Flow and process modelling of a Selective Membrane Capacitive Deionisation

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Abstract
Groundwater stores 97 % of the accessible global freshwater and is substantial for drinking water supply. Geological conditions, seawater intrusion or anthropogenic influences threaten the quality of groundwater by increased salt concentrations [1].
One of the emerging electrochemical desalination technologies is the membrane capacitive deionization (MCDI), which can be applied for slightly and moderate saline waters (TDS < 5 g/L) [2]. The energy demand is correlated to the amount ions removed, water recovery and ionic and electronic resistances.
The MCDI operates at a low potential with 1.2-2.0 V, making this process combined with an effective flow rate an energy efficient desalination process [3]. Within the joint project innovatION, funded by the German Federal Ministry of Education and Research (02WV1572A), a monovalent selective MCDI process with new selective membranes, new desalination modules and related flow and process model are developed. The desalination modules in laboratory and pilot scale are optimized, applying numerical flow simulations as Computational Fluid Dynamics (CFD) for the electrochemical cell.
Parameters improved are pressure loss and the flow distribution within one cell and a stack consisting of several cells. User defined functions (UDF) in ANSYS Fluent are used to implement the process model and for process and operating parameter optimization. Implementing the models using UDF takes advantage of the provided functions of ANSYS, like meshing, solvers, post-processing and direct coupling of flow and process model. The process model is based on the modified Donnan model for the electrode structures with micropores and overlapping electrical double layers (EDL) and is further extended with the Gouy-Chapman-Stern model, describing the ion distribution at planar surfaces without overlapping EDL [4]. In the presentation the approaches of flow and process models, the implementation as UDF and results are discussed.
Key words (5 max)

Electrochemical Membrane Process, MCDI, Selective Deionization, CFD

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