A multi-physics modelling tool for Reverse Electrodialysis

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Abstract

Reverse electrodialysis (RED) is a promising technology for generating electric power by the direct conversion of the chemical potential difference of two salt solutions (salinity gradient power). The stack is fed by the two solutions in alternated channels, separated by an alternated series of anion and cation exchange membranes. The selective ion transport across the membranes, from the concentrated channels towards the dilute ones, is converted at the electrodes (redox reactions) into a current of electrons supplying an external load. The process performance depends on a number of phenomena interacting at various scales. Fluid dynamics, stack geometry, membranes and operating conditions are the main aspects identifying the stack configuration and affect in a complex way the power output and the energy efficiency. A multi-physics model can be an effective predictive tool for the process design and optimization, passing through the modelling of a number of different phenomena involved, from the fluid dynamics, to the ions migration, from the solution/membrane equilibria to the ohmic phenomena, etc.

In this work, a multi-physics modelling approach has been developed for the RED process. Membranes were included in the computational domain and their behaviour was characterized by two parameters, i.e. the counterions/co-ions diffusion coefficient and counterions/co-ions mobility. These parameters were estimated starting from the available experimental information through an accurate model calibration. Moreover, the electroneutrality condition within the membranes took into account the concentration of the fix charges. Partition coefficients were used to relate the concentration at membrane-side to that at solution-side of the membrane-solution interfaces. At these interfaces, the jump of voltage was calculated as Donnan potential, i.e. by assuming the equilibrium condition between the two phases; the activity coefficients were assumed equal to 1.

Fluid dynamics, mass transfer and electric phenomena were modelled within the cell-pair by 2-D simulations allowing all controlling phenomena to be accurately predicted by providing the distribution of the main quantities computed (concentration, electric potential, fluxes profiles, current streamlines). As an example, the Donnan equilibria and relevant potential raise at IEM/solution interface were predicted for three different scenarios (i.e. Open Circuit, max Power output, short-cut circuit) as illustrated in Fig. 1.

The model was also adopted for analysing the difference in RED stacks equipped either with standard non-conductive spacers or with profiled membranes, in order to assess the main differences in behaviour and final performance. An interesting example of the effect of using profiled membranes on the internal current distribution is reported in Fig. 2.

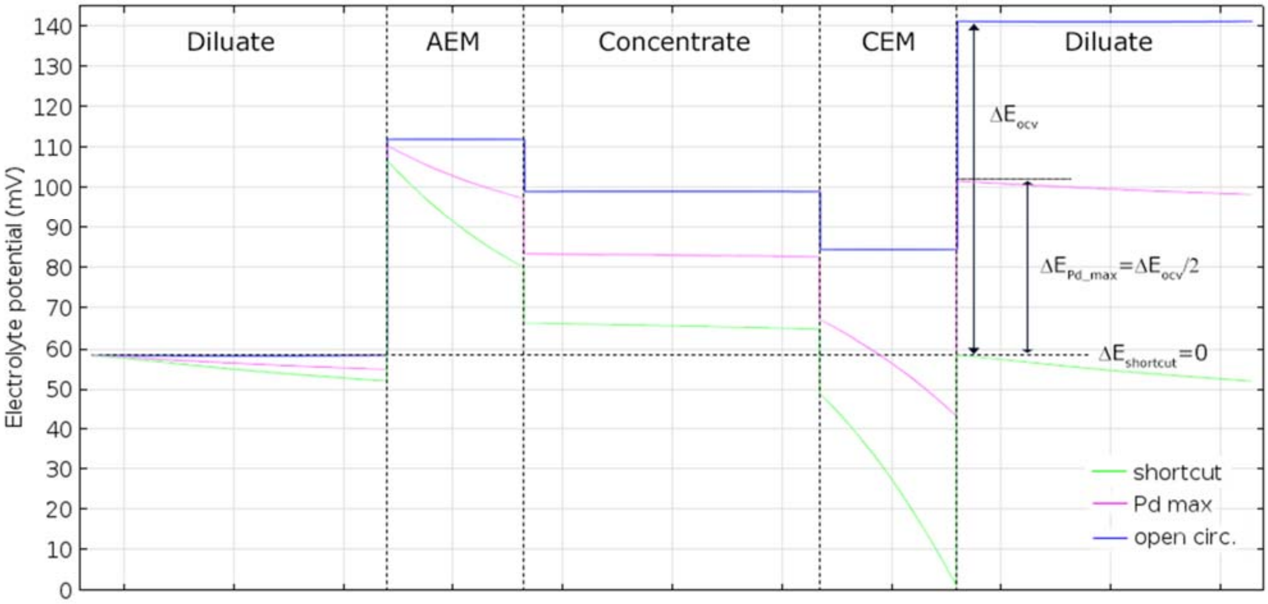

Fig.1. Electric potential profiles in a single cell pair, in conditions of open circuit, maximum power density and shortcut circuit. IEMs thickness 125 μm, channels thickness 270 μm, inlet feed conc. 0.5M-4M, temperature 20°C.

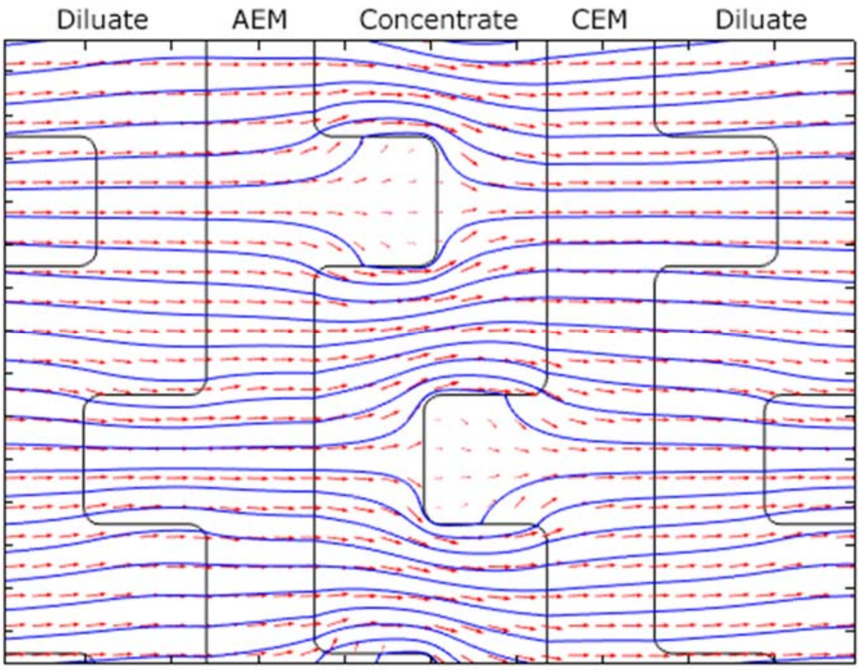

Fig. 2. Current density field for a RED cell equipped with profiled membranes. Current leaving a dilute channel tends to flow preferentially through the pins of the adjacent membrane; current leaving a concentrate channel tends to bypass the tip of the adjacent membrane. Simulation conditions: 1.2 mm x 1.2 mm x 10 cell pairs, IEMs thickness 125 μm (excluding pins), channels thickness 270 μm, inlet conc. 0.01M-4M, temperature 20°C.

Keywords: Reverse electrodialysis, multi-physics, profiled membranes, modelling