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Optimal Simulation of an Electrodialysis Reactor for the Desalination and Regeneration of Multi-Ionic Wastewater

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ABSTRACT

The objective of the present work is to optimize the simulation of an electrodialysis reactor for the desalination and regeneration of multi-ionic wastewater with high salt contents and conductivities, within the framework in the Sustainable Development Goal 6 (clean water and sanitation) and remarking the Electrodialysis (ED) as a highly energy-efficient and sustainable technology. The mathematical modelling has been carried out by using a semiempirical model that involves an algebraic system of differential equations, including mass and charge balances (taking into account the ions present in the wastewater: Na^+, Ca^{2+}, Mg^{2+}, Cl^-, SO_4^{2-}, and HCO_3^-), and the total electrodialysis stack voltage considering ohmic drops (in the dilute and concentrate compartments), the potential of membrane in each cell pair, and the electrode potentials. In the simulation process, different theoretical and experimental parameters are necessary such as number of cells, membrane working areas, efficiency, diffusion coefficients, molar conductivity at infinite dilution, etc.The experimental parameters have been obtained initially with a specially designed batch reactor printed with 3D technology, to imitate the hydrodynamics and the behavior of the industrial final reactor used. Additionally, to increase the accuracy of the simulation results, same parameters such as the resistance of the membranes (r_m), the transport numbers and the mass transfer coefficient (k_m) can be optimized by using a metaheuristic derivative-free optimizer, specifically a proprietary version of Particle Swarm Optimization (PSO) implemented in MatLab®.The results obtained yield a satisfactory reproduction of the observed experimental behavior, analyzing the evolution over time of the intensity, conductivity, and concentration of the concentrated and diluted currents, respectively. In addition, the evolution of the different contributions of the stack voltage and the membrane resistances are shown, in order to confirm the coherence of the results obtained.

Keywords: Wastewater, Modelling, Membranes, Process Design, Particle Swarm Optimization

INTRODUCTION

Wastewater Treatment Plants (WWTP) constantly receive water from industrial process that can present salinity levels from 1 wt % up to values similar to seawater (3.5 wt %) [1], including also domestic uses such as detergents or water softening processes [2], or waste derived from constructions and transportation activities [3]. This problem also occurs in coastal areas due to marine intrusion. On the other hand, waste water with high salinity degree released into the environment may cause damage by contaminating soils, surfaces, groundwater, or any water body with which they come into contact [4] There is evidence that it affects ecosystem processes by altering the decomposition of organic matter, biomass production, and reducing biodiversity [5].

Thus, in order to reuse any treated water as regenerated water for instance in urban cleaning tasks, garden watering, agricultural uses, etc., regulations must be followed to mitigate their impact. According to the FAO

(Food and Agriculture Organization), for conductivities higher than 3 mS/cm water must be under several restrictions and controls, between 0.7 and 3 mS/cm those restrictions are lower, and with electrical conductivities under 0.7 mS/cm there are any restriction [6].

In this context, electrodialysis (ED) appears as a very energy efficient and sustainable wastewater desalination treatment for those type of salinized water compared to other processes [7, 8]. Additionally, ED process is driven by an electric field and neutral species present in wastewater that may be associated with beneficial elements for plants, such as urea or organic nitrogen, are almost not altered by the process [9, 10, 11].

The ED process is conducted in a membrane stack (electrodialysis reactor) where two kind of exchange membranes: N+1 cation exchange membranes (CEM) and N anion exchange membranes (AEM) are alternatively located generating a series of N+1 compartment between two different consecutives membranes. A potential difference is applied across the membrane stack using two electrodes placed at the sides of it. The feed solution flows through the membranes, generating a dilute channel and a concentrate channel as a result of ion migration. The cathode is negatively charged, so cations migrate toward it by passing through the CEMs, but they cannot pass through the AEMs. Likewise, the positively charged anode attracts anions, which migrate toward it under the same selective transport mechanism [12].

To scale up an ED process without the need to perform many experimental tests at each stage of the scaling procedure, it is absolutely necessary to have a mathematical model to simulate the main characteristics of the process.

However, electrochemical processes are particularly complex to model due to their multiscale and multiphysics nature. In such processes, phenomena of different origins coexist, requiring the simultaneous consideration of thermodynamic and kinetic aspects together with the distribution of electric potential and ionic transport in the solution [13, 14]. In this sense, there are ED mathematical models capable of predicting the desalination rate and the current density [15] depending on the water composition, as well as the electrical energy consumption of the process [16].

In the case of the model presented by Ortiz et al. [16], parameters such as membrane resistance (Rm) and the potential difference between electrodes are introduced and assumed to be constant. The potential difference depends on the overpotential (μ), which also depends on the current density (j), the exchange current density (j0), and the Tafel slope (b). All of these parameters, including membrane resistance, vary depending on the type of electrolyte, its concentration and the hydrodynamics of the reactor. Treating these parameters as constants leads to a loss of accuracy in the results, for that, it is needed to determinate these parameters under specific operating conditions of each reactor or experiment.

Thus, this work presents a new modified and optimized version of the model developed by Ortiz [16, 17] further extended to a multi-ionic wastewater system. As case study, a Wastewater Treatment Plant in Santa Pola (Spanish east cost) has been selected where, even with effective tertiary treatment, the final water has conductivities between 4 and 7 mS/cm that hinder its reuse for purposes such as irrigation. Although the regulations considered these waters have high conductivity, for a desalination process they are relative low salinities.

MATHEMATICAL MODEL

The proposed model is structured into two blocks: one that defines mass transfer through mass balances equations, and another that is responsible for providing all the electrical data via the calculation of the total potential.

Mass balance

It is necessary to know the ionic composition of the solution, both in the reactor (concentrated and diluted compartments) and in the concentrated and diluted product tanks. To this end, the corresponding mass balances over the time are established. Assuming that the electrodialysis reactor and the reservoirs or tanks follow a perfectly mixed reactor model and that the compartments are equivalent, the following mass balances can be established for each cation (i) present in the concentrate and dilute compartments of the electrodialyzer, respectively:

$$NV_k \frac{dC_{conc,i}}{dt} = Q_{conc}C^0_{conc,i} - Q_{conc}C_{conc,i} + \\ +NA(J_i^{cat} - J_i^{an}) \qquad (1)$$

$$NV_k \frac{dC_{dil,i}}{dt} = Q_{dil}C^0_{dil,i} - Q_{dil}C_{dil,i} - NA(J_i^{cat} - J_i^{an}) \quad (2)$$

where N is the number of cells, V_k is the volume of the compartments (m^3), t is time (s), $C^0_{dil,\,i}$ and $C^0_{conc,\,i}$ are the initial concentrations or inlet concentrations of the ion i in the dilute and concentrate compartments, respectively, and $C_{dil,\,i}$ and $C_{conc,\,i}$ are the corresponding outlet concentrations (mol/m^3). Q_{dil} and Q_{conc} are the flow rates of the dilute and concentrate compartments (m^3/s), A is the electrode area (m^2), and $J_{cat,\,i}$ and $J_{an,\,i}$ are the fluxes of cations and anions of species i through the cation-exchange and anion-exchange membranes, respectively (mol/m^2).

For anions, the expression would be equivalent, but with the opposite sign for the ionic fluxes:

$$NV_k \frac{dC_{conc,i}}{dt} = Q_{conc}C^0_{conc,i} - Q_{conc}C_{conc,i} +$$

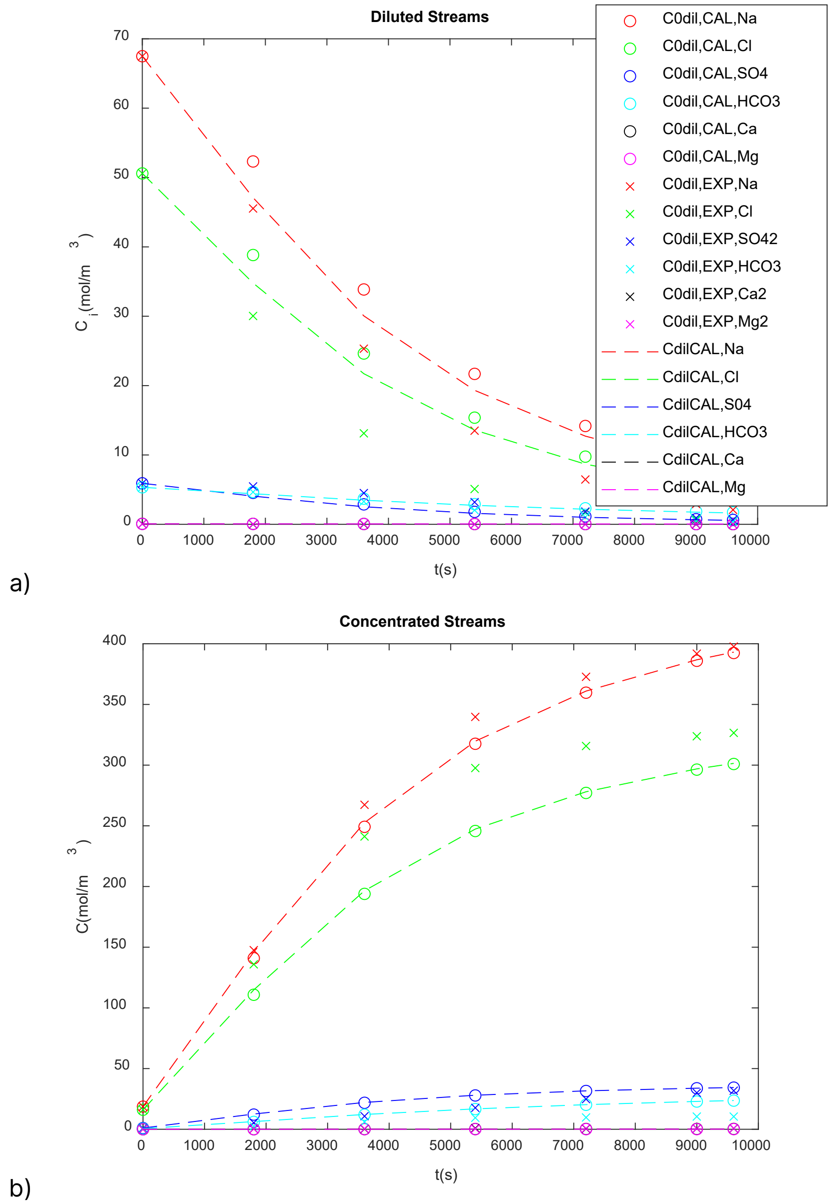

Figure 1. Composition profiles obtained for a sample with a initial conductivity of 6 mS/cm.

$$+NA(J_i^{an} - J_i^{cat}) \quad (3)$$

$$NV_k \frac{dC_{dil,i}}{dt} = Q_{dil}C^0_{dil,i} - Q_{dil}C_{dil,i} - NA(J_i^{an} - J_i^{cat}) \quad (4)$$

The ionic fluxes for ions i are given by the sum of the migration and diffusion components:

$$J_i^{cat} = \sum J_{i,mig}^{cat} + \sum J_{i,dif}^{cat} = \frac{\phi t_i^{cat}}{z_i F} j - D_i^{cat} \frac{C^{w,cat}_{conc,i} - C^{w,cat}_{dil,i}}{l_m^{cat}} \quad (5)$$

$$J_i^{an} = \sum J_{i,mig}^{an} + \sum J_{i,dif}^{an} = \frac{\phi t_i^{an}}{z_i F} j - D_i^{an} \frac{C^{w,an}_{conc,i} - C^{w,an}_{dil,i}}{l_m^{an}} \quad (6)$$

where ϕ is the experimental current efficiency, t^{cat}_i and t^{an}_i are the transport numbers of ion *i* in the cation-exchange and anion-exchange membranes, respectively, z_i is the ionic charge, *F* is Faraday's constant (C/mol), *j* is the current density (A/m^2), D^{cat}_i and D^{an}_i are the diffusion coefficients of ion *i* in the cation-exchange and anion-exchange membranes, respectively (m^2/s), $C^{w,\ cat}_{conc,\ i}$ and $C^{w,\ cat}_{dil,\ i}$ are the concentrations of ion *i* at the surface of the cation-exchange membrane for the concentrate and dilute compartments, respectively (mol/m^3), $C^{w,\ an}_{conc,\ i}$ and $C^{w,\ an}_{dil,\ i}$ are the analogous concentrations for the anion-exchange membrane, and l^{cat}_m and l^{an}_m are the thicknesses of the cation-exchange and anion-exchange membranes (m). This expression is equivalent for cations and anions, the only difference lies in the values of the corresponding parameters.

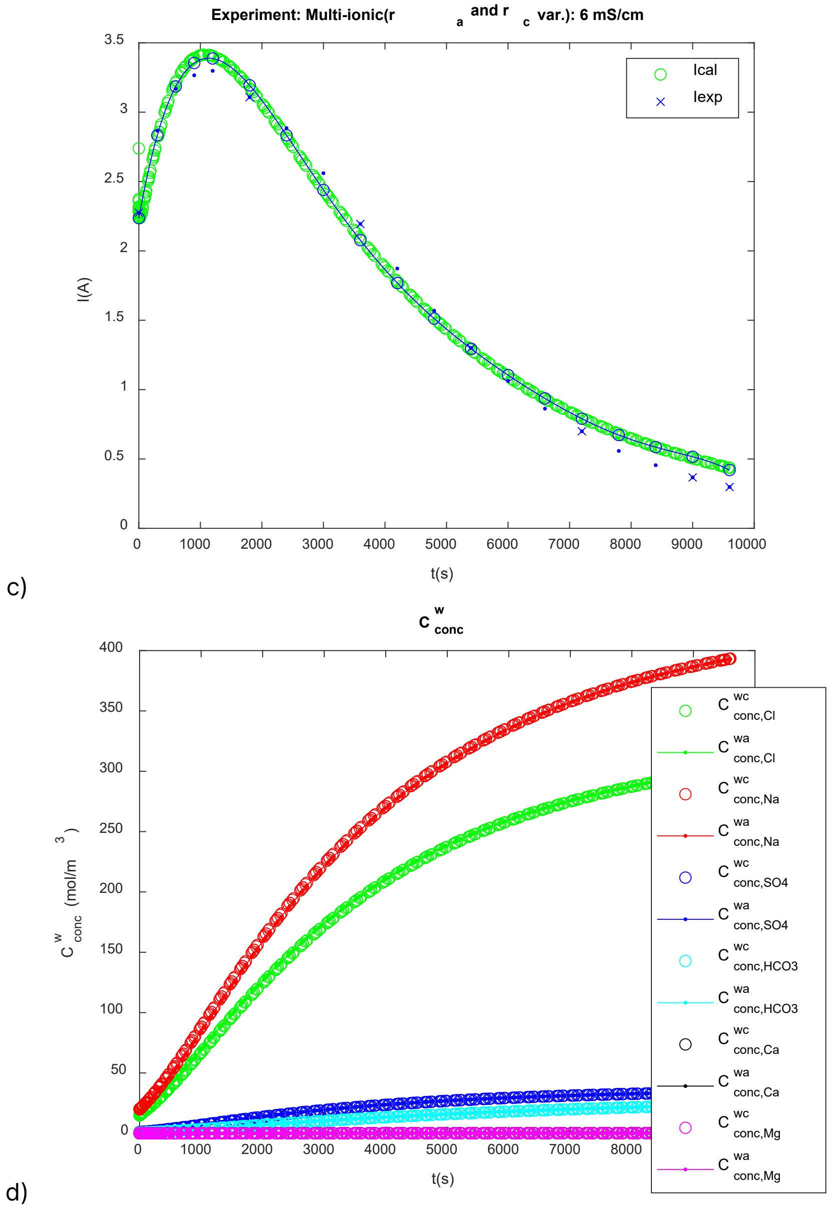

Figure 1(cont.). Intensity, membrane compositionc and potential profiles obtained for a sample with an initial conductivity of 6 mS/cm.

The corresponding concentrations in the membranes can be calculated as follows:

$$C^{wa}_{dil,i} = C_{dil,i} - \frac{\phi j}{|z_i| F k_m}\left(t^{ma}_{i,contra\ or\ co} t^{a}_{contra\ or\ co} - t^{dil}_i\right) \quad (7)$$

$$C^{wa}_{conc,i} = C_{conc,i} + \frac{\phi j}{|z_i| F k_m}\left(t^{ma}_{i,contra\ or\ co} t^{a}_{contra\ or\ co} - t^{conc}_i\right) \quad (8)$$

$$C^{wc}_{dil,i} = C_{dil,i} - \frac{\phi j}{|z_i| F k_m}\left(t^{mc}_{i,contra\ or\ co} t^{c}_{contra\ or\ co} - t^{dil}_i\right) \quad (9)$$

$$C^{wc}_{conc,i} = C_{conc,i} + \frac{\phi j}{|z_i| F k_m}\left(t^{mc}_{i,contra\ or\ co} t^{c}_{contra\ or\ co} - t^{conc}_i\right) \quad (10)$$

where the value of the transport numbers $t^{c\ or\ a}{}_{contra}$ is 0.999, with $t^{c\ or\ a}{}_{co} = 1 - t^{c\ or\ a}{}_{contra}$.

In the case of transport numbers, the general equations are:

$$t_i^{conc\ or\ dil} = \frac{|z_i| u_i\ C_i^{conc\ or\ dil}}{\sum_i |z_i| u_i\ C_i^{conc\ or\ dil}} \quad (11)$$

$$t^{ma\ or\ mc}_{app,i,contra\ or\ co} = \frac{|z_i| y_i^{contra\ or\ co} C^{wa\ or\ wc}_{conc\ or\ dil,i}}{\sum_i |z_i| y_i^{contra\ or\ co} C^{wa\ or\ wc}_{conc\ or\ dil,i}} \quad (12)$$

where y_i is a term related to ionic mobility in the membranes (if it were in solution, the notation would be u_i), and C_i is the ion concentration in the concentrate or dilute solution. This concentration may vary depending on whether it is in the membrane or in the solution [18].

The mass balances for the concentrate and dilute

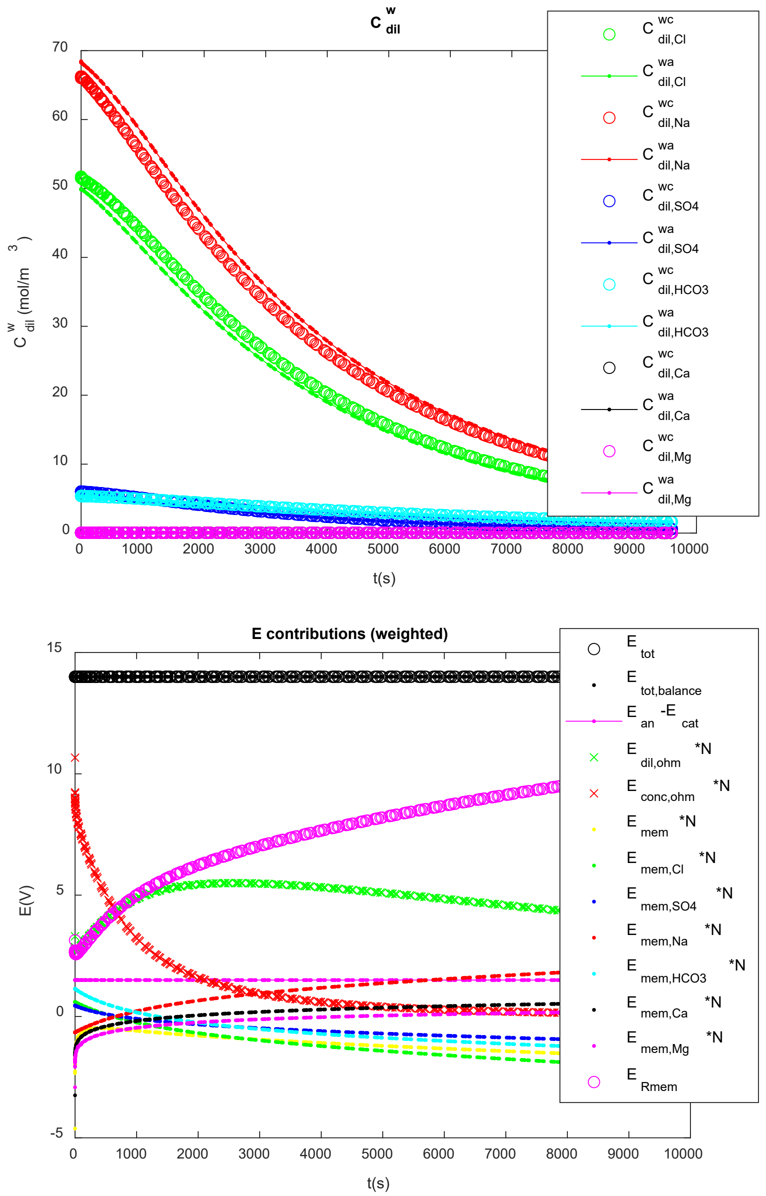

Figure 1(cont.). Intensity, membrane compositionc and potential profiles obtained for a sample with an initial conductivity of 6 mS/cm.

tanks can be expressed as follows:

$$\frac{C^0_{conc,i}V^T_{conc}}{dt} = Q_{conc}\left(C_{conc,i} - C^0_{conc,i}\right) \tag{13}$$

$$\frac{C^0_{dil,i}V^T_{dil}}{dt} = Q_{dil}\left(C_{dil,i} - C^0_{dil,i}\right) \tag{14}$$

where V^T_{dil} and V^T_{conc} are the volumes of the dilute and concentrate tanks, respectively (m³).

Electrical potential difference in the electrodialysis stack

The current intensity (I) that flows through the electrodialyzer is related to the applied electrical potential. The total electrical potential drop for an electrodialyzer can be obtained as follows:

$$\varphi_{tot} = (\varphi_{an} - \varphi_{cat}) + N\left(\varphi^{dil}_{ohm} + \varphi^{conc}_{ohm} + \varphi_{mem}\right) + + R_{mem} \cdot \frac{I}{A} \tag{15}$$

$$\text{with:}\ \varphi^{dil}_{ohm} = \frac{L\,I}{\Lambda_{dil}\,A};\ \varphi^{\mathrm{conc}}_{\mathrm{ohm}} = \frac{\mathrm{L\,I}}{\Lambda_{\mathrm{conc}}\,\mathrm{A}} \tag{16}$$

$$\varphi_{mem} = \sum_i^{ions} \frac{RT}{z_i F} \ln\left(\frac{C^{wc}_{conc,i}}{C^{wc}_{dil,i}}\frac{C^{wa}_{conc,i}}{C^{wa}_{dil,i}}\right) \tag{17}$$

where φ_{an} and φ_{cat} are the anode and cathode potentials, respectively (V), φ^{dil}_{ohm} is the ohmic drop in the dilute compartment (V), φ^{conc}_{ohm} is the ohmic drop in the

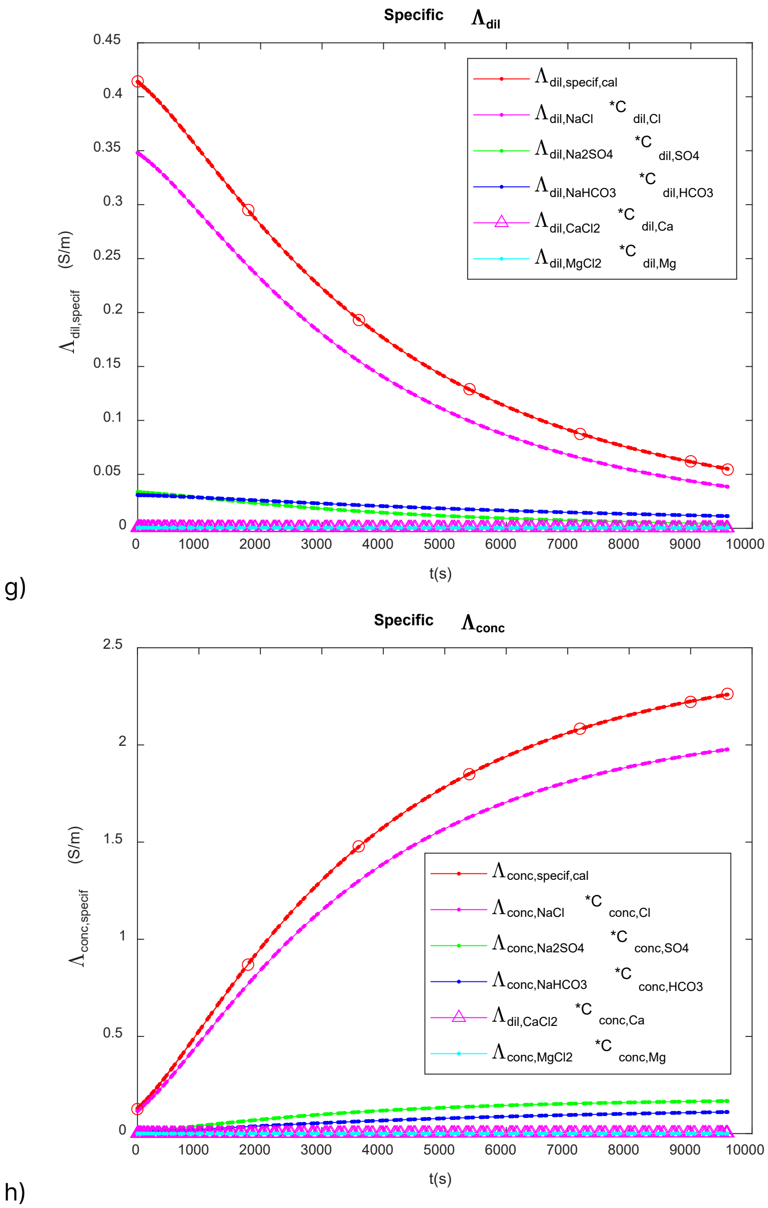

Figure 1.(cont.). Intensity, membrane compositionc and potential profiles obtained for a sample with an initial conductivity of 6 mS/cm.

concentrate compartment (V), φ_{mem} is the total membrane potential at each unit cell (V) due to the presence of all the ions present in the water, considering ideal mixture, Λ_{dil} and Λ_{conc} are the total specific conductivities (S/m) of the concentrated or diluted solution taking into account all the individual salts present in the solution (Table 1), respectively, *L* is the membrane gap, and $R_{mem} \cdot I/A$ is the term associated with the total resistance contributed by all the membranes (N+1 CEM, and N AEM), which has been obtained by correlation the experimental intensity values (obtained in A 3D printed reactor [18]) with the conductivity of the diluted solution [eq. 18] by using the proposed model and a proprietary version of Particle Swarm Optimization (PSO) implemented in MatLab®, that has been successfully used for the optimal design of different unit operations [19].

$$R_{mem} = Nra + (N+1)rc \tag{18}$$

with: $ra = 58.04\Lambda_{dil}^{-1.66}$; $rc = 120.46\Lambda_{dil}^{-1.42}$ and $\Lambda_{dil} = \sum_s^{Salts} \Lambda_s \, C_{dil,s}$.

RESULTS

To solve the obtained algebraic system of differential equations, additional equations and parameters are

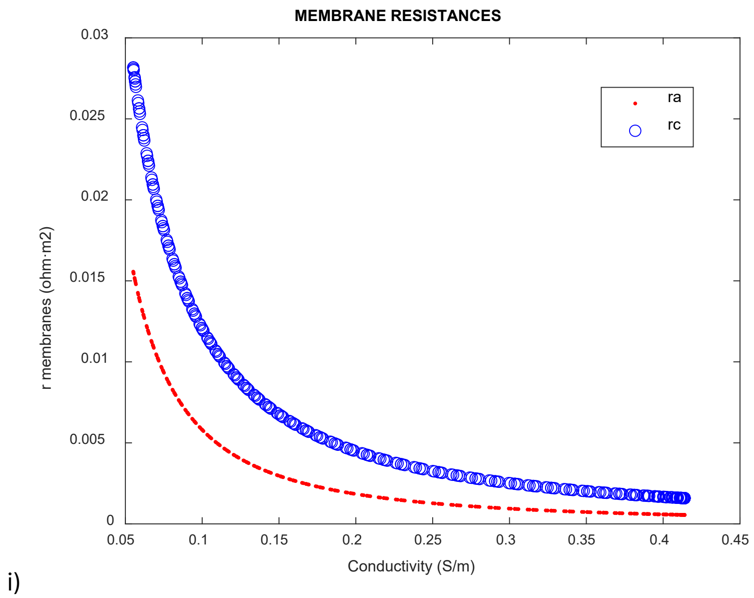

Figure 1.(cont.). Specific conductivities and membrane resistences profiles obtained for a sample with an initial conductivity of 6 mS/cm.

required (Tables 1-3), such as the characteristic parameter y, related to ion mobility in the membrane, the ion mobility in the solution u; the Falkenhagen equation for the molar conductivity of each salt of the solution (and its parameters B_0, B_1 and B_2), among others. Figures 1 show the main profiles obtained for the simulation of a case study with an initial conductivity of 6 mS/cm (concentration of the concentrated and diluted streams, intensity and, the different contributions of the stack voltage). As can be seen, the proposed model satisfactorily represents the experimental trends, analyzing the different evolutions over time, especially in the initial section up to approximately 3000 s, when a conductivity of less than 2.5 mS/cm is reached, which is the limit allowed for safe reuse of regenerated water in irrigation. However, future work should incorporate e.g. the non-ideality of the liquid mixture by using the corresponding activity coefficients in the calculation of the membrane potential.

Table 1. Parameters for Falkenhagen equation, with U= 4 Å. $\Lambda_{salt} = \Lambda_0 \text{-} (\mathrm{B}_1\Lambda_0 + \mathrm{B}_2)\frac{C_{salt}^{0.5}}{1+\mathrm{B}_0 U C_{salt}^{0.5}}$.

Salt	$\Lambda_0 \cdot 10^4$	B_0	B_1	$B_2 \cdot 10^4$
NaCl	126.45	0.358	0.240	60.32
Na_2SO_4	129.80	1.010	2.269	120.65
$NaHCO_3$	117.94	0.510	0.544	109.98
$CaCl_2$	135.77	1.336	1.986	120.65
$MgCl_2$	129.34	1.356	1.973	120.64

Table 2. Values of the parameters used in the model.

Parameter	Value	Parameter	Value
A (m^2)	0.02	Q (m^3/s)	5.56 10^{-5}
L_{an} (m)	$1.5 \cdot 10^{-4}$	φ_{tot} (V)	14
L_{cat} (m)	$1.6 \cdot 10^{-4}$	φ_{an} - φ_{cat} (V)	1.5
L (m)	0.001	Φ(exp.)	0.87
N	10	k_m	0.0005
V_k ($m^{3)}$	$1.96 \cdot 10^{-5}$	F (C/mol)	96485
V^T_{conc} (m^3)	0.004	R (J(mol K)	8.31
V^T_{dil} (m^3)	0.025	T (K)	298.15

Table 3. Data for streams without pressure change. Molar ionic conductivities and limiting diffusion coefficients in water at 298 K [20]. Characteristic parameter (*y*) related to ion mobility in ion-exchange membranes [17], and ionic mobilities (*u*) in water at 298 K [21, 22].

Ion	$\lambda \cdot 10^{-4}$ (m^2S/mol)	$D \cdot 10^{-9}$ (m^2/mol)	*y* *contra / co*	$u \cdot 10^{-8}$ (m^2/sV)
Ca^{2+}	118.94	1.584	0.3/0.1	6.17
Mg^{2+}	106	1.412	0.1/0.03	5.50
Na^+	50.08	1.334	0.7/0.1	5.19
Cl^-	76.31	2.032	1/0.1	7.90
HCO^{-3}	44.5	1.185	0.5/0.3	4.61
$SO2^{-4}$	160	2.13	1/0.1	8.29

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