MODELLING OF UNDERLIMITING AND OVERLIMITING CURRENT TRANSPORT IN ELECTRODIALYSIS: CHALLENGES AND OPPORTUNITIES

BRAM DE JAEGHER, WIM DE SCHEPPER, INGMAR NOPENS, AND ARNE VERLIEFDE

Abstract. Electrodialysis (ED) is a membrane separation technology that employs an electric field and ion-exchange membranes to separate charged components in solution. ED is a highly efficient and selective technology with prominent industrial applications in the desalination of brackish and seawater to drinking water, the demineralisation of whey proteins and the stabilisation of wine. The development of an efficient and generic model for ED could facilitate the design and operation of ED facilities and is of great interest to science and industry. The system is governed by the Poisson-Nernst-Planck equations, a singulary perturbed system of partial differential equations that is notoriously difficult to solve. Several simplifications can be made to alleviate the computational burden, i.e. at underlimiting conditions (no diffusive mass transfer limitations) the local electroneutrality principle is valid and a description based on the Laplace-Nernst-Planck equations with one-way momentum coupling is adequate [1]. At overlimiting currents (significant mass transfer limitations), the formation of a space charge region generates electroconvective vortices that need to be accounted for but the computational cost is high. The driving force of these vortices localises closer to the system boundaries with increasing salt concentrations and even with simplified boundary conditions [2] the mesh requirements are too stringent to simulate realistic electrolyte conditions. It remains a challenge to simulate ED in overlimiting conditions at realisitic electrolyte concentrations within a reasonable timeframe. However, an opportunity arises to employ the Reynolds-averaging framework as has been done for electromagnetic and buoyancy forces [3]. Several closure terms will have to be modelled.

Keywords: Electrodialysis, Fluid dynamics, Reynolds-averaging, Singularly pertubed PDEs

Minisymposium: Numerical Methods for Water Resources

References

[1] A. Campione, L. Gurreri, M. Ciofalo, et al. Electrodialysis for water desalination: A critical assessment of recent developments on process fundamentals, models and applications. *Desalination*, 434:121-160, 2018.
[2] A. M. Uzdenova, A. V. Kovalenko, M. Kh. Urtenov and V. V. Nikonenko Theoretical analysis of the effect of ion concentration in solution bulk and at membrane surface on the mass transfer at overlimiting currents., *Russian Journal of Electrochemistry*, 53(11):1254-1265, 2017.
[3] D. R. Wilson, T. J. Craft, H. Iacovides Application of RANS turbulence closure models to flows subjected to electromagnetic and buoyancy forces., *International Journal of Heat and Fluid Flow*, 49:80-90, 2014.

BIOMATH, Department of Data Analysis and Mathematical Modelling, Ghent University, Coupure links 653, 9000 Ghent, Belgium
E-mail address: Bram.DeJaegher@UGent.be

VITO Flemish Institute for Technological Research, Boeretang 200, 2400 Mol, Belgium
E-mail address: Wim.DeSchepper@vito.be

BIOMATH, Department of Data Analysis and Mathematical Modelling, Ghent University, Coupure links 653, 9000 Ghent, Belgium
E-mail address: Ingmar.Nopens@UGent.be

PaInT, Department of Applied Analytical and Physical Chemistry, Ghent University, Coupure links 653, 9000 Ghent, Belgium
E-mail address: Arne.Verliefde@UGent.be