Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supplementary information

Life cycle assessment of salinity gradient energy recovery by reverse electrodialysis in a seawater reverse osmosis desalination plant

Carolina Tristán, Marta Rumayor, Antonio Dominguez-Ramos, Marcos Fallanza, Raquel Ibáñez, Inmaculada Ortiz*

* Corresponding author: ortizi@unican.es
Department of Chemical and Biomolecular Engineering, University of Cantabria, Av. Los Castros 46, 39005 Santander, Spain.

S1 RED stack´s electrical parameters

Table S1 summarises the electric current and voltage values at the RED stack's electrodes, estimated with the RED's model [1], under optimum gross power conditions in Scenarios a and b.

Table S1 Electrical parameters of the commercial RED stacks under maximum power conditions in Scenarios a and b: Current density, current and terminal potential.

RED stack	Scenario	I_d (A m^{-2})	I (A)	E (V)
Lab-scale				
#1	a	40.8	0.82	1.5
#2				19.1
Product-scale				
#3	a	40.3	7.06	75.1
	b	36.0	6.31	67.4

I_d: Current density, current per effective membrane area per cell pair.
E: RED stack terminal voltage.

S2 Life cycle inventory: RED stack's components.

Table S2 Inventory for the production of a 1 m^2 CEM.

Description	Amount	Unit	Source/Comments
Materials			
Cationic resin	4.2×10^{-2}	kg	CH: cationic resin production (ecoinvent 3.5)[2]
Processes			
Extrusion, plastic film	4.2×10^{-2}	kg	RER: extrusion, plastic film (ecoinvent 3.5)[3]

CH: Switzerland; RER: Europe

Table S3 Inventory for the production of a 1 m^2 AEM.

Description	Amount	Unit	Source/Comments
Materials			
Anionic resin	4.2×10^{-2}	kg	CH: anionic resin production (ecoinvent 3.5)[4]
Processes			
Extrusion, plastic film	4.2×10^{-2}	kg	RER: extrusion, plastic film (ecoinvent 3.5)[3]

CH: Switzerland; RER: Europe

Table S4 Inventory for the production of a 1 kg spacer.

Description	Amount	Unit	Source/Comments
Materials			
PES	3.5×10^{-1}	kg	Baseline scenario GLO: polysulfone production, for membrane filtration production (ecoinvent 3.5)[5]
PP	3.5×10^{-1}	kg	Sensitivity analysis RER: polypropylene production, granulate (ecoinvent 3.5)[6]
Silicone	6.5×10^{-1}	kg	All scenarios RER: silicone product production (ecoinvent 3.5)[7]
Processes			
Injection moulding	1.0	kg	All scenarios RER: injection moulding (ecoinvent 3.5)[8]

RER: Europe; GLO: global

Table S5 Inventory for the production of a 1 m^2 electrode.

Description	Amount	Unit	Source/Comments
Materials			
Titanium	9.2	kg	GLO: titanium production, primary (ecoinvent 3.5)[9]
Ruthenium	7.0×10^{-3}	kg	ZA: ruthenium ts (GaBi)[10]
Iridium[a]	3.0×10^{-3}	kg	ZA: ruthenium ts (GaBi)[10]
Processes			
Metal working	9.2	kg	RER: metal working, average for metal product manufacturing (ecoinvent 3.5)[11]

RER: Europe; ZA: South Africa;

[a] Not available in any database assumed equal as Ruthenium. They are both platinum group metals (PGM). Hence, they have similar physical and chemical properties and tend to occur together in the same mineral deposits.

Table S6 Inventory for the production of a 1 kg endplate.

Description	Amount	Unit	Source/Comments
Materials			
PP	1.0	kg	RER: polypropylene production, granulate (ecoinvent 3.5)[6]
Processes			
Injection molding	1.0	kg	RER: injection moulding (ecoinvent 3.5)[8]

RER: Europe

S3 Maximum energy available for conversion: Gibbs free energy of mixing

The maximum specific energy –the energy per initial volume of the diluate solution– available for conversion in the RED system is given by thermodynamics as follows [12]:

$$\frac{\Delta G_{mix}}{V_{LC}} = \nu\, R\, T \left(C_{LC} \ln \frac{C_{LC}}{C_M} + \frac{1 - \Phi}{\Phi}\, C_{HC} \ln \frac{C_{HC}}{C_M} \right) \tag{1}$$

$$C_M = \Phi\, C_{LC} + (1 - \Phi)\, C_{HC} \tag{2}$$

$$\Phi = \frac{V_{LC}}{V_{HC} + V_{LC}} \tag{3}$$

where ΔG_{mix} is the change in the Gibbs free energy of mixing (J), R is the gas constant (8.314 J mol^{-1} K^{-1}), T is the absolute temperature (K), ν is the number of ions each salt molecule dissociates into (2 for NaCl aqueous solutions), V is the initial volume (m^3) and C the concentration of the concentrate (HC stands for high concentration) and the diluate (LC denote low concentration) aqueous solution before mixing completely (mol m^{-3}). The concentration of the mixed solution in thermodynamic equilibrium C_M (mol m^{-3}) is given by eq. (2). Φ, calculated using eq. (3), is the volumetric ratio of the diluate solution to the total volume of the system.

The Gibbs free energy expressed in terms of the functional unit in the SWRO-RED's system assessment, i.e. 1.0 m^3 of freshwater produced by the SWRO plant, is defined considering 1.4 m^3 per cubic meter of freshwater of concentrate and diluate stream is fed to the SGE-RED plant in Scenario 1 and 0.7 $m^3\ m^{-3}$ in Scenario 2. Regarding RED's operational scenarios, in Scenario a ($v_{HC} = v_{LC} = 3$ cm s^{-1}) the volumetric ratio is equal to 2, whereas in Scenario b ($v_{HC} = 0.6$ cm s^{-1} and $v_{LC} = 1.2$ cm s^{-1}) $\Phi = 0.65$.

Supplementary references

1 R. Ortiz-Imedio, L. Gomez-Coma, M. Fallanza, A. Ortiz, R. Ibañez and I. Ortiz, *Desalination*, 2019, **457**, 8–21.

2 A. Primas, *cationic resin production, CH*, ecoinvent database version 3.5.

3 R. Hischier, *extrusion, plastic film, RER*, ecoinvent database version 3.5.

4 A. Primas, *anionic resin production, CH*, ecoinvent database version 3.5.

5 M. Dussault, *polysulfone production, for membrane filtration production, GLO*, ecoinvent database version 3.5.

6 R. Hischier, *polypropylene production, granulate, RER*, ecoinvent database version 3.5.

7 N. Jungbluth, *silicone product production, RER*, ecoinvent database version 3.5.

8 R. Hischier, *injection moulding, RER*, ecoinvent database version 3.5.

9 M. Dussault, *titanium production, primary, GLO*, ecoinvent database version 3.5.

10 Process data set: Ruthenium; mining, transport, separation: mechanical separation, smelting, magnetic separation, chemical refining; production mix, at plant; 12.37 g/cm3, 101.07 g/mol (en), http://gabi-documentation-2019.gabi-software.com/xml-data/processes/1080b451-f8d5-4404-bdce-eb5e1127a4db.xml, (accessed 12 December 2019).

11 R. Steiner, *metal working, average for metal product manufacturing, RER*, ecoinvent database version 3.5.

12 N. Y. Yip and M. Elimelech, *Environ. Sci. Technol.*, 2012, **46**, 5230–5239.