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NOVEMBER 8–11, 2020
PRAGUE, CZECH REPUBLIC
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BOOK OF ABSTRACTS

On-line International Conference
on Membrane Processes

8-11, November 2020

Prague, Czech
Republic

Organized by CZECH MEMBRANE PLATFORM,

www.czemp.cz

Book of Abstracts, MELPRO Conference, 2020
Edited by Czech Membrane Platform
Published by Czech Membrane Platform in 2020
Printed by Academic and Medical Conference Agency
1st edition, 100 copies

Abstracts, except for their headings, are printed without editing.

ISBN 978-80-907673-3-1
ISSN 2694-8958

A VALIDATED MULTI-SCALE MODEL OF A NOVEL ELECTRODIALYTIC ACID-BASE FLOW BATTERY

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Abstract: Electrical energy storage is crucial for a deeper penetration of intermittent renewable energies, e.g. solar and wind. The Acid/Base Flow Battery (AB-FB) is a novel, sustainable, environmental-friendly storage technology with high energy density[1]. The process is based on reversible electrodialytic techniques that convert the electrical energy in the chemical energy associated to pH gradients and *vice versa*. The bipolar membrane electrodialysis process operates in the charge phase, while the bipolar membrane reverse electrodialysis in the discharge phase. The stack consists of repetitive units, called triplets, made up of an anion-exchange membrane, a bipolar membrane, and a cation-exchange membrane, separated by spacers forming the channels where the acid, base and salt solutions flow.

This work presents for the first time an experimentally validated AB-FB process model along with a sensitivity analysis. The model is based on a multi-scale simulation strategy, where four different dimensional scales are integrated within a comprehensive simulation tool with distributed parameters. The lowest hierarchical level concerns the channels. It includes CFD simulations for the estimation of polarization phenomena and pressure losses, and the correlations for the physical properties of the solutions. The middle-low hierarchical level simulates the triplets, by computing mass balances, membrane fluxes, electrical resistance and electromotive force. The middle-high scale simulates the stack by an electrical sub-model intended to compute the shunt currents, and by a hydraulic sub-model to calculate pressure losses. Finally, the highest hierarchical level simulates the external hydraulic circuit including dynamic mass balances in the tanks.

The model was validated against an original experimental campaign, showing a good agreement. A broad sensitivity analysis was performed in order to explore the behavior of the battery under several scenarios. The model outcome illustrates how stack geometry, operating parameters and battery layouts (e.g. open-loop vs closed-loop operations) can affect the process performance. By adopting some measures to tackle the shunt currents and taking thermodynamic advantages from open-loop operations, the round trip efficiency reached values up to 70%. This original model will orient the identification of optimized and competitive AB-FB systems.

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A PROCESS MODEL OF ELECTRODIALYSIS INCLUDING MEMBRANE DEFORMATION EFFECTS

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Abstract: Electrodialysis (ED) is an electro-driven process that makes use of ion exchange membranes (IEMs) under an applied electric field. The main application of ED is the desalination for drinking water production. A transmembrane pressure (TMP) distribution may arise in ED stacks due to an uneven pressure distribution in the two fluid channels, thus causing membrane/channel deformation and flow redistribution. This can occur in large-scale non-parallel configurations, e.g. cross-flow arrangements. Detrimental effects of membrane deformation have widely been studied with reference to several membrane processes. However, this aspect has been neglected in ED applications.

In this work, a novel process model of ED units including the effects of membrane deformation is presented[1]. The model was developed with a multi-scale architecture. The model simulates the fluid-structure interaction (i.e. membrane deformation and flow redistribution) in a cell pair[2] based on correlations from small-scale numerical simulations (structural mechanics and computational fluid dynamics)[3,4]. Then, transport and electrochemical phenomena occurring in ED systems are simulated. Cross-flow ED units were simulated in two-dimensions (length and width). Results showed that mild deformations have a negligible impact on the ED process performance. However, configurations prone to larger deformations (e.g., thin membranes) exhibited more significant effects, with an increase in the specific energy consumption. The same approach can be used for other configurations (e.g. counter-flow and asymmetrical channels in parallel flow) and for reverse electrodialysis.

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