

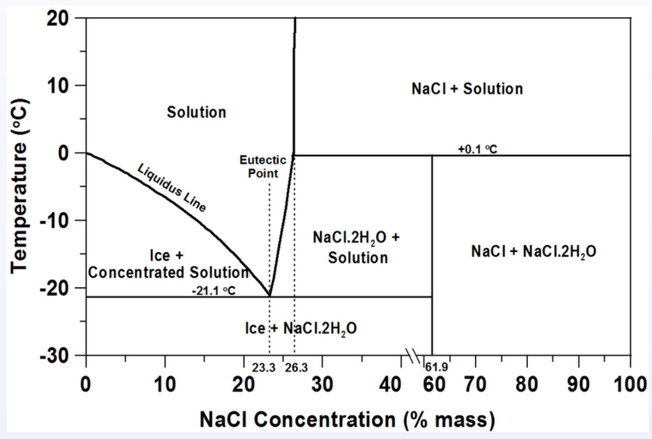

Figure: NaCl-water phase diagram

Results & Discussion

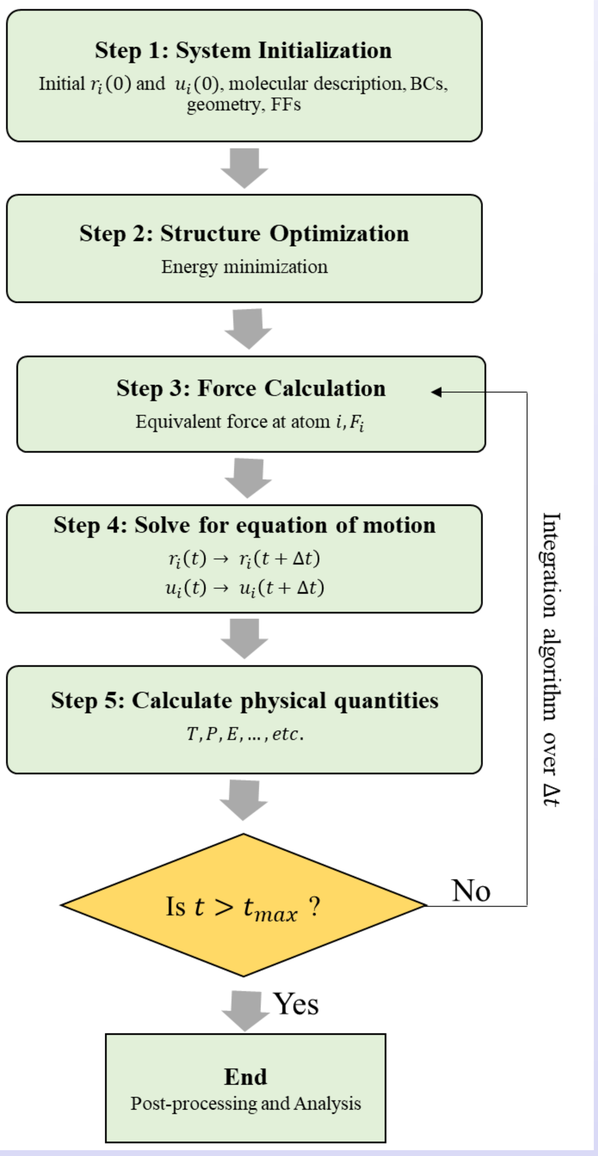

Figure: Molecular dynamics flow chart

Interatomic potential:

$$U(r) = \sum_{i}^{on} \sum_{j}^{a\ on\ b} \frac{k_C q_i q_j}{r_{ij}} + \frac{A}{r_{OO}^{12}} - \frac{B}{r_{OO}^{6}}$$

MD Methodology:

Temperature equilibration at 273 K (NVT) → Pressure equilibration at 1 bar (NPT) → Progressive freezing from 273K to 233K (NVT)

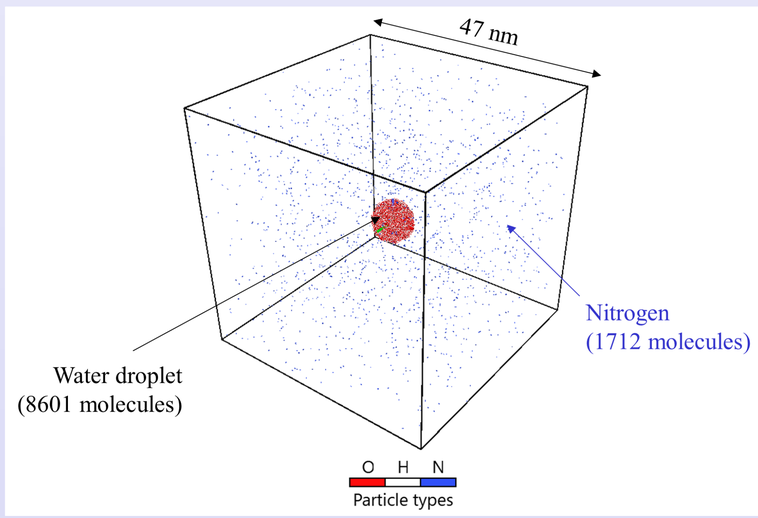

Figure: Initial state- equilibrated at 1 bar 273K

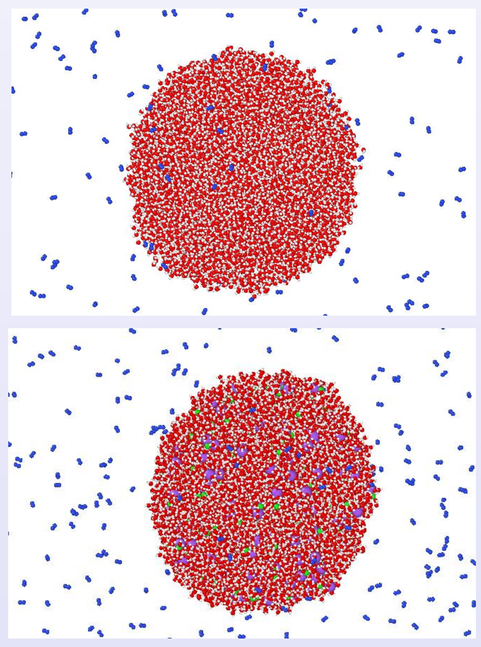

Figure: Top: pure water droplet. Bottom: 70 g/L brine droplet equilibrated at 1 bar 273K

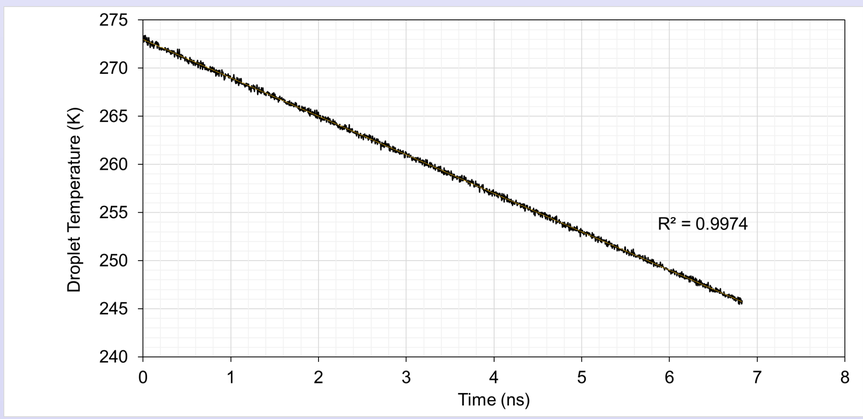

Figure: Time evolution of water temperature

Radial distribution function (RDF):

$$g(r) = \frac{V}{N^2} \sum_{i=1} \sum_{j \neq i} \delta(r - r_{ij})$$

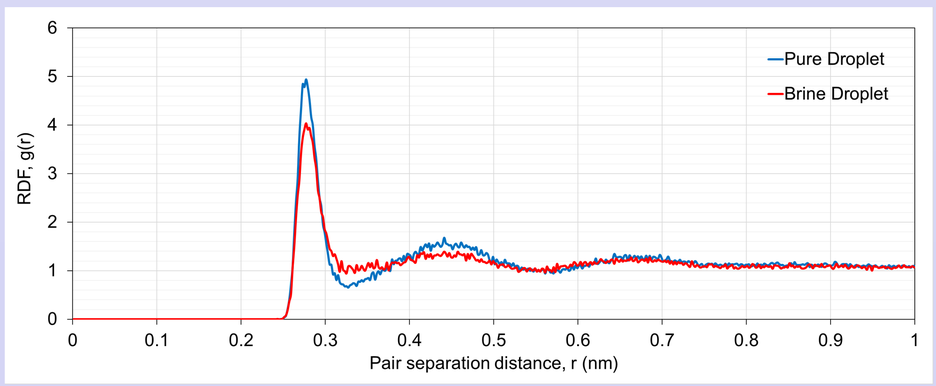

Figure: Pair-wise normalized RDF of O-O equilibrated pure water and brine droplets

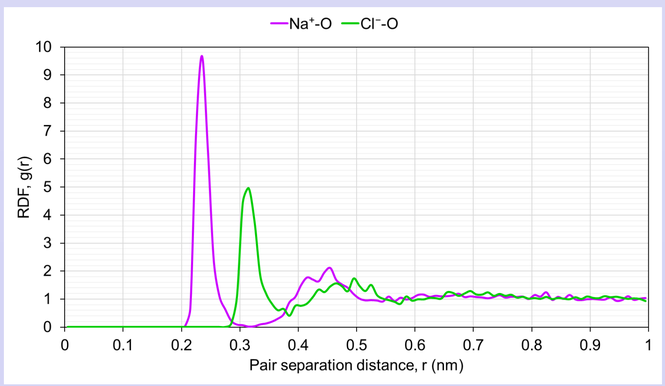

Figure: Normalized RDF of Na+ and Cl- ions with oxygen atoms of brine water droplet at 273 K

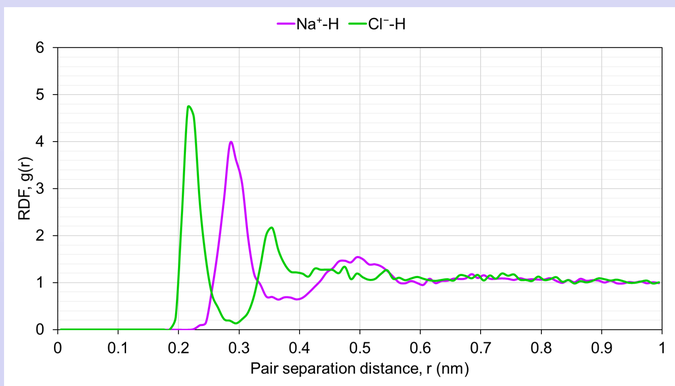

Figure: Normalized RDF of Na+ and Cl- ions with hydrogen atoms of brine water droplet at 273 K

Conclusions

- This study provides a fundamental understanding of SWRO brine treatment based on molecular dynamics simulation of brine/pure water droplet freezing.
- The findings reveal that the presence of dissolved NaCl in water droplets enhances ice nucleation, indicating the potential for effective salt removal during freezing.
- The presence of Na+ and Cl- ions disrupts the hydrogen bond network of water molecules, leading to changes in the arrangement and orientation of neighboring water molecules.
- RDF between Na-O indicates a stronger and more pronounced interaction between sodium ions and oxygen atoms, suggesting a higher affinity and binding propensity between these species.

The authors would like to express appreciation for the support of Khalifa University (ESIG-2023-013)