Modelling of Electrodialysis units by a multi-scale process simulator

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Drinking water production by desalination is an interesting alternative to face water scarcity issues. Electrodialysis (ED) is an electro-membrane process that is actually gaining attention as a competitive alternative for seawater and brackish water desalination due to recent developments in manufacturing of high performance ion exchange membranes (IEMs). In this context, a suitable process simulator can be a very effective tool in order to drive the design of optimized ED systems.

In this work a novel mathematical model of ED units was developed by a hierarchical simulation strategy of separation of scales, in order to address the full simulation problem. The model was implemented in *PSE gPROMS Modelbuilder*. In the lower-hierarchy model, transport phenomena of salt and water were simulated within the whole cell pair of an electrodialyser. Then, the higher-hierarchy model describes the behaviour of the stack. The model is based on mass balance equations and phenomenological expressions of fluxes that describe transport phenomena along channels and across IEMs. In addition, Kirchhoff's law together with the Nernst's law for the non-Ohmic voltage drop was used to determine the electrical behaviour of the equivalent circuit. Finally, the model makes use of CFD correlations from a lower scale as input data in order to predict the effect of concentration polarization and the contribution of pumping to the energy consumption.

Co-current, counter-current and crossflow configurations were simulated, by obtaining the distribution of current density/voltage and concentration along the channels. Finally, total resistance, total power consumption and specific energy consumption were computed. Several simulations were carried out by changing the operating conditions and the stack features. Simulation results showed a good agreement with experimental findings as obtained from the literature, demonstrating that the model is able to adequately capture the phenomenological description of the ED process.

Keywords: Electrodialysis, Multi-scale, Process simulator.

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