DESALINATION USING POLYELECTROLYTE HYDROGELS

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When the gel is put into contact with aqueous salt solution, it absorbs a solution with the ion composition different from the original one. The absorbed solution can be easily squeezed out from the gel by means of sieve or microfiltration membrane. In our previous work we proposed a fully reversible desalination cycle made of compression and swelling steps, which can in principle work on ideal thermodynamic efficiency. In this work we simulate the desalination process using theoretical and coarse-grained models of gel and prove the concept by experiment.

We used Monte Carlo and molecular dynamics molecular simulations in the reaction ensemble to predict the degree of ionization of the weak polyelectrolyte hydrogel when it is put in contact with salt solution, and calculate the salt partitioning between the gel and bulk salt solution.

We constructed laboratory apparatus based on swelling and pressing cycles of the gel. First, we let the polyelectrolyte gel swell with salt solution of defined concentration. Then we press the gel and the liquid is released. Due to the ion exchange in polyelectrolyte hydrogel, this released liquid has lower salt concentration than the initial one. We measure the salinity of the solution before and after this procedure and we compare the results with theoretically obtained salt partitioning. We also measure the pressure applied on the gel and corresponding gel volume and compare these results with respective computational results.