Water desalination using polyelectrolyte hydrogel. Gibbs ensemble modelling

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Recently polyelectrolyte hydrogels have been proposed as draw agents for reverse osmosis desalination techniques. Indeed, polyelectrolyte hydrogels have the ability to absorb a big amount of water across forward osmosis membrane as a result of their swelling pressure. The insoluble cross-linked network of the gel enables dewatering under the influence of stimuli (thermal and/or mechanical). On the other hand, the network structure of a polymer hydrogel from a thermodynamic perspective is already an osmotic membrane. So hydrogel microparticles may allow to completely avoid the osmotic membranes in forward osmosis and use microfiltration instead. By this article, we present our recent theoretical study of the use of polyelectrolyte hydrogel for water desalination. We modeled the thermodynamic equilibrium of coexistence of the gel and the aqueous salt solution in the so-called closed ensemble, in which the total amount of ions is assumed to be constant. We modeled the compression of the gel and the associated with that release of the solution. We have shown that the squeezed out solution has a little lower salinity than that the gel was equilibrated with. Also, we performed a set of simulations modeling the process of continuous decrease of water salinity up to freshwater concentrations.

Keywords: desalination, hydrogel, polyelectrolye, simulation

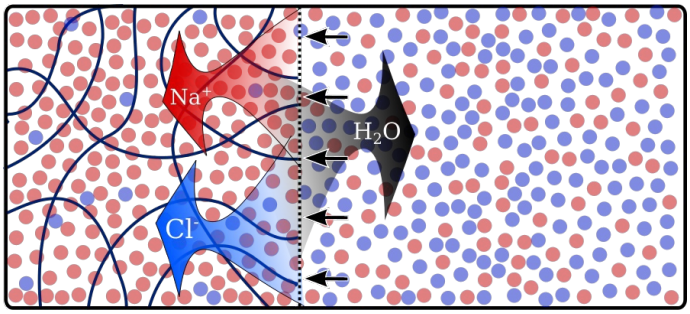

Figure 1. *The compression of the gel affects the salinity of the solution*

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References

[1] Rud, O., Borisov, O., Košovan, P. (**2018**). Thermodynamic model for a reversible desalination cycle using weak polyelectrolyte hydrogels. *Desalination*, 442, 32–43.
[2] Rud, O. V., Landsgesell, J., Holm, C., Košovan, P. (**2021**). Modeling of weak polyelectrolyte hydrogels under compression – Implications for water desalination. *Desalination*, 506, 114995.