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Electrodialysis with capacitive electrodes (CED): hierarchical process modelling for water desalination

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Introduction

Membrane desalination processes play a crucial role in the current scenario of drinking water production. In particular, electrodialysis (ED) is currently spreading as a viable alternative to other membrane desalination processes, also thanks to the recent developments in ED process equipment. One of the most interesting developments is represented by the use of capacitive electrodes instead of Faradaic electrode compartments (Barber *et al.* 2014). In the literature, this possibility has been mainly explored with capacitive de-ionisation and Reverse ED, showing advantages such as absence of unstable or hazardous products (i.e. Cl_2) and reduction of electrode potential drop (Vermaas *et al.* 2012; Vermaas *et al.* 2013). In order to avoid charge saturation, ED with capacitive electrodes (CED) needs a periodical polarity switch, a feature that is already applied for fouling prevention in most industrial ED units. To the authors' knowledge no CED models can be found in literature. Therefore, the present work describes the development of the first dynamic model for CED.

Modelling approach

A one-dimensional hierarchical CED model has been developed. The lower hierarchy model of the cell pair is based on partial differential mass balance equations and phenomenological expressions of fluxes that account for transport phenomena through the membranes. In addition, CFD-derived correlations are used to characterise polarization phenomena. At the higher scale of the stack, multiple pairs are considered to constitute the stack along with the capacitive electrodes. An equivalent circuit describing the electrical behaviour of the system was adopted in order to account for the dynamic behaviour of capacitive electrodes, simulated with a series of a capacitor and a resistor. In this way, it was possible to model the intrinsically transient behaviour of typical CED operation.

Results and Discussion

The model was implemented in *PSE gPROMS ModelBuilder*, where a set of dynamic simulations was performed. As a consequence, it was possible to extensively analyse the dynamic behaviour of a CED unit, including also the polarity inversion step.

Figure 1.b shows simulation results for a typical CED operation using electrodes with a specific capacity of 1.2 F/cm^2 and an areal resistance of 13 $\Omega\cdot$cm^2. A 24 cell pairs unit with a constant applied voltage of 5V is simulated. During the first part of the cycle

the voltage drop at the electrodes increases due to charge accumulation. As a consequence, the voltage drop of cell pairs and the current decrease, causing the outlet concentration of Stream 1 (i.e. the diluate) to increase until it exceeds 500 ppm. At this point, the polarity is switched by applying an opposite voltage. For this reason, all fluxes are inverted (Figure 1.a) as well as the two streams. The immediate response to the switch is characterised by a sudden peak of high negative current after which a normal operation is gradually restored. It is worth noting that the electrodes potential drop remains positive in the first part of the inverted operation, as the accumulated charge is being desorbed from the electrodes. This justifies the absolute value of voltage applied to the membrane pile being higher than the external applied voltage.

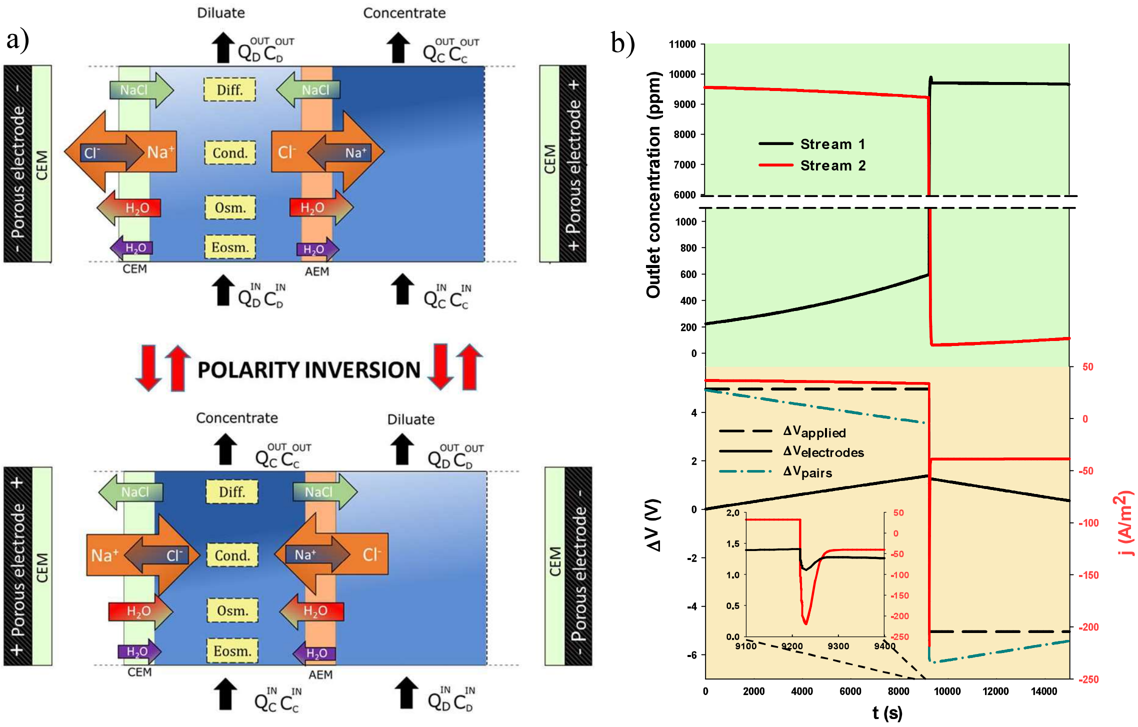

Figure 1. a) Schematics of a CED unit working in both polarities. b) Time distribution of applied voltage, current density and outlet concentrations in a typical CED operating cycle.

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