Up-scaling reverse electrodialysis

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Supporting information

1. S1. Gibb´s Free Energy of Mixing

In this research, the molar flow rate has been used to calculate the Gibb's free energy of mixing. Therefore, the Gibb's free energy is expressed as a power, which for efficiency calculations can be combined with the power produced by the RED stack.

To calculate the Gibb's free energy available in both the inlet and outlet solutions, the following formula is used:

$$\Delta G = -\Delta S \cdot T \qquad \textit{Eq.S1}$$

Where ΔG is the available Gibb's free energy of mixing in (J/s) or (W), ΔS is the change in entropy when the solutions would be fully mixed (J/(s·K)) and T is the absolut temperature (K). The available entropy can be calculated as follows:

$$\Delta S = S_m - S_c - S_d \qquad \textit{Eq.S2}$$

S is the entropy of the individual solutions in (J/(s·K)), the subscripts m, c and d indicate fully mixed, concentrated and diluted solution, respectively. The entropy of each of these individual solutions can be calculated using the following expression:

$$S = -N_{total} \cdot R \cdot \sum_i (x_i \cdot \ln x_i) \qquad \textit{Eq.S3}$$

Where, N_{total} is the amount of moles in the solution expressed as a molar flowrate (mol/s), R is the universal gas constant (8.314 J/(mol·K)) and x is the mole fraction of species Na^+, Cl^- and H_20.

The total amount of moles in the solution is depending on the concentration of the solution. Based on experimental obtained data of the molality and density of sodium chloride solution at 298 K, a fit has been made of the molarity with the total amount of moles. Based on the molality of sodium chloride, the total molality (m_{total}) of solution can be calculated:

$$m_{total} = \frac{1000 - m_{NaCl} \cdot mm_{NaCl}}{mm_{H_2O}} + m_{NaCl} \qquad \textit{Eq.S4}$$

Where m_{NaCl} is the molality (mol/kg) of sodium chloride, mm_{NaCl} is the molar mass of sodium chloride (g/mol) and mm_{H2O} is the molar mass of water [g/mol]. The nominator calculates the mass of water in a solution of one kilogram (g/kg), by subtracting the mass of sodium chloride (g) from the mass of the solution (1000 g). Dividing by the molar mass of water gives the molality of water in the solution. Adding the molality of sodium chloride gives the total molarity of the solution [mol/kg].

$$M_{total} = m_{total} \cdot \rho \qquad \textit{Eq.S5}$$

Multiplying the total molality with the density (kg/l) gives the total amount of moles (M_{total}) per liter solution (mol/l). With the density of sodium chloride solutions related to the molality of sodium chloride, a plot can be made of the total amount of moles as a function of the molarity of sodium chloride. A 4th degree polynomial is fitted on this data (R^2 = 0.9998), to get a correlation between the molarity and the total amount of moles per liter of solution. This correlation is used to calculate the total amount of moles based on the measured concentration.

With the calculated total amount of moles per liter, also the molar fractions of each of the species can be calculated. By multiplying the total amount of moles per liter (mol/l) with the measured flow rate (l/s), the molar flow rate N_{total} can be calculated (mol/s) following;

$$N_{total} = M_{total} \cdot \Phi \qquad \textit{Eq.S6}$$

The molar flow rate of sodium and chloride can also be calculated using a formula analogue to the formula above. Only substituting the total amount of moles for the molarity of sodium and chloride. The molar flow rate of water can then be calculated by subtracting the molar flow rate of sodium and chloride from the total molar flow rate.

$$N_{H_2O} = N_{total} - N_{Na^+} - N_{Cl^-} \qquad \textit{Eq.S7}$$

The molar fractions x (-) of each of the species Na^+, Cl^- and H_20, can then be calculated as follows:

$$x_i = \frac{N_i}{N_{total}} \qquad \textit{Eq.S8}$$