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A 2-D model of electrodialysis stacks including the effects of membrane deformation

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ABSTRACT

Membrane-based processes have gained a relevant role in many engineering applications. Much effort has been devoted to thoroughly understand the fundamental phenomena behind them. However, membrane deformation has been taken into consideration only recently, although much evidence has shown its impacts in many applications. This work presents a novel 2-D, multi-scale, semi-empirical process model able to predict the behaviour and the performance of Electrodialysis (ED) systems in cross-flow configurations in the presence and absence of local membrane deformations. The model exploits the results and the simulation approaches of previous fluid-structure investigations performed by the authors. Low-scale numerical simulations are coupled with a high-scale model to predict the redistribution of channel height, flow rate, friction coefficient and Sherwood number in ED stacks caused by local membrane deformations. Finally, salt and water fluxes, mass balances and electrochemical quantities are computed to assess the performances of cross-flow ED stacks. Different test cases have been simulated for the desalination of seawater by two-stage ED. Interestingly, membrane deformation is found to reduce, albeit slightly, the energy consumption. More pronounced effects are expected if thinner or less stiff membranes are used.

Keywords

Ion exchange membrane, profiled membrane, transmembrane pressure, membrane deflection, desalination

1. Introduction

In the last 60 years, membrane-based separation processes have been established as promising technologies in a broad range of applications, e.g. potable water production from seawater and brackish water [1,2], wastewater treatment [3,4], food engineering [5], energy production from non-conventional sources [6,7] and biomedical applications [8]. The key components of these processes are the membranes, which allow the permeation of a chemical species to be controlled [9]. In recent years, much effort has been devoted to improve membrane properties, allowing membrane-based processes to become increasingly competitive in all their fields of application.

In this context, many studies have been focused on the better understanding of the fundamental physical, thermo-dynamical and electrochemical phenomena characterizing the functioning of many membrane processes. However, only recently the mechanical behaviour of membranes has been taken into account. From a mechanical point of view, membranes are very thin elements, whose mechanical response can be studied as that of thin plates, having no bending stiffness, undergoing large deflections. Membranes are mainly made of polymeric materials, which have low mechanical properties in terms of Young modulus and yield stress. This makes the membrane prone to deform when subjected to even small loads. Moreover, due to their small elastic region (low yield stress), the membranes' deformation may likely be irreversible.

In membrane-based processes, a pressure difference between two solutions, flowing in two fluid channels separated by a membrane, may arise. This pressure difference is referred to as transmembrane pressure, TMP. Experimental evidence has shown the significant effects of TMP in many membrane technologies, as briefly reviewed here below.

A water flux decline was detected in Reverse Osmosis (RO) seawater treatment working at 6900 kPa [10]. The authors attributed this phenomenon also to membrane deformation, which causes membranes to be squeezed through the permeate spacer thus leading to a reduction of the membrane active area.

In Forward Osmosis, the effects of membrane draw channel contraction caused by membrane deformation have been investigated experimentally and numerically in a system equipped with a dot geometry spacer in the draw channel [11]. Membrane deformation was not simulated, but ellipsoidal-shaped membrane deformation was assumed to occur through the

dot-spacer supports. The membrane was found to stretch from 0 to 67.7% of the nominal channel height under a TMP between 0 and 145 kPa. Shear rates along the membrane surface and fluid flow regime in deformed channels were also studied by performing CFD simulations showing complex effects of membrane deformation on them.

In Assisted Forward Osmosis, two different permeate spacer types were investigated to address membrane deformation issues [12]: (1) a commercial 1.2 mm diamond-type mesh spacer and (2) a finer porous frit support. Hydraulic pressure impact was investigated in a pressure range between 200 and 600 kPa. Using the frit support, pure water permeability and salt permeability were almost constant in all the pressure range investigated, while they both increased when the system was equipped with the commercial spacer. Digital images of the membranes, taken after tests at 600 kPa, clearly showed that this behaviour was mainly related to membrane deformation.

Membrane deformation phenomena have also been largely reported in Pressure Retarded Osmosis (PRO) [13–21]. The most appropriate PRO setup, to be used for high pressure operations, was investigated in [16]. Results showed that, when a critical limit pressure of 5520 kPa was exceeded, the water flux drastically increased, indicating excessive membrane deformation. In addition, results suggested that the use of small opening spacers, although leading to higher shadow effects, guarantees a better mechanical stability of the membranes avoiding their collapse. Similar findings were also shown in [17,18] working at lower pressures of 2000-2500 kPa.

In pressure-retarded membrane distillation, the performance of a system was investigated in a pressure range between 0 and 1000 kPa using tricot-type spacers with small openings (< 0.35 mm) [22]. No power output and a considerable water vapour flux reduction were detected working at a pressure higher than 200 kPa. Concave and convex deformed shapes of the membranes were optically observed. Further analysis also showed that coarse net-type spacers (openings > 0.35 mm) caused much more severe membrane deformation leading to membrane damage even at pressure values lower than 200 kPa.

In permeate gap membrane distillation with simultaneous fresh water and energy production, the performance of a unit using two different membranes was investigated adopting assembled package layers of diamond shape mesh plastic spacer and stainless steel woven mesh with 0.154 mm aperture [23]. The membranes tested could only withstand pressures lower than 200 kPa and the system produced a much lower power density than that theoretically predicted.

In many other membrane-based processes, membrane deformation issues have also been reported, e.g. liquid-to-air membrane energy exchangers [24] and proton exchange membranes for fuel cells [25,26].

This short literature review clearly shows that membrane deformation phenomena may have a significant impact on the performances of membrane-based processes.

In electro-membrane processes, such as Electrodialysis (ED) and Reverse Electrodialysis (RED), trans-membrane pressures are usually smaller than those considered in the above studies, and are mainly caused by the frictional losses occurring in the fluids flowing on the opposite sides of each membrane. However, many practical (R)ED working conditions could lead to non-negligible TMP values. Novel ED stack configurations have been investigated in [27] in order to reduce the energy demand of ED stacks for brackish water desalination. Lab-scale experiments performed using parallel- and counter- flow ED stacks showed that counter-flow configuration allowed a 10-30% reduction of the energy consumption with respect to that of the parallel-flow arrangement. TMP values lower than 30 kPa were measured during the experiments. In RED applications, the power generation performance of a bench-scale RED stack (40 m²) has been investigated in [28]. The RED stack was fed using natural seawater RO brine and sewage-treated water (STW). Results showed that at a given STW flow rate, the RED stack was able to produce higher gross power densities as the RO brine flow rates increased. The authors did not give an estimation of the TMP values in the stack; however, they attributed the increase of the gross power densities to a possible contraction of the STW channel, which caused a reduction of the Ohmic stack resistance, when the RO brine solution was pumped at higher flow rate than that of the STW solution. Many other practical (R)ED working conditions where non-negligible TMP values could arise have been also identified by the present authors in [29–31]. In this context, the present work aims at presenting a comprehensive process model tool, which can be used for the design of an ED stack (and of a RED stack, just making a few adjustments) taking into account also membrane deformation phenomena.

1.1 Modelling of Electrodialysis systems

Electrodialysis is an electrochemical process in which an external electric potential is used as the driving force [32]. ED has been established to be a promising technology for drinking water production through the desalination of brackish water or even seawater sources. In an ED stack, a couple of anion and cation exchange membranes (*AEMs* and *CEMs*) are alternatively piled and separated by means of net-spacers or membrane built-in profiles (profiled membranes), which define the fluid channels where solutions flow. Profiled membranes have

recently attracted the attention of both academics and industrials as a promising alternative to classical flat membranes and net-spacers. Although profiled membrane have not been commercialized yet, many experimental and modelling works have shown their beneficial effects in ED and RED processes [33]. In ED, when an external potential is applied to the system, an ionic current is induced, leading ions to migrate from one solution to the adjacent ones through the membranes. In the process, ion concentration increases in one solution (concentrate solution, *CON*), while it decreases in the other one (diluate solution, *DIL*). A couple of an *AEM* and a *CEM* together with one *CON* and one *DIL* channel form the so called “cell pair”, which represents the fundamental repetitive unit of an ED stack. ED stacks can be made from a few, e.g. 10-50 at lab scale, to hundreds of cell pairs, e.g. 500 at industrial scale. Electrode compartments are placed at the two external sides of a stack to allow the conversion of the external electric current into ion fluxes in the stack via redox reactions. A schematic representation of an ED stack is shown in Figure 1.

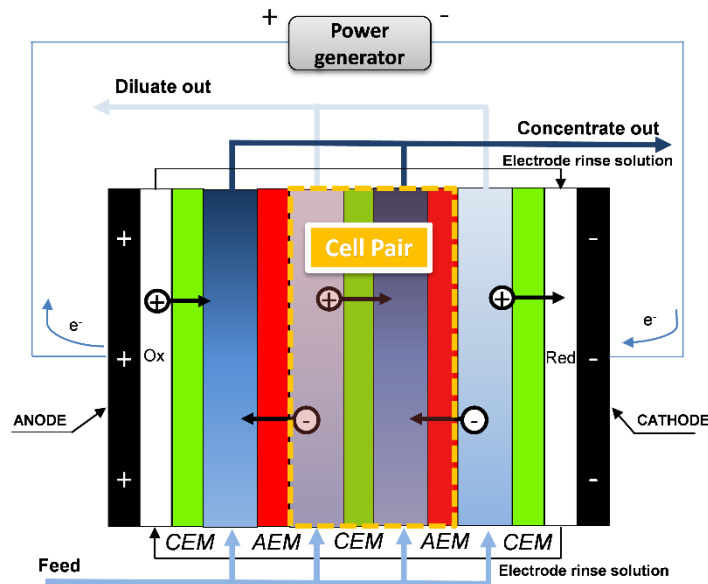


Figure 1. Schematic representation of an Electrodialysis stack. Adapted from [2].

Many numerical and theoretical models have been developed to study and design of ED systems, including very simplified and advanced theoretical models [2]. In particular, simplified models are based on many assumptions and usually employ a lumped parameters approach. They have been proposed for a preliminary design of specific ED stacks relying on experimentally determined parameters [34,35].

Conversely, advanced models give a more accurate description of the functioning of a system by taking into account spatial effects and non-ideal phenomena. They can be divided into two sub-categories: theoretical and semi-empirical models.

Theoretical models aim at describing ED, but also RED, phenomena based on rigorous theories by solving a complex set of equations [36–40] (i.e. the Nernst-Planck equation, or even the more complex Stefan-Maxwell equations). However, they require a large amount of computational power and several thermodynamic and electrochemical parameters which are difficult to be found, and their application is usually limited to the simulation of a small-scale portion of a real stack.

Semi-empirical models, instead, aim at describing a (R)ED stack at its whole scale, taking spatial effects into account, but have to use empirical information for membrane properties (e.g. salt permeability, ohmic resistance, osmotic permeability, etc.) and for local hydraulic and mass transfer characteristics of the channels (permeability, limiting current density, Sherwood number) [41–44]. As an alternative to empirical input, these models can use correlation obtained from the small-scale simulation of specific phenomena, e.g. by means of Computational Fluid Dynamics [45–49] (multi-scale approach).

As far as ED/RED modelling is concerned, with a few exceptions [50,51], most of the proposed semi-empirical models are one-dimensional. A 2-D approach allows the study of more stack configurations (such as the cross-flow one) besides the classical parallel- and counter-flow arrangements. The present work introduces a novel 2-D semi-empirical, multi-scale model to address the performance of ED stacks in cross-flow configurations with and without membrane deformation phenomena.

In regard to the membrane deformation treatment, a multi-scale modelling approach is exploited. In previous work [29,30] coupled mechanical and fluid dynamics simulations were conducted using a Finite Element (FE) / Finite Volume (FV) method as implemented in the commercial software Ansys Mechanical® and Ansys CFX®. At this stage, the study was conducted at the low scale of a periodic repetitive unit of a fluid channel bounded by two membranes (unit cell), shown in Figure 2. In particular, results were obtained for Overlapped Crossed Filament (OCF) profiled membranes having a pitch P (distance between two consecutive filaments) of 1.6 mm and a channel height H of 0.2 mm, leading to a P/H ratio equal to 8.

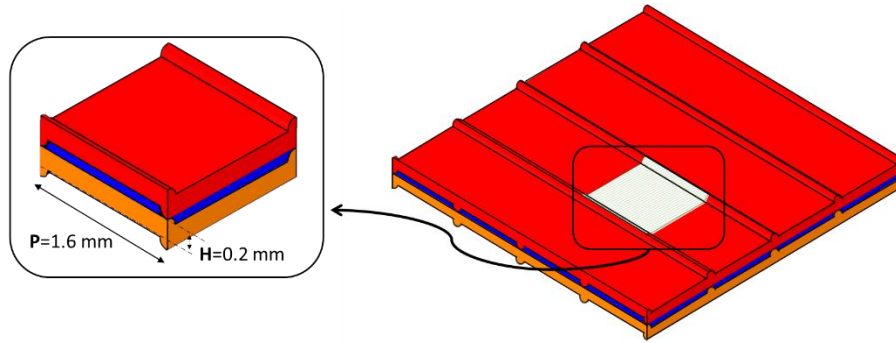


Figure 2. Sketch of a channel bounded by two Overlapped Crossed Filament (OCF) profiled membranes with $P/H = 8$. The detail of a unit cell is illustrated on the left. Adapted from [29].

A one-way fluid-structure approach was employed to study the effect of membrane deformation due to the action of an imposed TMP (simulated as the difference between external and internal pressure) varying between -40 kPa and 40 kPa. Results were the fluid dynamics and mass transport properties of the corresponding deformed fluid channel for each deformed configuration simulated.

Based on these results, a full two-way fluid-structure interaction model was developed in [31] to assess membrane deformation effects on the flow re-distribution at the higher scale of a whole cell pair. This was carried out by developing an original closed-loop iterative algorithm, which takes into account the local change of the channel's hydraulic permeability as a function of the local transmembrane pressure (TMP), which, in its turn, varies with the local flow rate and eventually with the channel's permeability. No effects on mass transfer rates were considered in [31].

The present work adds the last piece of the puzzle by integrating the approach in [31] with a 2-D modelling of the main physical and electrochemical phenomena of the ED process, including deformation effects on mass transfer. The result is a comprehensive modelling tool, which encloses most of the previous modelling approaches to assess the performance of ED stacks in terms of energy requirements and product quality either in the presence or in the absence of membrane deformation. In this work, the model was employed for the analysis of ED units equipped with the above-mentioned OCF profiled membranes with $P/H=8$ (Figure 2) [29,31], which have been developed in the framework of the REvived water project [52]. The simulations have been performed both neglecting and including deformation and its effects. As OCF profiled membranes suitable for assembling large ED units were not available, the ED model was validated, in the absence of membrane deformation, against experimental results collected with a large-scale conventional ED stack equipped with flat membranes and woven spacers.

2. Modelling

The present model simulates transport and electrochemical phenomena occurring in ED stacks, computing the distribution of the main variables in a cell pair (assumed to be representative of the whole stack) and assessing the process performance, e.g. the energy consumption. As mentioned before, to describe the effect of membrane deformation a multi-scale approach is employed. Specifically:

- (i) At the lowest scale, FE-FV simulations provide channel deformation, friction coefficients and Sherwood numbers as functions of the transmembrane pressure (TMP) in the fluid channels.
- (ii) At the higher scale of the cell pair, the equations expressing mass balances, transport phenomena, solutions and membrane properties are solved, taking into account (if required) the local flow redistribution in the channels due to local membrane deformations.
- (iii) Finally, at the highest scale of the stack, the ED performance is predicted for any number of cell pairs, taking into account the resistance of the electrode compartments.

The main model assumptions are:

1. Each channel is simulated as a porous isotropic medium with locally variable porosity ε and hydraulic permeability K ;
2. binary electrolyte solutions (specifically, NaCl) are considered;
3. steady-state regime is assumed;
4. all cell pairs behave in the same way;
5. empirical expressions for the limiting current density are not used;
6. parasitic currents are not considered;
7. manifolds are not included in the model.

In regard to assumption 5, it should be observed that, in the absence of specific correlations for the limiting current density, the model allows the current density to grow until either concentration at the diluate-membrane interfaces becomes zero. It is known that this condition (diffusion limited current density) is never actually attained in real ED, and that empirical correlations are required to predict more realistic limiting current density values.

2.1 Basic equations of the ED model

In a two-dimensional approach, the distribution of all variables is evaluated over the length (L) and width (W) of a channel. Considering a cross-flow arrangement, as shown in Figure 3, the concentrate solution (CON) may be assumed to flow (on average) from left to right, parallel

to the x -axis, while the dilute solution (DIL) may be assumed to flow (on average) from top to bottom, parallel to the y -axis.

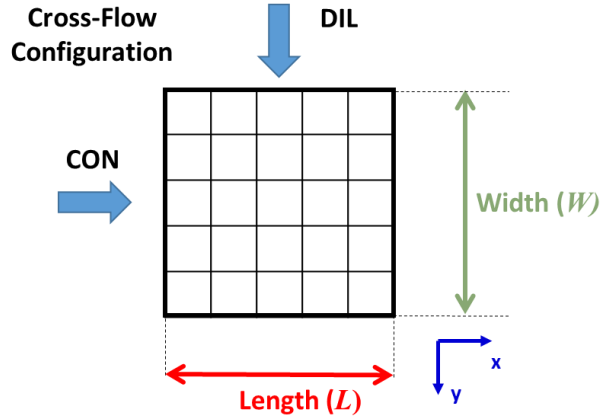


Figure 3. Computational domain of the developed model for a 2-D cross-flow configuration.

Under the assumption of constant density solutions, differential mass balances for the salt and water species in the concentrate and diluate channels can be written as:

$$\frac{\partial U_x^{CON}(x, y) C^{CON}(x, y)}{\partial x} + \frac{\partial U_y^{CON}(x, y) C^{CON}(x, y)}{\partial y} = + \frac{1}{H} N_{SALT}^{TOT}(x, y); \quad (1)$$

$$\frac{\partial U_x^{CON}(x, y)}{\partial x} + \frac{\partial U_y^{CON}(x, y)}{\partial y} = + \frac{1}{H} J_w^{TOT}(x, y); \quad (2)$$

$$\frac{\partial U_x^{DIL}(x, y) C^{DIL}(x, y)}{\partial x} + \frac{\partial U_y^{DIL}(x, y) C^{DIL}(x, y)}{\partial y} = - \frac{1}{H} N_{SALT}^{TOT}(x, y); \quad (3)$$

$$\frac{\partial U_x^{DIL}(x, y)}{\partial x} + \frac{\partial U_y^{DIL}(x, y)}{\partial y} = - \frac{1}{H} J_w^{TOT}(x, y); \quad (4)$$

where:

- $U_x^{SOL}(x, y)$ and $U_y^{SOL}(x, y)$ are the local superficial velocities (in m/s) along x and y in the channel SOL , which can be either CON (concentrate channel) or DIL (dilute channel). They represent averages over the nominal (undeformed) channel thickness H ;
- $C^{SOL}(x, y)$ is the local salt concentration (also averaged over the channel thickness H) in the SOL (CON or DIL) channel, in mol/m³;
- $N_{SALT}^{TOT}(x, y)$ is the local transmembrane molar salt flux (a detailed description can be found in the Appendix A), summed over both membranes, taken in absolute value and expressed in mol/(m² s).
- $J_w^{TOT}(x, y)$ is the local transmembrane volumetric water flux (a detailed description can be found in the Appendix A), summed over both membranes, taken in absolute value and expressed in m³/(m² s), i.e. in m/s.

In the ED system, a potential voltage drop V is applied by a power supply to the electrodes in order to obtain the desired desalination degree of the dilute (DIL) feed solution. In the model, the potential voltage drop V is assumed to be constant (i.e. independent of x and y) at the electrodes. At the stack level, the number of cell pairs and the electrode compartments have to be taken into account in order to simulate the whole electrical circuit.

The local current density $i_c(x, y)$ can be computed by using the Kirchhoff's second law:

$$i_c(x, y) = \frac{V - \eta(x, y)N_{cp}}{R_{blank} + R_{TOT}(x, y)N_{cp}} \quad (5)$$

where N_{cp} is the total number of cell pairs, $\eta(x, y)$ is the non-Ohmic voltage drop in a cell-pair, R_{blank} is the electric resistance of the electrode compartments and $R_{TOT}(x, y)$ is the total electrical resistance of a cell pair. More details are reported in the Appendix A.

The total power consumption of an ED process P_{el} can be expressed as:

$$P_{el} = VI + P_{pump} \quad (6)$$

where I is the overall current calculated as the integral of the current density (i_c) over the active area of the membrane, while P_{pump} is the total pumping power. This latter quantity is quite cumbersome to compute in the presence of trans-membrane fluxes (due to osmotic and electro-osmotic effects) which make the flow rate of either solution differ from inlet to outlet, especially in the present, two-dimensional domain. A crude approximation is

$$P_{pump} = \frac{\Delta p^{CON} Q_{TOT,av}^{CON}}{\eta_{pump}^{CON}} + \frac{\Delta p^{DIL} Q_{TOT,av}^{DIL}}{\eta_{pump}^{DIL}} \quad (7)$$

in which Δp^{SOL} is the inlet-to-outlet distributed pressure drop associated with either solution (singular losses in the manifolds and in the piping are not included in the present model), while $Q_{TOT,av}^{SOL}$ is the flow rate in either channel, averaged between inlet and outlet and summed up over the N_{cp} cell pairs (assumed identical in the present model).

Finally, two other important parameters can be introduced to quantify the efficiency of an ED stack [47]:

- The energy consumption per unit volume of product E_{spec} :

$$E_{spec} = \frac{P_{el}}{Q_{TOT,OUTLET}^{DIL}} \quad (8)$$

where $Q_{TOT,OUTLET}^{DIL}$ is the overall diluate outlet flowrate from all cell pairs.

- The apparent product flux J_p :

$$J_p = \frac{Q_{TOT,OUTLET}^{DIL}}{2LWN_{cp}} \quad (9)$$

which can be useful in order to calculate the total membrane area required to obtain a certain flow rate of desalinated water.

For the sake of clarity, Table 1 summarizes all the constants employed for membrane and channels features. The correlations used for the physical and transport properties of NaCl solutions are reported in the Appendix B.

Table 1. Values of the fixed quantities employed in the model. Many of these parameters were taken from [53].

Quantity	Value	Unit
Temperature	25	°C
Nominal channel height H (<i>DIL</i> and <i>CON</i>)	200×10^{-6} [29,31]	m
Undeformed channel porosity ε (<i>DIL</i> and <i>CON</i>)	0.9 [29,31]	-
Membrane thickness (<i>AEM</i> and <i>CEM</i>)	120×10^{-6} [29,31]	m
Salt diffusivity, D_{Salt}^{IEM} (<i>AEM</i> and <i>CEM</i>)	$4E^{-12}$ [53]	m ² /s
<i>AEM</i> permselectivity, α_{AEM} (constant)	0.969 [53]	-
<i>CEM</i> permselectivity, α_{CEM} (constant)	0.975 [53]	-
Water permeability in the <i>AEM</i> , $L_{p,AEM}$	6.29 [53]	ml/m ² h bar
Water permeability in the <i>CEM</i> , $L_{p,CEM}$	7.79 [53]	ml/m ² h bar
Membrane resistance (<i>AEM</i> and <i>CEM</i>), R^{IEM}	See Eq.(A.9)	Ω m ²
Blank resistance, R_{blank}	2×10^{-3} [53]	Ω m ²

2.2 Model validation

The electrochemical part of the model was validated by comparison with experimental results provided by the REDstack (Sneek, The Netherlands) company for an ED square cross-flow stack of 0.44 m side with 288 cell pairs. The stack was equipped with woven spacers (Deukum GmbH, Germany) having $P/H=2$, a volume porosity of 0.712, a nominal channel height H of 260 μ m and 90° angled filaments. Fujifilm Type 10 Ion Exchange Membranes, (FUJIFILM Manufacturing Europe B.V., Tilburg, The Netherlands), whose properties are used in the simulations, were adopted. Both salt solutions were fed at a superficial velocity (U^{sol}) of 1 cm/s and at an initial solution concentration of 513.34 mol/m³ (30 g/l). The applied voltage V was made to vary between 0 and ~65 V. The temperature was measured to increase from 18 to 22°C during the experiments due to the passage of electric current, and these changes (which

affect solution and membrane properties and also the electromotive force) were explicitly included in the simulations. The empirical correlations for the solution and the membrane resistances are reported in the Appendix B. The voltage data provided do not take electrode losses into account, thus null blank resistance (R_{blank}) was set in the simulation. In order to account for the different spacer configuration with respect to the OCF profiled membranes discussed so far, the Sherwood number and friction factor dependence on the fluid velocity appropriate to channels filled with woven spacers, as obtained in [46], were implemented in the model.

The test conditions (woven spacers of small P/H , moderate flow velocities) are such that no significant membrane/channel deformation is expected to have occurred. Therefore, no membrane deformation was taken into account in the simulations. Comparison between the experimental and the numerical current-voltage and outlet concentration-current curves are shown in Figure 4.

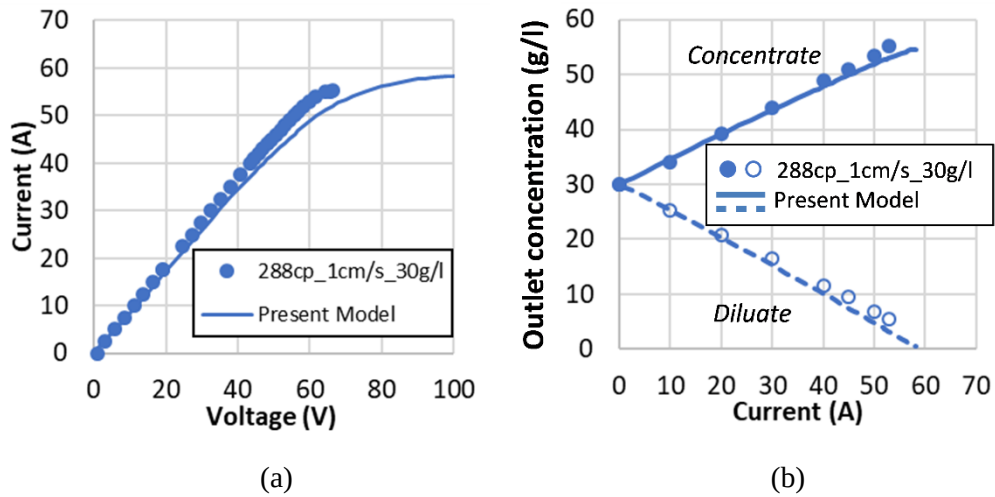


Figure 4. Experimental results (symbols) and predictions by the present model (lines) for an ED cross-flow stack. (a) current-voltage curves; (b) outlet concentration-current curves. In graph (b), solid lines and symbols represent the concentrate outlet concentration, while dashed lines and hollow symbols represent the diluate outlet concentrations.

From Figure 4, it can be observed that the model predictions are in very good agreement with the experiments, both in terms of electric variables and of outlet concentrations, though approaching limiting current conditions generates a slight deviation of model results from experimental data.

3 Model results

3.1 No membrane deformation

To investigate the process performances of cross-flow ED stacks for seawater desalination (inlet solutions concentrations of 513.34 mol/m^3 , i.e. 30 g/l) depending on the size and the operating conditions, a first parametrical study was carried out neglecting deformation effects. As discussed in Section 2, limiting current density conditions are not well reproduced by the model. Therefore, in order to avoid simulating working conditions where limiting current density may arise, it was decided to simulate two consecutive ED stacks in series with the same features, except the inlet solutions concentrations. Specifically, the first stack was fed by salt solutions of initial concentration of 513.34 mol/m^3 (30 g/l). In this stack, a first desalination step took place reducing the concentration of one of the two streams to 85.5 mol/m^3 (5 g/l). The outlet solutions were then directly pumped into the second stack, which completed the desalination process by reducing the diluate solution concentration to 8.55 mol/m^3 (0.5 g/l). The number of cell pairs was fixed at 400 for each case and each stack. All results were obtained for OCF profiled membranes with $P/H=8$, see Figure 2, having an equivalent undeformed channel height h^{sol} of $180 \mu\text{m}$.

As far as the parametrical study is concerned, the length (L) and the width (W) of the stacks were made to vary between 0.1 and 0.6 m . Moreover, the inlet velocity of the concentrate, v_c , and dilute, v_d , solutions in the first stack were made to vary between 1 and 5 cm/s . The total voltage drop V at the electrodes of each stack yielding an outlet diluate concentration of 85.5 mol/m^3 for the first stack and 8.55 mol/m^3 for the second stack was assessed in each simulated case. All other quantities were kept fixed at the values listed in Table 1. Eight different cases were investigated, as listed in Table 2.

Table 2. Eight ED stack configurations investigated in 2-stage desalination.

<i>Cases</i>	#1	#2	#3	#4	#5	#6	#7	#8
<i>Quantities</i>								
$L \text{ [m]}$	0.2	0.4	0.6	0.6	0.6	0.6	0.6	0.6
$W \text{ [m]}$	0.6	0.6	0.6	0.35	0.15	0.6	0.6	0.6
$v_c \text{ [cm/s]}$	5	5	5	5	5	3	1	1
$v_d \text{ [cm/s]}$	1	1	1	1	1	1	1	3

Results in terms of specific energy consumption E_{spec} , apparent flux J_p , overall electric current of the first I_1 and second I_2 stack, voltage drop at the first V_1 and second V_2 stack, diluate Ohmic resistance of the first R_1^{DIL} and second R_2^{CON} stack and diluate flow rate at the outlet of the second stack, $Q_{TOT,OUTLET,2}^{DIL}$, are reported in

Table 3. Ohmic resistances of the *CON* channels are not reported since they are small and play a minor role in the overall voltage drop.

It should be noted that Eqs. (8) and (9) were modified as follows to address the performances of the two consecutives stacks.

- Specific energy consumption:

$$E_{spec}^{TOT} = \frac{P_{el,1} + P_{el,2}}{Q_{TOT,OUTLET,2}^{DIL}} \quad (10)$$

where $P_{el,1}$ and $P_{el,2}$ are the electric power of the first and second stack, respectively, while $Q_{TOT,OUTLET,2}^{DIL}$ refers to the overall diluate outlet flowrate of the second stack.

- Apparent product flux J_p^{TOT} :

$$J_p^{TOT} = \frac{Q_{TOT,OUTLET,2}^{DIL}}{A^{TOT}} \quad (11)$$

where A^{TOT} is the total membrane area calculated as $A^{TOT} = N_{stacks} 2N_{cp} LW$, where N_{stacks} is the total number of stacks used in the desalination process, i.e. 2.

Table 3. Main results obtained for eight cross-flow 2-stage test cases in the absence of deformation.

Cases	#1	#2	#3	#4	#5	#6	#7	#8
Quantities								
L [m]	0.2	0.4	0.6	0.6	0.6	0.6	0.6	0.6
W [m]	0.6	0.6	0.6	0.35	0.15	0.6	0.6	0.6
v_c [cm/s]	5	5	5	5	5	3	1	1
v_d [cm/s]	1	1	1	1	1	1	1	3
E_{spec}^{TOT} [kWh/m ³]	2.27	2.30	2.33	3.03	5.67	2.39	2.66	5.03
J_p^{TOT} [l/m ² h]	2.66	2.66	2.65	4.64	11.0	2.63	2.57	8.01
I_1 [A]	17.8	35.7	53.5	53.0	52.7	53.6	53.9	160
I_2 [A]	3.45	7.03	10.6	9.92	9.41	10.7	11.2	30.2
V_1 [V]	48.7	49.1	49.4	71.8	148	50.1	52.8	121

V_2 [V]	83.9	84.9	85.9	92.3	128	88.1	96.6	130
R_1^{DIL} [Ω]	0.114	0.114	0.113	0.106	0.102	0.113	0.112	0.103
R_2^{DIL} [Ω]	1.455	1.447	1.440	1.174	0.944	1.450	1.482	1.042
$Q_{TOT,OUTLET,2}^{DIL}$ [l min ⁻¹]	8.52	17.0	25.4	26.0	26.4	25.3	24.7	76.9

Results suggest that the stack length (L , which is the length of the concentrate channel and the width of the diluate channel) does not significantly affect the process performances (E_{spec}^{TOT} and J_p^{TOT}). In fact, E_{spec}^{TOT} and J_p^{TOT} are almost the same for cases #1-3.

The stack width (W , which is the width of the concentrate channel and the length of the diluate channel) considerably influences the process parameters, see results of cases #3, 4 and 5. Specifically, E_{spec}^{TOT} and J_p^{TOT} are found to increase as the stack width W decreases. This can be explained considering that the stack width decreases from case #3 to case #5, while the diluate flow rate is almost constant at each case. This yields a reduction of the residence time of the dilute solution in the stack, which, in turn, causes an increase of the external potential to guarantee the same diluate outlet target concentration.

The specific energy consumption and the apparent flux change slightly when the concentrate solution velocity v_c varies, see cases #3 and 6-7. Conversely, E_{spec}^{TOT} and J_p^{TOT} are significantly affected by the diluate velocity v_d (cases #7-8). The effects of v_d exhibit an opposite trend with respect to that of the stack width W . Specifically, an increase of the diluate velocity causes an increase of both E_{spec}^{TOT} and J_p^{TOT} . This trend can be attributed to the change of the diluate solution residence time, as discussed for the influence of W .

It should be also noted that the comparison of cases #3 through 5, differing only in the stack width, illustrates the potential economic usefulness of a parametrical study such as the one conducted here. Although the reduction of the stack width yields an increase of the specific energy consumption, the desalination process requires less membrane area while demanding less concentrate flow rate and providing comparable outlet diluate flow rates (higher water recovery). This aspect may be taken into account in an economic optimization analysis, where the most convenient stack configuration is sought.

3.2 Effects of membrane deformation

The eight ED test cases presented above were also simulated taking into account membrane deformation effects. In particular, two membrane deformation conditions were investigated: (i) mild deformation and (ii) heavy deformation.

3.2.1 Mild deformation effects

To take membrane deformation into account, stationary flow and channel height distributions were first evaluated for each of the above mentioned eight cross-flow 2-stage cases by computing step I before performing steps II and III, as described in the Section A.3 in the Appendix A. Quantities like the local hydraulic permeability K , the porosity ε and the equivalent channel height h^{SOL} resulting from the TMP-induced deformation were obtained by using correlations derived from previous local-scale studies of the fluid-structure interaction for the same membrane/channel geometry [29].

Table 4 reports the same quantities of Table 3 determined for all the eight cases taking deformation into account. In addition, the computed mean equivalent channel heights of the diluate channel for both stacks $\langle h_1^{DIL} \rangle$, $\langle h_2^{DIL} \rangle$ are also reported.

Table 4. Main results obtained for eight cross-flow test cases in the presence of deformation.

<i>Cases</i>	#1	#2	#3	#4	#5	#6	#7	#8
<i>Quantities</i>								
L [m]	0.2	0.4	0.6	0.6	0.6	0.6	0.6	0.6
W [m]	0.6	0.6	0.6	0.35	0.15	0.6	0.6	0.6
v_c [cm/s]	5	5	5	5	5	3	1	1
v_d [cm/s]	1	1	1	1	1	1	1	3
E_{spec}^{TOT} [kWh/m ³]	2.26	2.28	2.31	2.99	5.53	2.37	2.64	4.98
J_p^{TOT} [l/m ² h]	2.68	2.66	2.69	4.65	11.2	2.66	2.60	8.10
I_1 [A]	17.9	35.6	53.7	52.9	52.7	53.7	54.1	160
I_2 [A]	3.52	7.04	10.7	9.92	9.52	10.8	11.3	30.5
V_1 [V]	48.7	48.8	49.3	71.2	146	50.0	52.7	120
V_2 [V]	83.4	84.4	85.5	91.3	124	87.7	96.2	129
R_1^{DIL} [Ω]	0.113	0.112	0.111	0.105	0.100	0.112	0.113	0.105
R_2^{DIL} [Ω]	1.44	1.42	1.40	1.14	0.92	1.43	1.48	1.04

$Q_{TOT,OUTLET,2}^{DIL} [l \min^{-1}]$	8.58	17.0	25.8	26.0	26.8	25.5	24.9	77.7
$\langle h_1^{DIL} \rangle [\mu m]$	179	176	180	173	173	177	180	184
$\langle h_2^{DIL} \rangle [\mu m]$	179	176	173	173	172	177	180	183

The comparison of Tables 3 and 4 shows that membrane deformation alters only mildly the process performances. Interestingly, the specific energy consumption decreases in all cases, while the apparent flux increases. The most affected configuration is that of case #5, where the specific energy consumption is found to be almost 2.50% lower than in the undeformed case. To better understand this behavior, for the sake of brevity, only diluate concentration and current density maps of the second stack of case #5 are shown in Figure 5, comparing undeformed and deformed channels, as these variables are the most affected by the membrane deformation phenomena.

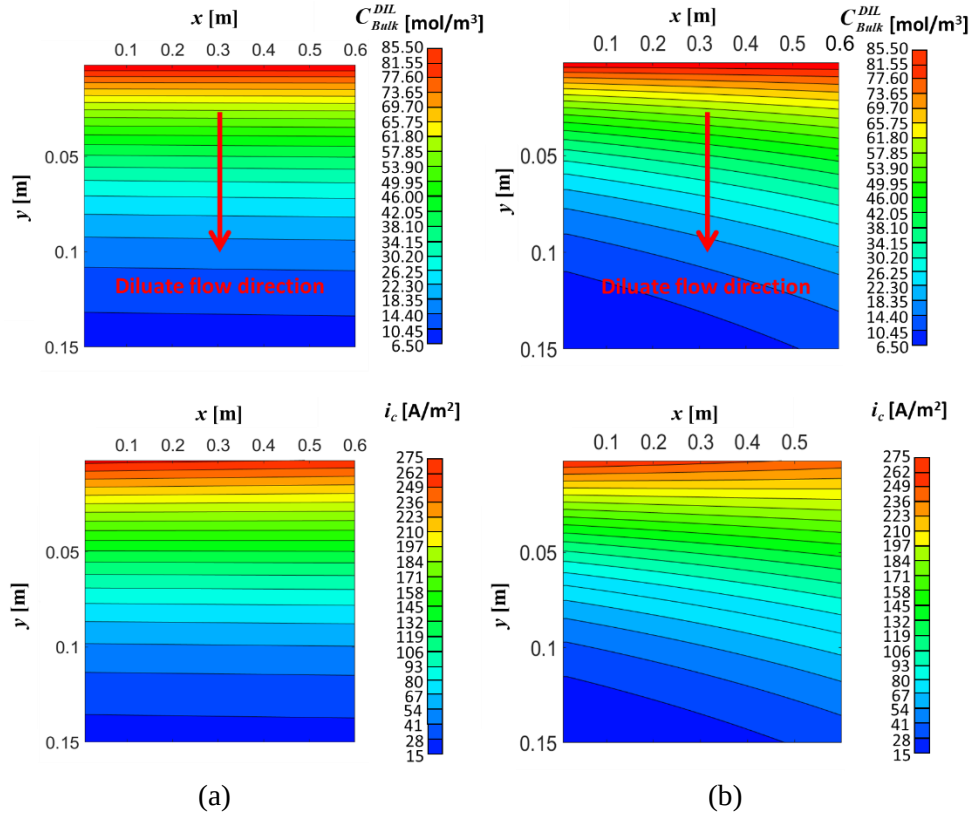


Figure 5. Maps of the diluate concentration C_{Bulk}^{DIL} (top row) and of the current density i_c (bottom row) for the second cross-flow stack of case #5 without (a) and with (b) membrane deformation.

As can be seen in Figure 5, concentration and current density iso-lines are not straight anymore in the presence of deformation. In particular, iso-lines show a significant deflection close to the channel outlet. To further investigate the reason of this behavior, maps of the diluate

superficial velocity along the main flow direction (y-axis) and of the equivalent channel height in the presence of membrane deformation are shown in Figure 6.

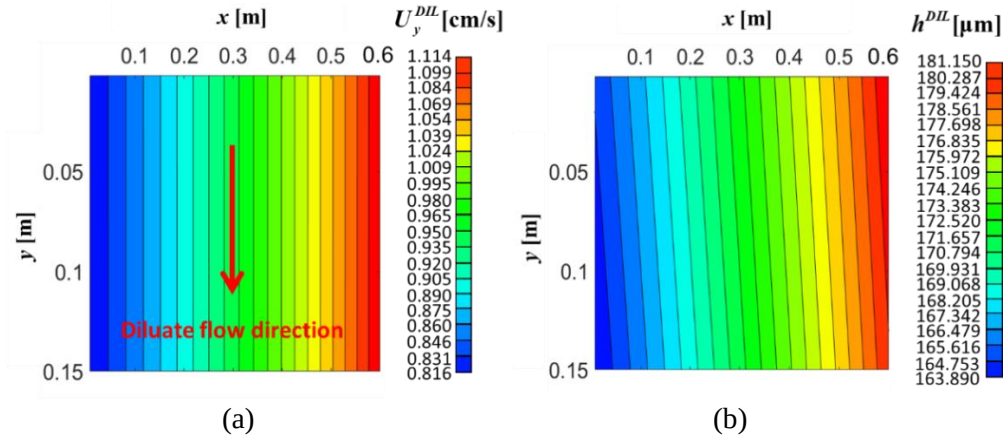


Figure 6. Maps of (a) diluate superficial velocity along the main flow direction (y-axis), and (b) channel height for the cross-flow case #5 in the presence of membrane deformation.

As it can be seen in Figure 6(a), the superficial velocity is 26.7% lower in the left side of the channel with respect to the right side, consistent with the distribution of the channel height, Figure 6(b), and thus of the hydraulic permeability. As a consequence, the residence time is higher in the left part of the stack compared to the right part. This favors the desalination process in the left side, so that local concentrations decrease more rapidly here along the flow direction y than in the right side, as shown in the top row of Figure 5(b). Moreover, the low-velocity area is larger than the high-velocity area, thus increasing the mean residence time. Note that the diluate channel is almost all compressed, and the average equivalent channel height is $172 \mu\text{m}$.

3.2.2 Heavy deformation effects

Based on the above results, it may be concluded that membrane deformation has negligible effects in ED applications for the geometry, membrane thickness t and membrane Young modulus E selected in this study (OCF $P/H=8$, $t=120 \mu\text{m}$, $E=150 \text{ MPa}$). However, deformation effects might be larger for a different choice of these quantities.

In particular, treating either membrane portion included in a unit cell (Figure 2) as a non pre-stressed square flat membrane of side length $2a$ subjected to a uniformly distributed load $q=\text{TMP}$, having all edges clamped and undergoing large deflections, an approximate estimation of the deflection w_0 at the center of the membrane surface is given by [54]:

$$w_0 = f(\nu) \left(\frac{qa^4(1-\nu)}{Et} \right)^{1/3} \quad (12)$$

where ν is the Poisson ratio and $f(\nu) \approx 0.800 + 0.062\nu$. For example, for membranes three times thinner than the above OCF ones, i.e. 40 μm , or characterized by a Young modulus three times smaller, i.e. 50 MPa, any given deformation would be obtained under a load three times smaller. Membranes with a thickness of 40 μm or less represent a promising alternative in ED and RED applications due to their lower electrical resistance [55].

In the light of these considerations, a preliminary investigation was carried out on the effects of more severe membrane deformations than those considered in Section 3.2.1. To this purpose, fictitious correlations for the channel hydraulic permeability (K) and the equivalent channel height (h^{SOL}) as functions of TMP were built to characterize less stiff membranes. The used criterion consisted in assuming that all effects caused by a given TMP in the OCF membranes previously simulated at the unit cell scale must occur in less stiff membranes at TMP/3. Table 5 reports the resulting correlations along with those for the actual OCF membranes with $t=120\text{ }\mu\text{m}$, $E=150\text{ MPa}$ considered so far. For the sake of simplicity, no change was made in the correlations used to express the Sherwood numbers as functions of TMP, due to the small influence of this quantity on the overall stack performance.

Table 5. Channel hydraulic permeability K and equivalent height h^{SOL} as functions of TMP for OCF profiled membranes at $P/H=8$ and fictitious less stiff membranes. In the equations, TMP is in kPa.

	OCF $P/H=8$ membranes	Less stiff membranes
K [m^2]	$2.4055 \cdot 10^{-13} \cdot \text{TMP}^2 - 3.4005 \cdot 10^{-11} \cdot \text{TMP} + 1.6560 \cdot 10^{-9}$	$2.27 \times 10^{-12} \times \text{TMP}^2 - 1.03 \times 10^{-10} \times \text{TMP} + 1.6560 \cdot 10^{-9}$
h^{SOL} [m]	$6.00 \times 10^{-10} \times \text{TMP}^2 - 1.13 \times 10^{-6} \times \text{TMP} + 1.80 \times 10^{-4}$	$1.89 \times 10^{-9} \times \text{TMP}^3 - 7 \times 10^{-9} \times \text{TMP}^2 + -3.57 \times 10^{-6} \times \text{TMP} + 1.80 \times 10^{-4}$

Only results for *case #5*, which showed the highest membrane deformation effects among the eight configuration studied in section 3.1, will be presented. Table 6 reports the same quantities as Table 4 but comparing the cases of undeformed membranes, actual deformed membranes (mild deformation), and fictitious deformed membranes (heavy deformation).

Table 6. Main results obtained for case #5 under the three conditions of no deformation, mild deformation (actual OCF membranes) and heavy deformation (fictitious membranes).

Quantities	Undeformed	Mild Deformation	Heavy Deformation
E_{spec}^{TOT} [kWh/m ³]	5.669	5.527	5.361
J_p^{TOT} [l/m ² h]	11.00	11.17	11.02

I_1 [A]	52.68	52.75	51.20
I_2 [A]	9.415	9.523	9.331
V_1 [V]	147.6	146.0	143.9
V_2 [V]	127.7	124.5	122.4
$\langle h_1^{DIL} \rangle$ [μm]	180.0	172.5	160.3
$\langle h_2^{DIL} \rangle$ [μm]	180.0	172.1	159.5
R_1^{DIL} [Ω]	0.102	0.100	0.110
R_2^{DIL} [Ω]	0.944	0.923	0.950
$Q_{TOT,OUTLET,2}^{DIL}$ [l min^{-1}]	26.4	26.81	26.45

Results in Table 6 show that heavy membrane deformation conditions can influence the process' performances. Specifically, the total energy consumption decreases of more than 5% with respect to the undeformed case. The reason is the stronger redistribution of the fluid velocity with respect to the “mild deformation” case discussed in Section 3.2.1, as shown by the diluate concentration and current density maps in the second stack of case #5 reported in Figure 7. Note that in the heavy deformation case the diluate superficial velocity along the y-axis is more than twice higher in the right side of the channel than in the left side, thus strongly influencing the residence time. As a result, concentration and current density iso-lines are much more deflected than in the case of mild deformation of Figure 5. Table 6 shows also that the behavior of several quantities (among which J_p^{TOT}) is not monotonic with the amplitude of the deformation.

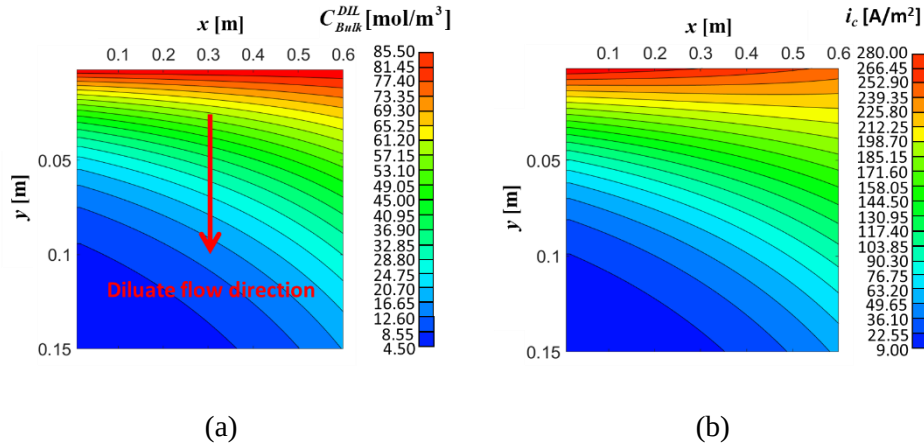


Figure 7. Maps of diluate concentration C_{Bulk}^{DIL} (a) and current density i_c (b) for the second cross-flow stack of case #5 in the presence of heavy membrane deformation (compare with Figure 5).

Conclusions

In this paper, a novel 2-D, multi-scale, semi-empirical process model has been presented for the simulation of cross-flow Electrodialysis (ED) systems in the presence and absence of membrane deformation. The model is based on a multi-scale approach allowing the study of membrane deformation phenomena by exploiting results and modelling approaches of previous fluid-structure investigations performed by the authors. Specifically, at the lowest scale of a small repetitive unit of a fluid channel bounded by two profiled membranes, fluid dynamics and mass transport properties of deformed fluid channels have been taken into account using correlations previously determined by one-way coupled structural/fluid-dynamics simulations regarding Overlapped Cross Filaments (OCF) profiled membranes. At the higher scale of a whole channel dimension, an original previously developed two-way fluid-structure algorithm has been used to calculate the fluid, mass transfer characteristics and channel height redistribution in ED stacks considering the local membrane deformation. Finally, at the highest scale of an ED stack, all physical and electrochemical phenomena of the ED process have been computed to assess the performance of cross-flow ED stacks. In a first set of simulations without considering membrane deformation, the process performances of cross-flow ED systems have been investigated profiled membranes have been investigated for a two-stage desalination of seawater by changing the stack size and operating conditions. The use of shorter diluate channels increased the specific energy demand (due to a higher voltage) for a desalination process requiring, however, less membrane area and providing higher water recovery. Then, the same ED stack configurations have been simulated by including local membrane deformations. In this case, results have shown that membrane deformation did not affect significantly the process performances. In particular, the specific energy consumption decreased of $\sim 2.5\%$ in the most affected configuration with respect to its undeformed case. However, the use of thinner or less stiff membranes than the OCF ones (thickness lower than $120\text{ }\mu\text{m}$ and Young modulus lower than 150 MPa) could lead to more severe membrane deformations and, thus, to larger effects on the process performance. In this regard, a preliminary investigation has shown that the specific energy consumption could decrease up to $\sim 5\%$ with respect to the undeformed case.

The paper presents a novel tool to support the design and the optimisation of cross-flow ED stacks and profiled membranes or spacers. Helpful information could be collected to guide membrane manufacturers and stack designers, especially in the early stages of the development of novel membranes or stacks. ED tests performed with stacks equipped with segmented

electrodes could integrate and further validate the present model by providing experimental data on the distribution of the current density.

Authors would also stress that, although the modelling tool has been presented for ED applications, the fundamental idea behind the simulation approach can be readily extended to the analysis of any other membrane-based process, where a differential pressure can generate local deformation of membranes and channels geometry.

Acknowledgements

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Appendix A: ED model equations and numerical details

This Appendix reports equations of the ED model not included in Section 2.1 and other numerical details.

A.1 Mass fluxes in a cell pair

In a repetitive unit of an ED stack, i.e. the cell pair, two transmembrane mass fluxes occur across each membrane: the water and the ion fluxes.

The total transmembrane water flux can be expressed as the sum of two terms:

$$J_w^{TOT}(x, y) = J_w^{OSM}(x, y) + J_w^{E.OSM}(x, y) \quad (A.1)$$

accounting for osmotic and electro-osmotic transport mechanisms, respectively.

The osmotic term, $J_w^{OSM}(x, y)$, describes the water transport due to the interfacial osmotic pressure gradient between concentrate and dilute solutions across the membranes:

$$J_w^{OSM}(x, y) = L_{p,AEM} [\pi_{AEM}^{CON}(x, y) - \pi_{AEM}^{DIL}(x, y)] + L_{p,CEM} [\pi_{CEM}^{CON}(x, y) - \pi_{CEM}^{DIL}(x, y)] \quad (A.2)$$

where

- $L_{p,IEM}$ is the osmotic water permeability coefficient of a generic Ion Exchange Membrane (*IEM*), i.e. either the cation- or the anion-exchange membrane (*CEM* or *AEM*), whose value is usually given in ml/(m² h bar) but is expressed here in SI units m³/(m² s Pa).
- $\pi_{IEM}^{SOL}(x, y)$ is the osmotic pressure evaluated at the concentration $C_{IEM}^{SOL}(x, y)$ occurring at the interface between the generic *IEM* membrane and the generic *SOL* solution (solution side). For simplicity, osmotic pressures were calculated here by the van't Hoff law $\pi_{IEM}^{SOL} = 2RTC_{IEM}^{SOL}$.

The second transport mechanism, i.e. electro-osmosis, refers to the migration of water molecules coupled with the ions' transport. The electro-osmotic term can be expressed as:

$$J_w^{E.OSM}(x, y) = n_h N_{SALT}^{TOT}(x, y) \frac{M_w}{\rho_w} \quad (A.3)$$

where n_h is the hydration number, here assumed to be equal to 7, while M_w and ρ_w are the water molecular weight (in kg/mol) and density (in kg/m³). n_h has been fixed as the average of the hydration number of sodium ion (equal to 6) and that of chloride ion (equal to 8) [56,57].

In regard to the total salt flux $N_{SALT}^{TOT}(x, y)$, it accounts for the Coulombic, or migrative, flux $N_{Coul}^{TOT}(x, y)$ and the diffusive $N_{Diff}^{TOT}(x, y)$ flux:

$$N_{SALT}^{TOT}(x, y) = N_{Coul}^{TOT}(x, y) - N_{Diff}^{TOT}(x, y) \quad (A.4)$$

It is worth noting that the ion diffusive flux occurs from the concentrate channel to the diluate one. Therefore, in ED, it has to be subtracted from the Coulombic ion flux, which is directed from the dilute solution to the concentrated one. The Coulombic flux represents the main salt transport contribution and is proportional to the local ionic current density i_c . For monovalent ions, under the assumption of unitary membrane perm-selectivity, the Na^+ ions flux $N_{Coul}^{Na^+}(x, y)$ through a *CEM*, or the Cl^- ions flux $N_{Coul}^{Cl^-}(x, y)$ through an *AEM*, which corresponds to the total Coulombic flux, can be expressed by the Faraday law as:

$$N_{Coul}^{Na^+ \text{ or } Cl^-}(x, y) = \frac{i_c(x, y)}{z_{Na^+ \text{ or } Cl^-} F} \quad (A.5)$$

where F is the Faraday constant (96,485 C/mol), $i_c(x, y)$ is the local ionic current density in A/m² and $z_{Na^+ \text{ or } Cl^-}$ is the ion valence, i.e. +1 and -1 for Na^+ and Cl^- , respectively.

As already discussed, the diffusive flux describes the salt back-diffusion through the membrane due to the concentration difference between the channels. The diffusive flux through a single membrane can be written as:

$$N_{Diff}^{IEM}(x, y) = \frac{D^{IEM}}{t} [C_{IEM}^{CON}(x, y) - C_{IEM}^{DIL}(x, y)] \quad (A.6)$$

where D^{IEM} (in m²/s) is the salt diffusivity in a generic *IEM* membrane of thickness t . Two diffusive fluxes, one at the *AEM* and one at the *CEM*, have to be taken into account, so that $N_{Diff}^{TOT}(x, y) = N_{Diff}^{AEM}(x, y) + N_{Diff}^{CEM}(x, y)$.

A.2 Electric variables, Ohmic and non-Ohmic resistances

In ED systems, the overall voltage drop over a cell pair V_{cp} , independent of x and y , can be expressed as:

$$V_{cp} = \eta(x, y) + R_{TOT}(x, y)i_c(x, y) \quad (A.7)$$

The term $\eta(x, y)$ is the non-Ohmic voltage drop and $R_{TOT}(x, y)i_c(x, y)$ is the Ohmic loss in the cell pair R_{TOT} is the total areal resistance of the cell pair and can be expressed as:

$$R_{TOT}(x, y) = R^{CEM}(x, y) + R^{AEM}(x, y) + R^{DIL}(x, y) + R^{CON}(x, y) \quad (A.8)$$

where $R^{CEM}(x, y)$ and $R^{AEM}(x, y)$ are the areal electrical resistances of the membranes, while $R^{DIL}(x, y)$ and $R^{CON}(x, y)$ are the areal electrical resistances of the channels.

By following the results of the experimental measurements performed by Galama *et al.* [58], $R^{IEM}(x, y)$ can be approximated as:

$$R^{IEM}(x, y) = a^{IEM} + b^{IEM} \left[C_{IEM}^{DIL}(x, y) \right]^{-c^{IEM}} \quad (A.9)$$

where a^{IEM} , b^{IEM} , c^{IEM} are constants, which can be empirically determined. In the present simulations, a was set equal to 1.89×10^{-4} and $1.77 \times 10^{-4} \Omega \text{ m}^2$, for the *CEM* and *AEM* membranes, respectively. These values are the areal membrane resistances measured at the standard concentration of 0.5M NaCl. Moreover, b and c are equal to 7×10^{-3} (in the appropriate units) and 1.25, for both *AEM* and *CEM*. The constants were taken from [47].

In regard to the channel areal resistance, it can be estimated by:

$$R^{SOL}(x, y) = \frac{h^{SOL}(x, y)}{\kappa^{SOL}(x, y) \varepsilon^2(x, y)} \quad (A.10)$$

where $\kappa^{SOL}(x, y)$ is the electrical conductivity of the solution, which is a function of the local salt concentration (as expressed by Eqs. (B.2-3) in the Appendix B), $\varepsilon(x, y)$ is the local channel volume porosity, defined with reference to the unit cell as the ratio between fluid volume and total volume of the undeformed channel without profiles, while $h^{SOL}(x, y)$ is the local equivalent channel thickness, defined as the ratio of fluid volume to projected area of a unit cell. The fluid volume (V_f) under deformed condition is a function of the local TMP [31]. In the present work, it is computed by a polynomial approximation of results obtained for a variety of membrane profiles by the one-way coupled fluid-structure simulations described in [29,30]. In particular, for the OCF profiled membranes with $P/H=8$ considered here, the dependence of V_f , h^{SOL} and ε on TMP is reported in the Appendix C, Eqs. (C.2)-(C.4).

Eq. (A.10) is, of course, only a crude approximation for the Ohmic resistance of the solution flowing in its channel, based, in particular, on the assumption that membrane profiles do not contribute significantly to the total conductance. In order to accurately investigate its validity, its predictions were compared with accurate 3D numerical solutions of the Laplace equation for the electrical potential [46]; only minor discrepancies were obtained, thanks also to the fact that the OCF geometry investigated ($P/H=8$) is characterized by a channel porosity close to 0.9, so that the accurate modelling of the profiles is not a crucial issue.

In Eq. (A.7), both non-Ohmic voltage drop $\eta(x, y)$ and Ohmic resistances were presented. With regard to $\eta(x, y)$, it is given by the back electro-motive force originated from the salt

concentration gradient over the perm-selective membranes. $\eta(x, y)$ can be divided into two contributions associated with (i) the concentration gradient between the two solutions bulks $\varphi(x, y)$ and (ii) its increment due to concentration polarization phenomena in the boundary layer $\eta_{BL}(x, y)$.

Therefore, the total non-Ohmic voltage drop can be written as:

$$\eta(x, y) = \varphi(x, y) + \eta_{BL}(x, y) \quad (\text{A.11})$$

Specifically, the first contribution for a single membrane IEM is calculated [32] as:

$$\varphi_{IEM}(x, y) = (\alpha_{IEM}) \frac{RT}{F} \ln \left(\frac{\gamma^{CON}(x, y) C_{Bulk}^{CON}(x, y)}{\gamma^{DIL}(x, y) C_{Bulk}^{DIL}(x, y)} \right) \quad (\text{A.12})$$

where α_{IEM} is the perm-selectivity of a generic membrane, which is correlated to the ability of the membrane to block the passage of co-ion through itself (assumed constant in the model); T is the temperature; R is the gas constant; γ^{CON} and γ^{DIL} are the salt activity coefficients in the *CON* and *DIL* solutions, calculated using Eqs. (B.6)-(B.7) (Appendix B), which depend on the solution bulk concentration ($C_{Bulk}^{CON}(x, y)$ and $C_{Bulk}^{DIL}(x, y)$). Taking into account both *AEM* and *CEM* membranes, one has: $\varphi(x, y) = \varphi_{AEM}(x, y) + \varphi_{CEM}(x, y)$.

The second contribution in Eq. (A.11) accounts for concentration polarization phenomena. Concentration polarization phenomena are caused by the different kinetics of ion transport in solutions and in membranes [2]. In particular, polarization phenomena can be defined as: “the concentration profile that has a higher (or lower) level of solute nearest to the upstream membrane surface compared with the more-or-less well-mixed bulk fluid far from the membrane surface” [59]. In the case of the ED process, salt concentration increases at the membrane surface in the concentrate channel and reduces at the membrane surface in the diluate channel causing a non-Ohmic voltage drop that intensifies the back electromotive force. In the description of a cell pair, four non-Ohmic voltage drops arise, one for each membrane/solution interface. The increase of non-Ohmic voltage drop associated to the concentration polarization in the boundary layers ($\eta_{BL}(x, y)$) is given by the sum of the four contributions:

$$\eta_{BL}(x, y) = \eta_{AEM}^{CON}(x, y) + \eta_{CEM}^{CON}(x, y) + \eta_{AEM}^{DIL}(x, y) + \eta_{CEM}^{DIL}(x, y) \quad (\text{A.13})$$

where the single boundary layer voltage drop $\eta_{IEM}^{SOL}(x, y)$ at the generic *IEM* membrane, i.e. *AEM* or *CEM*, in contact with the generic solution *SOL* (*CON* or *DIL*), can be calculated as [46]:

$$\eta_{IEM}^{SOL}(x, y) = -\alpha_{IEM} \frac{RT}{F} \ln(\theta_{IEM}^{SOL}(x, y)) \quad (\text{A.14})$$

where $\theta_{IEM}^{SOL}(x, y)$ is the so-called polarization coefficient determined at the membrane-solution interface as:

$$\theta_{IEM}^{CON}(x, y) = \frac{C_{Bulk}^{CON}(x, y)}{C_{IEM}^{CON}(x, y)} \text{ and } \theta_{IEM}^{DIL}(x, y) = \frac{C_{IEM}^{DIL}(x, y)}{C_{Bulk}^{DIL}(x, y)} \quad (A.15)$$

Note that, $\theta_{IEM}^{CON}(x, y)$ and $\theta_{IEM}^{DIL}(x, y)$ are always smaller than one. The polarization coefficient is purposely introduced to distinguish the two contributions to the non-Ohmic voltage drop [2]. In Eq. (A.15), the effects of the activity coefficients are neglected.

To determine the polarization coefficients in Eq. (A.15), information about $C_{IEM}^{CON}(x, y)$ and $C_{IEM}^{DIL}(x, y)$ is needed. To this aim, the *Sherwood* number equation presented in [46] is employed:

$$Sh_{IEM}^{SOL}(x, y) = \left| \frac{(N_{Diff}^{IEM}(x, y) + 0.5 \times N_{Coul}^{TOT}(x, y)) 2H}{(C_{Bulk}^{SOL}(x, y) - C_{IEM}^{SOL}(x, y)) D^{SOL}(x, y)} \right| \quad (A.16)$$

where $D^{SOL}(x, y)$ is the salt diffusivity in the generic solution *SOL*, whose dependence on the solution concentration is expressed in Eqs. (B.4)-(B.5). The term $N_{Diff}^{IEM}(x, y) + 0.5 \times N_{Coul}^{TOT}(x, y)$ represents the diffusive salt flux in the generic solution *SOL* in contact with the generic membrane *IEM*, which can be found by taking into account the flux continuity at the solution-membrane interface.

Rearranging Eq. (A.16) and taking into account Eq. (A.15), the polarization coefficients for the two solutions can be calculated as:

$$\theta_{IEM}^{CON}(x, y) = 1 / \left[1 + \frac{(N_{Diff}^{IEM}(x, y) + 0.5 \times N_{Coul}^{TOT}(x, y)) 2H}{Sh_{IEM}^{CON}(x, y) C_{Bulk}^{CON}(x, y) D_{Salt}^{CON}(x, y)} \right] \quad (A.17)$$

$$\theta_{IEM}^{DIL}(x, y) = 1 - \frac{(N_{Diff}^{IEM}(x, y) + 0.5 \times N_{Coul}^{TOT}(x, y)) 2H}{Sh_{IEM}^{DIL}(x, y) C_{Bulk}^{DIL}(x, y) D_{Salt}^{DIL}(x, y)} \quad (A.18)$$

Thus, the voltage drop $\eta_{IEM}^{SOL}(x, y)$ can be obtained from Eq. (A.14).

A.3 Resolution algorithm

In order to solve the water and salt mass balance equations (1)-(4) taking account of the constitutive equations (A.1)-(A.18) and Eq. (5), a finite difference approach, similar to that used in [31], is adopted. The two *CON* and *DIL* channels of a cell pair, of overall size $L \times W$, are divided into a number of rectangular blocks along the x (N_{Block}^x) and y (N_{Block}^y) directions, of

size $\Delta x = L / N_{Block}^x$ and $\Delta y = W / N_{Block}^y$. Figure A.1 presents a sketch of a cell pair along with a detail of the computational molecules adopted in the present work to compute spatial derivatives in Eqs. (1-4).

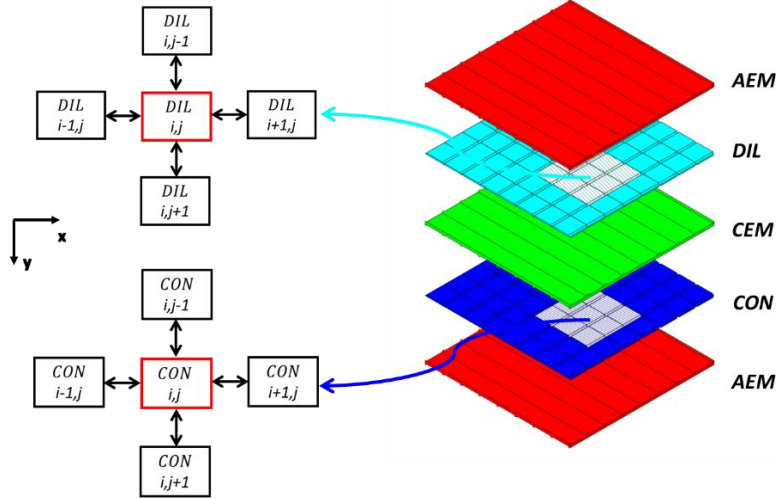


Figure A.1. Schematic representation of a cell pair made of a diluate channel (*DIL*), a concentrate channel (*CON*), an *AEM* and a *CEM* (a further *AEM* membrane is added only to illustrate the periodicity of the cell pair). In addition, details of the computational molecules adopted for the discretization of Eqs. (1-4) in both channels are reported on the right. Adapted from [31].

With reference to the computational molecules shown in Figure A.1, multiplying all terms in Eqs. (1)-(4) by the nominal volume of a block, $H\Delta x\Delta y$, approximating the derivatives by finite differences, and neglecting in each channel the components of the velocity along the direction orthogonal to the main flow, with reference to the flow configuration of Figure 3, the following salt / water discrete mass balance equations are obtained:

$$C_{Bulk;i,j}^{CON} \cdot Q_{i,j}^{CON;x} - C_{Bulk;i-1,j}^{CON} \cdot Q_{i-1,j}^{CON;x} = N_{SALT;i,j}^{TOT} \cdot \Delta x \Delta y \quad (A.19)$$

$$Q_{i,j}^{CON;x} - Q_{i-1,j}^{CON;x} = J_{W;i,j}^{TOT} \cdot \Delta x \Delta y \quad (A.20)$$

$$C_{Bulk;i,j}^{DIL} \cdot Q_{i,j}^{DIL;y} - C_{Bulk;i,j-1}^{DIL} \cdot Q_{i,j-1}^{DIL;y} = -N_{SALT;i,j}^{TOT} \cdot \Delta x \Delta y \quad (A.21)$$

$$Q_{i,j}^{DIL;y} - Q_{i,j-1}^{DIL;y} = -J_{W;i,j}^{TOT} \cdot \Delta x \Delta y \quad (A.22)$$

where $Q_{i,j}^{CON;x}$ is the flow rate in the *CON* channel, directed along *x* from block (*i*, *j*) to block (*i*+1, *j*) while $Q_{i,j}^{DIL;y}$ is the flow rate in the *DIL* channel, directed along *y* from block (*i*, *j*) to block (*i*, *j*+1). $J_{W;i,j}^{TOT}$ is the specific trans-membrane water flux (in m/s) from the diluate to the concentrate channel in block (*i*, *j*). $N_{SALT;i,j}^{TOT}$ is the specific trans-membrane salt flux, in

mol/(m²s), from the diluate to the concentrate channel in block (i,j) . Finally, $C_{Bulk;i,j}^{SOL}$ is the bulk salt concentration, in mol/m³, in the generic *SOL* channel (either *CON* or *DIL*) in block (i,j) .

The fluid flow may have a nonzero component in the direction orthogonal to the main flow. However, our previous investigation on cross-flow configurations with uniform conditions at the inlet (velocity) and at the outlet (pressure) [31] revealed that such secondary velocity components are still three orders of magnitude lower than the streamwise component even in the presence of relevant TMP values (see Figure 12(f) in [31]). This consideration justifies the assumption made here.

Eqs. (A.19)-(A.22) are $4N$ equations in $4N$ unknowns, where $N = N_{Block}^x \cdot N_{Block}^y$: N concentrations in the *CON* channel, N concentrations in the *DIL* channel, N flow rates along x in the *CON* channel and N flow rates along y in the *DIL* channel.

All the terms in the constitutive Eqs. (A.1)-(A.18) and Eq. (5) are evaluated at each grid block taking into account the local concentration of the two solutions.

In order to couple Eqs. (A.19)-(A.22) with Eqs. (A.1)-(A.18) and Eq. (5), thus determining the steady-state distributions of all variables for a chosen ED stack configuration, an iterative procedure is employed. In particular, the algorithm can be divided into four main steps:

I. Starting from a tentative pressure distribution in the two channels, the local TMP is evaluated in each block. The local hydraulic permeability K resulting from the TMP-induced deformation is then calculated by using K -TMP correlations, Eq. (C.1) in the Appendix C, derived from previous local-scale studies of the fluid-structure interaction for the same OCF geometry [29]. The simplified (Darcyan) model described in Section 2.4 of ref. [31] is then used to compute the flow rates Q . At this stage, trans-membrane water fluxes are neglected.

II. All the other distributed variables are then computed by the ED process model solving Eqs. (A.1)-(A.18) and Eq. (5) in conjunction with the salt balance equations (A.19) and (A.21) for the chosen value of the applied voltage and of the number of cell pairs.

Step II is iterated until a desired convergence criterion is satisfied. More specifically, at the beginning of step II uniform block concentrations, equal to the inlet values ($C_{Inlet}^{DIL}, C_{Inlet}^{CON}$), are imposed in both channels at each grid block, and the same values are also assumed for the membrane-solution interfacial concentrations (no concentration polarization).

Then, the solution's properties and activity coefficients are calculated by the correlations reported in the Appendix B, Eqs. (B.1)-(B.7). The channels' Ohmic resistances are evaluated

by Eq. (A.10), taking into account the channel equivalent height and local porosity, which are computed from the TMP distribution obtained in step I using Eqs. (C.3) and (C.4) in the Appendix C. Membrane resistances are calculated by Eq. (A.9) and thus the cell pair resistance can be obtained by Eq. (A.8). The non-Ohmic voltage drop φ and η are evaluated by Eqs. (A.12) and (A.11) at each grid block. Note that the voltage drop due to concentration boundary layers η_{BL} and also φ are zero at the first iteration, since bulk and interfacial concentrations are the same. The local current density i_c is obtained from Eq. (5).

By knowing the current density and solution concentrations, total salt and water fluxes are calculated using Eqs. (A.1-A.6). Thus, polarization coefficients and η_{BL} can be found by Eqs. (A.13), (A.14), (A.17), (A.18) by using Eqs. (C.5)-(C.18) to calculate Sherwood numbers as functions of local TMP. Note that η_{BL} is actually used at the next iteration to compute η .

Finally, from Eqs. (A.19) and (A.21) new concentration values at each i, j block are found. Step II terminates when the maximum difference between old and new concentrations over all grid blocks ($e = |C_{New}^{SOL} - C_{Old}^{SOL}|$) becomes less than 10^{-3} M.

III. Flow rates of step I are re-calculated using the water balance equations (A.20) and (A.22) taking into account the trans-membrane water fluxes calculated in step II.

Then, the solution concentrations ($C_{New,2}^{SOL}$) are again calculated from the mass balances of Eqs. (A.19) and (A.21), taking into account the new flow distribution. Finally, the difference between the new concentration values and those of step II are calculated over all grid blocks as $e_2 = |C_{New,2}^{SOL} - C_{New}^{SOL}|$. If the maximum difference is higher than 10^{-3} M, the flow distribution is updated in step II and new concentrations are found. Otherwise, the final solution is attained. For the sake of clarity, Figure A.2 presents the flow chart of Steps II and III.

IV. Finally, the process' performances are evaluated by solving Eqs. (6)-(9).

It should be noted that, in a more complete procedure, membrane deformation (deformed membrane shape) would be updated (step I) considering the calculated flow rates of step III, which take into account water transmembrane fluxes. However, this step has been neglected in the present version of the model in view of the small influence of the trans-membrane water flow rate with respect to the main water flow rate along the channels. A more detailed discussion of this issue was presented in [31].

The procedure was implemented in the MATLAB® environment. The simulations were performed by a desktop computer equipped with a 4-core (8 threads) intel i7-6700 CPU (3.4 GHz, max 4.0 GHz) and 32 GB RAM memory. By neglecting deformation, the overall computing time for a 2-stage ED process providing the desired outlet concentration was of ~300 core-seconds. By including deformation, the overall computing time was of ~5.6 core-hours, whose main portion is taken by the evaluation of the inlet conditions (pressure) ensuring the same flow rate of the undeformed case.

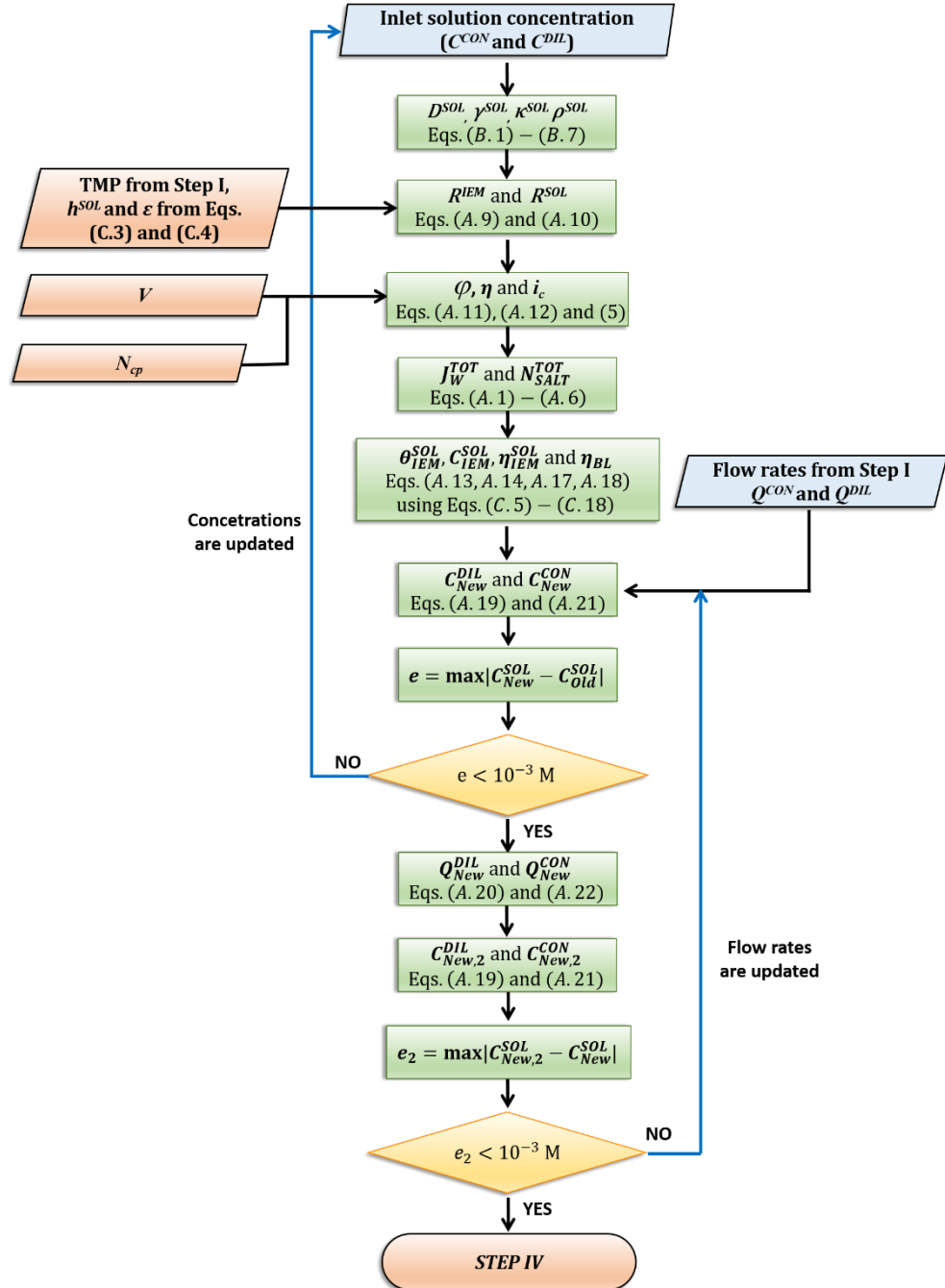


Figure A.2. Flow chart of steps II and III of the iterative algorithm used for the 2-D process model of ED stacks.

A.4 Grid dependence analysis

In order to determine the most suitable grid size that satisfies the trade-off between computing time and accuracy in the simulation of cross-flow configurations, a sensitivity analysis of the model predictions on the grid resolution was carried out. In this grid dependence analysis, membrane deformation effects were taken into account. Five grids were investigated: 40×40, 80×80, 120×120, 180×180 and 240×240 blocks. All simulations were conducted for ED stacks equipped with OCF profiled membranes with P/H=8, see Figure 2, assuming:

- inlet solutions concentrations of 513.34 mol/m³ (30 g/l);
- length and width of the stack equal to 0.6 m;
- inlet mean concentrate and diluate velocities of 5 cm/s;
- 400 cell pairs;
- an applied voltage drop V able to desalinate the diluate up to an outlet concentration of 8.5 mol/m³ (0.5 g/l).

Moreover, the parameters in Table 1 were used. Table A.1 and Figure A.3 present the results of the above mentioned grid-dependence analysis. Reported discrepancies are with respect to the finest grid (240×240).

Table A.1. Grid dependence for the cross-flow configuration.

$N_{Block}^x = N_{Block}^y$	40	80	120	180	240
Quantities					
C_{OUTLET}^{CON} [M]	969.41	966.59	965.76	965.21	964.93
Discrepancy %	0.464	0.172	0.086	0.029	0.000
$Q_{TOT,OUTLET}^{CON}$ [l min ⁻¹]	151.16	152.52	152.96	153.27	153.43
Discrepancy %	-1.480	-0.593	-0.306	-0.104	0.000
$Q_{TOT,OUTLET}^{DIL}$ [l min ⁻¹]	130.11	131.67	132.16	132.51	132.69
Discrepancy %	-1.944	-0.769	-0.399	-0.136	0.000
V [V]	260.15	254.99	253.70	252.90	252.50
Discrepancy %	3.030	0.986	0.475	0.158	0.000
i_c [A m ⁻²]	839.75	831.52	828.73	827.19	826.43
Discrepancy %	1.612	0.616	0.278	0.092	0.000

Note that C_{OUTLET}^{CON} is calculated as the mean concentration value at the outlet of the concentrate channel; $Q_{TOT,OUTLET}^{CON}$ is the overall concentrate outlet flowrate, calculated as the flow rate at the outlet of the channel and multiplied by the total number of cell pairs (N_{cp}).

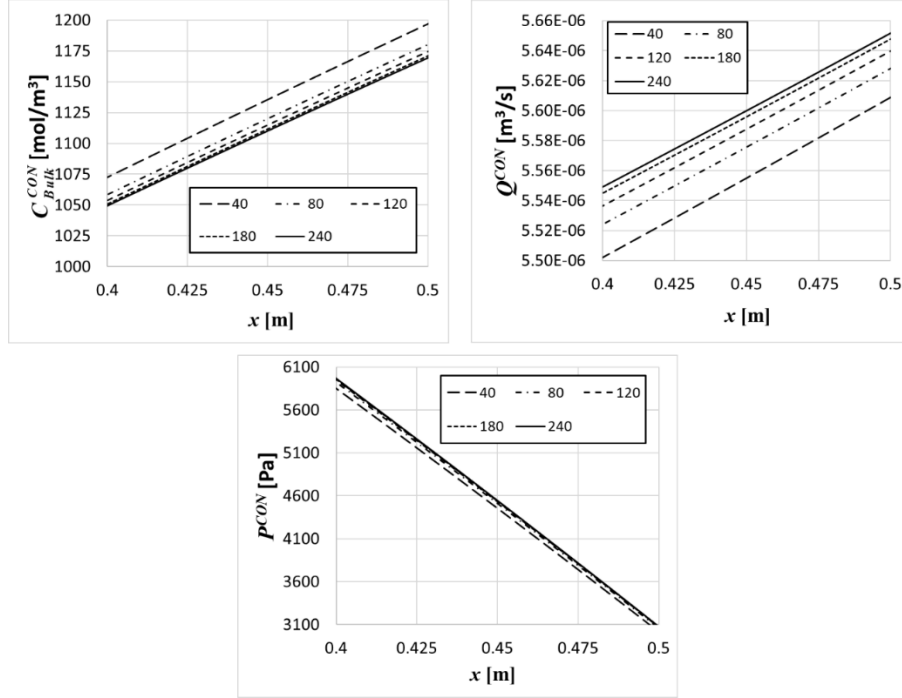


Figure A.3. Comparison among results of the present model obtained with different discretization degrees: concentration, flow rate and pressure profiles of the concentrate solution along a line placed at 2.5 cm from the top of the channel. Quantities in the region of the channel between 0.4 and 0.5 m are reported.

Results show that the 80×80 grid can be employed, as discrepancies lower than 1% are obtained with respect to the finest grid. Note that all the results shown hereinafter are obtained using the 80×80 grid.

Appendix B: Correlations used for the physical and transport properties of NaCl solutions.

In the following appendix, the correlations for the physical and transport properties of NaCl solutions used in the present model are reported. All the correlations (B.1-7) refer to a temperature T_0 of 25 °C and are taken by Annex 1 in [46].

- Solution density ρ^{sol} (kg/m³):

$$\rho^{sol} = 5.94 \times 10^{-11} C^3 - 1.032 \times 10^{-6} C^2 + 4.097 \times 10^{-2} C + 997 \quad (B.1)$$

- Solution electrical conductivity κ^{sol} (S/m):

$$\log_{10}(\kappa^{SOL}) = -0.0027373(\log_{10}(C))^3 - 0.0059675(\log_{10}(C))^2 + 0.98994(\log_{10}(C)) - 1.9074 \quad C \leq 1000 \quad (B.2)$$

$$\log_{10}(\kappa^{SOL}) = -1.3893(\log_{10}(C))^3 + 13.252(\log_{10}(C))^2 - 41.277(\log_{10}(C)) + 43.011 \quad C \leq 1000 \quad (B.3)$$

• Salt diffusion D^{SOL} (m²/s):

$$D^{SOL} = 1.47 \times 10^{-9} + 0.13 \times 10^{-9} e^{(-C/70)} \quad C \leq 400 \quad (B.4)$$

$$D^{SOL} = -2.87262 \times 10^{-21} C^3 + 2.03219 \times 10^{-17} C^2 - 8.44113 \times 10^{-15} C + 1.4705 \times 10^{-9} \quad C > 400 \quad (B.5)$$

• Salt activity coefficients γ^{SOL} (dimensionless):

$$\gamma^{SOL} = 0.64 + 0.189e^{-C/260} + 0.1605e^{-C/20} \quad C \leq 1200 \quad (B.6)$$

$$\gamma^{SOL} = 0.64 + 0.189e^{-C/260} + 0.1605e^{-C/20} + 1.051 \times 10^{-7} (C - 1200)^{1.8} \quad C > 1200 \quad (B.7)$$

As discussed in Section 2.2, the temperature varied during the experiments used for model validation from 18 to 22 °C. In order to properly simulate the experimental conditions, empirical correlations for solution and membrane resistances as functions of the temperature were employed taking into account the change of these variables with respect to the values measured at the reference temperature:

• Solution electrical conductivity as a function of the temperature (°C):

$$\kappa^{SOL}(T) = \kappa^{SOL}(T_0) \frac{0.1692 \cdot T_0 + 4.7276}{0.1692 \cdot T + 4.7276} \quad (B.8)$$

• Membrane resistance as a function of the temperature (°C):

$$R^{IEM}(T) = R^{IEM}(T_0) \frac{0.0023 \cdot T^2 - 0.1799 \cdot T + 5.1795}{0.0023 \cdot T_0^2 - 0.1799 \cdot T_0 + 5.1795} \quad (B.9)$$

Eqs. (B.8) and (B.9) were provided by the REDstack company.

Appendix C: Correlations for membrane deformation

In the following appendix correlations for hydraulic permeability, equivalent channel height, volume porosity and Sherwood number as a function of TMP are reported. Correlations were obtained for the OCF unit cell geometry of Figure 2 by performing computational fluid-structural one-way simulations [29]. Note that in the correlations TMP is in kPa and positive value of TMP causes the compression of a channel.

• Hydraulic channel permeability (m²):

$$K = 2.40 \cdot 10^{-13} \cdot \text{TMP}^2 - 3.40 \cdot 10^{-11} \cdot \text{TMP} + 1.66 \cdot 10^{-9} \quad (C.1)$$

- 869 • Unit cell fluid volume (mm³):
- 870 $V_f = 1.53 \cdot 10^{-6} \cdot \text{TMP}^2 - 2.89 \cdot 10^{-3} \cdot \text{TMP} + 0.46$ (C.2)
- 871 • Equivalent channel height, in μm , calculated as the unit cell fluid volume over the cell
- 872 projected area (2.56 mm²):
- 873 $h^{SOL} = 6.00 \times 10^{-4} \times \text{TMP}^2 - 1.13 \times \text{TMP} + 180$ (C.3)
- 874 • Channel porosity calculated as the ratio between unit cell fluid volume over total cell
- 875 volume of the undeformed channel without profiles (0.512 mm³):
- 876 $\varepsilon = 3.00 \cdot 10^{-6} \cdot \text{TMP}^2 - 5.64 \cdot 10^{-3} \cdot \text{TMP} + 0.90$ (C.4)
- 877 • Sherwood number (Sh) from [29] considering a fluid flow attack angle of 45°:
- 878 • TMP=0
- 879 $\text{Sh} = 0.346 \times \ln(\text{Re}) + 9.552;$ (Re $\leq$ 17.5) (C.5)
- 880 $\text{Sh} = 5.314 \times \ln(\text{Re}) - 4.636;$ (Re > 17.5) (C.6)
- 881 • TMP=10 kPa
- 882 $\text{Sh} = 0.414 \times \ln(\text{Re}) + 10.121;$ (Re $\leq$ 14.3) (C.7)
- 883 $\text{Sh} = 4.498 \times \ln(\text{Re}) - 0.723;$ (Re > 14.3) (C.8)
- 884 • TMP=20 kPa
- 885 $\text{Sh} = 0.417 \times \ln(\text{Re}) + 11.072;$ (Re $\leq$ 11.52) (C.9)
- 886 $\text{Sh} = 3.906 \times \ln(\text{Re}) + 2.616;$ (Re > 11.52) (C.10)
- 887 • TMP=30 kPa
- 888 $\text{Sh} = 0.462 \times \ln(\text{Re}) + 11.685;$ (Re $\leq$ 9.2) (C.11)
- 889 $\text{Sh} = 2.750 \times \ln(\text{Re}) + 6.615;$ (Re > 9.2) (C.12)
- 890 • TMP=-10 kPa
- 891 $\text{Sh} = 0.440 \times \ln(\text{Re}) + 8.934;$ (Re $\leq$ 21.3) (C.13)
- 892 $\text{Sh} = 6.608 \times \ln(\text{Re}) - 9.812;$ (Re > 21.3) (C.14)
- 893 • TMP=-20 kPa
- 894 $\text{Sh} = 0.359 \times \ln(\text{Re}) + 8.318;$ (Re $\leq$ 25.37) (C.15)
- 895 $\text{Sh} = 6.905 \times \ln(\text{Re}) - 12.797;$ (Re > 25.37) (C.16)
- 896 • TMP=-30 kPa
- 897 $\text{Sh} = 0.363 \times \ln(\text{Re}) + 7.807;$ (Re $\leq$ 29.8) (C.17)
- 898 $\text{Sh} = 7.778 \times \ln(\text{Re}) - 17.292;$ (Re > 29.8) (C.18)
- 899 where Re is the local Reynolds number:

$$\text{Re} = \frac{\rho U 2H}{\mu} \quad (\text{C.19})$$

In Eq. (C.19) μ is the viscosity of the generic solution *SOL* (*DIL* or *CON*), assumed to be constant (0.0089 Pa s) in the model.

NOMENCLATURE

$C^{DIL}, C^{CON}, C^{SOL}$	Concentration of <i>DIL</i> , <i>CON</i> or generic <i>SOL</i> (<i>DIL</i> or <i>CON</i>) solutions	mol/m ³
$C_{Bulk}^{SOL}, C_{IEM}^{SOL}$	Concentration in the bulk of a generic solution <i>SOL</i> and at the a generic membrane <i>IEM</i> -solution interface	mol/m ³
D^{IEM}, D^{SOL}	Salt diffusivity in a generic <i>IEM</i> and solution <i>SOL</i>	m ² /s
E_{spec}	Energy consumption per unit volume of product	kWh/m ³
F	Faraday constant (96,485)	C/mol
H	Undeformed nominal channel thicknesses	m
h^{SOL}	Equivalent fluid channel thickness of a generic solution <i>SOL</i>	m
I	Overall stack electric current	A
i_c	Ionic current density	A/m ²
$N_{SALT}^{TOT}, N_{Coul}^{TOT}, N_{Diff}^{TOT}$	Total, Coulombic and diffusive salt fluxes	mol/(m ² s)
J_p	Apparent product flux	l/(m ² h)
$J_W^{TOT}, J_W^{E.OSM}, J_W^{OSM}$	Total, osmotic and electro-osmotic water fluxes	m ³ /(m ² s)
K	Channel hydraulic permeability	m ²
L	Fluid channel length	m
$L_{p,IEM}$	Water permeability coefficient of a generic <i>IEM</i>	ml/(m ² hbar)
M_w	Water molecular weight	kg/mol
N_{Block}^x, N_{Block}^y	Number of rectangular blocks	-
N_{cp}	Total number of cell pairs	-
n_h	Hydration number	-
P	Profiled membrane pitch	m
P_{el}, P_{pump}	Electric and pumping power consumption	W
Q^{CON}, Q^{DIL}	<i>CON</i> and <i>DIL</i> solution flow rates	m ³ /s
$Q_{TOT,av}^{CON}, Q_{TOT,av}^{DIL}$	Average overall (stack) <i>CON</i> and <i>DIL</i> solution flow rates	m ³ /s
$Q_{TOT,OUTLET}^{DIL}$	Overall diluate outlet flow rate	m ³ /s
R	Universal gas constant (8.314)	J/(mol K)
$R^{CON}, R^{DIL}, R^{SOL}$	Areal resistance of <i>CON</i> , <i>DIL</i> and generic <i>SOL</i> solutions	Ω m ²
$R^{CEM}, R^{AEM}, R^{IEM}$	Areal resistance of <i>CEM</i> , <i>AEM</i> and generic <i>IEM</i> membranes	Ω m ²
R_{TOT}, R_{blank}	Total areal resistance of a cell pair and electrode compartments	Ω m ²

Re	Reynolds number	-
Sh	Sherwood number	-
T	Temperature	K
t	Membrane thickness	m
U_x^{SOL}, U_y^{SOL}	Superficial velocities along x and y in the channel SOL	m/s
V_f	Volume of fluid channels	m ³
V, V_{cp}	Potential voltage drop applied by a power supply and voltage drop over a cell pair	V
v_c, v_d	Inlet velocities of the CON and DIL solutions	m/s
W	Fluid channel width	m
x	Component of Cartesian coordinate system	m
y	Component of Cartesian coordinate system	m

905

906 **Greek symbols**

α_{IEM}	Perm-selectivity of a generic IEM	-
$\gamma^{CON}, \gamma^{DIL}$	Salt activity coefficients in CON and DIL solutions	-
ε	Channel porosity	-
$\eta, \eta_{BL}, \eta_{IEM}^{SOL}$	Total non-Ohmic voltage drop, non-Ohmic voltage drop due to concentration polarization and voltage drop at each SOL/IEM interface	V
θ_{IEM}^{SOL}	Polarization coefficient at the generic SOL/IEM interface	-
κ^{SOL}	Electrical conductivity of the generic SOL	S/m
μ	Fluid viscosity	Pa s
π_{IEM}^{SOL}	Osmotic pressure at the at the generic SOL/IEM interface	Pa
ρ^{SOL}, ρ_w	SOL and water density	kg/m ³
φ	Non-ohmic voltage drop due to fluid concentration gradient	V
$\Delta x, \Delta y$	Length and width of rectangular blocks	m
$\Delta p^{CON}, \Delta p^{DIL}$	Pressure drops in the CON and DIL channels	Pa

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908 **Acronyms and abbreviations**

AEM	Anion Exchange membranes
BL	Boundary Layer
Blank	Electrode compartments
CEM	Cation Exchange Membranes
CFD	Computational fluid dynamics
CON	Concentrate solution
CP	Cell pair
DIL	Diluate solution
ED	Electrodialysis
FE	Finite Element Method
FV	Finite Volume Method

IEM	Generic Ion Exchange Membrane (AEM or CEM)
RED	Reverse Electrodialysis
SOL	Generic Solution (CON or DIL)
TMP	Transmembrane pressure

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