Analysis and validation of the hydrodynamics of an electrodialysis cell using computational fluid dynamics

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HIGHLIGHTS

- Hydrodynamics and mass transfer in a electrodialysis reactor was studied via CFD.
- The theoretical results show a good correlation with those obtained experimentally.
- Theoretical and experimental mass transfer coefficients differ in max 16%.
- Major differences in the mass transfer coefficients are in the low velocity zones.
- CFD has shown the influence of the hydrodynamic regime on the process efficiency.

ARTICLE INFO

ABSTRACT

Due to the shortage of drinking water and the deterioration in its quality several processes have been developed to remove the ions and impurities contained. A technology used for the ions removal is the electrodialysis, which uses an electric field gradient and ion-exchange membranes to promote the movement of ions from treated water to a suitable compartment.

Studies carried out using this technology have shown the influence of the hydrodynamic regime on the efficiency, mass transfer rate on the process and its influence on the concentration polarization.

Using the finite element method, this work describes the hydrodynamic behavior and mass transfer in a filter press type electrodialysis reactor using computational fluid dynamics and experimental validation of the results obtained with CFD.

The theoretical results show a good correlation with those obtained experimentally for hydrodynamics, from which the validation of the mass transfer and the distribution of potential on the electrodes and the solution is possible. A second validation is made by comparing theoretical and experimental mass transfer coefficients obtaining a maximum error of 16%.

1. Introduction

Water electrochemical treatment using ion-exchange material has a wide use in electrodialysis [1,2] and electrodeionization [3,4]. Both techniques utilize electrical current as the main driving force in matter separation so mass transfer of charged particles is important. In fact electrodeionization is a processes combining ion-exchange with electrodialysis. The knowledge of hydrodynamics for both systems allows the improvement of the performance of the processes as a whole [5,6]. The performance of electrodialysis process depends on several parameters such as applied potential or current, or hydrodynamics in the diluted compartment. The hydrodynamics in the diluted compartment is influenced by flow entrance effects. Given that electrodeionization combines ion-exchange and electrodialysis, it is important to take into account the inlet and outlet geometry of the electrodializer [7].

The design of the necessary components of an electrodeionization reactor is very similar to those used for a conventional electrodialysis, resulting in the possibility to use the same strategy for the design of the reactor given that EDI configuration was developed to improve the electrical conductivity drawback at ED cell [5]. There are some published works available that study the effects of the geometry of the electrodializer over different process parameters. Pawlowsi et al. [8] studied a reverse electrodialysis process using various concentrations of NaCl solutions and studied the ohmic and non-ohmic resistances in the stack varying the hydrodynamic conditions (1.5 cm s^{-1}). Using a chronopotentiometric study they determined the thickness of the boundary layer finding that the process is strongly influenced by the inlet effects. The presence of spacers reduces the thickness of this boundary layer increasing the ohmic resistance on the membrane. In

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their findings they suggest that the length of the electrodializer is not bigger than the zone in which the inlet is influencing. Zourmand et al. [9] developed a bidimensional, stationary, isothermal model to predict the mass transport of an ion in the electrodializer considering the concentration polarization phenomena and its influence in ion separation. This model includes the Navier-Stokes and Nerst-Planck equations. These equations where solved using the finite element method and CFD on the dilute and concentrated compartment and the membranes, being capable of predicting the local concentrations and ion fluxes, electric potential and velocity distribution in the electrodializer. This mathematical model is limited to current densities below the limiting diffusion current and neglecting the effect of the spacers. Turek and Mitko [10] developed a model to measure the RTD in a working reactor to assess the effect of the applied current on the ion migration and the electroosmotic flux of the water. The change of the RTD in the concentrated compartment was confirmed in the 0.38–0.84 cm s^{-1} range observing a substantial longitudinal dispersion, being the objective of this methodology to obtain a method that allows to predict the probability of the formation of crystals on the membrane.

There are few studies that have reported the impact of hydrodynamics on the efficiency of an electrodialysis reactor; however it is a fundamental design parameter. Furthermore, published studies show the global influence of hydrodynamic on the rate of mass transfer efficiency of the process and its relationship to concentration polarization. Often optimizations or appropriate scaling are not possible since the measured response of the studied parameter (hydrodynamic regime) does not allow to visualize or predict local variations, its effects and how to modify them. Due to the complexity involved on the analysis of fluid flow equations when the geometry of the system is complicated, computational tools have been developed such as Computational Fluid Dynamics (CFD), that help describing the hydrodynamics in the compartment globally and locally, as well as mass transfer (without requiring a large number of experimental tests) [11].

The aim of this paper is to propose a simple methodology for the experimental and theoretical description of an electrodialysis/ electrodeionization reactor using Digital Image Analysis and Computational Fluid to validate the results. The knowledge gain from this paper will allow a better understanding of the mass transfer phenomena in an electrodeionization reactor.

2. Methodology

The reactor used consists of DSA and a stainless steel cathode, the reactor compartments are delimited by ion exchange membranes and the compartments formed between the membranes are of 50×80 mm
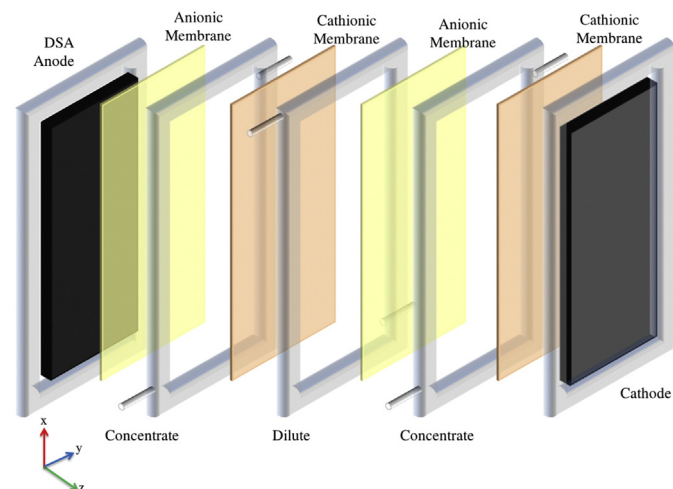

Fig. 1. Schematic illustration of the reactor geometry.

(Fig. 1). The fluid is fed by an inlet of 3 mm diameter located in the lower compartment using a hose with a diameter of 1.6 mm and a discharge identical to the inlet located at the top of the compartment. For the hydrodynamics study, the continuity equation and the momentum balance for a steady-state incompressible flow are solved. Calculating the Reynolds number a value of $Re = 17$ for a mean residence time of 1 min was obtained, therefore, a laminar model was considered to simulate de system.

Simulations were carried on with a mesh conformed for 172,161 tetrahedral and hexahedral elements, which provides sufficient detail in the areas with the highest gradients of speed and concentration. Simulations were carried out with an Intel Core™ 2 Duo CPU T 5570 a 2.00 Ghz processor and 16GB of RAM. Details of the additional parameters used for the simulation can be found on Table 1.

A 6 mm gap between spacers and an open channel configuration were used due to their availability since this configuration was a first test to assess the feasibility of the electrodializer for an electrodeionization process (including further modelling).

To describe the effect of the hydrodynamic over mass transfer it is necessary to know the flow distribution inside the cell. The validation of the simulated hydrodynamic results was made using a flow distribution technique, replacing the ion-exchange membranes and electrodes by transparent acrylic plates that allowed to obtain a video showing the hydrodynamic behavior inside the reactor, then to carry on the Digital Image Analysis, a pulse of 1.0 mL of a blue dextran solution (50 g L^{-1}) was introduced in an injection port located 25 diameters away from the input. Once the reactor was operating at steady state the flow distribution was recorded digitally using a Canon Digital Video GL2 3CCD camcorder.

The experimental results were compared with the simulated velocity profiles, determined by drawing a plane in the center of the channel ($z = 3$ mm) and plotting the velocity profile of the cell with respect to x axis, using data from simulation and local variations considering the fluid velocity. The experimental trajectory of the fluid was obtained by separating the video in to frames of 720×480 pixels and tracking the path of the dye frame by frame that it was injected into the system.

The validation of the simulated results was obtained by comparing experimental and simulated data. Detailed analysis allowed the detection of stagnant areas, channeling and flow distribution to optimize the reactor operation.

The simulation of the primary current distribution was performed using COMSOL Multiphysics 4.3a.

The imposed voltage on the simulated electrodialysis cell was 4.2 V for the steel cathode and a voltage of 0 to the anode, and the current density in the cathode was 2.5 A m^{-2}.

The mass transport in the cell was modeled under a current density of 2.5 A m^{-2} at laminar hydrodynamic conditions using results obtained for the flow distribution and potential distribution of previous simulations. For the Nernst-Planck equation the velocity term in the portion of the convection contribution is obtained from the simulation of hydrodynamics, and the term of potential is obtained from the simulation of the potential distribution.

For the bulk of the solution, the Nernst-Planck equation considering diffusion, migration and convection was used, to solve the boundary

Table 1
Simulation parameters and geometry dimensions.

Reaction compartment volume	2.4×10^{-5} m^3
Height and width of the compartment	0.08×0.05 m
Thickness of the compartment	6×10^{-3} m
Inlet and outlet diameter	1.6×10^{-3} m
Thickness of the ion-exchange membranes	1.5×10^{-4} m
Fluid viscosity	8.82×10^{-4} Pa s
Fluid density	994.4 kg m^{-3}
Operation flow	
2.5×10^{-2} L min^{-1}	
Residence time	1 min