Maxwell-Stefan modelling of ion transport in a Nafion membrane

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Abstract title	MAXWELL-STEFAN MODELLING OF ION TRANSPORT IN A NAFION MEMBRANE
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Background

Cation-exchange membranes are used in electrolysis processes to separate anodic and cathodic products due to their high selectivity of positive ions. The principle of all cation-exchange membranes is the combination of mass and electrical charge transport by cations through the perm-selective membrane applying electrical potential gradient. A nafion membrane with sulfonic groups separating sodium chloride and sodium hydroxide of higher concentration solutions is studied in this paper.

Aims

The aim is to investigate the membrane resistance to transport of ions in a nafion membrane by mathematical modeling of ion transport through the membrane under high current and concentration conditions.

Methods

For prediction of ion transport inside the membrane appropriate mass transport and equilibrium models are required. The mass transfer can be modeled using either the Nernst-Planck or the Maxwell-Stefan equations [1]. The Nernst-plank equation neglects the interactions of ions and according to literature it is valid for system of dilute concentrations [2]. The Maxwell-Stefan equation takes the interaction of different species into account. However, it requires reliable data for diffusion coefficients [3]. In this paper, a mathematical model of ion transport in the membrane is developed based on the Maxwell-Stefan equation. In addition, the boundary conditions are determined with the Donnan equilibrium [4,5]. Solving the Maxwell-Stefan equations requires the selection of a component that is not calculated from the molar flux equations, but from the Gibbs-Duhem rule that the sum of mole fractions is unity. For charged components an additional condition is the electroneutrality.

Results

We show that the Maxwell-Stefan equation is sensitive for the choice of component that is eliminated (Figure 1-2). When no current is applied Na^+ ions are expected to diffuse from cathode to anode and the current density should force them toward the cathode. Also, increasing the current density causes higher driving force for OH^- ions to diffuse back and less Cl^- ions to diffuse into the membrane.

Summary/Conclusion

The model in case of Na^+ elimination predicts that increasing the current density results in more transport of Na^+ ions from cathode to anode compartment. This can be due to the fact that the potential gradient which forces Na^+ ions to transport toward cathode is not predicted by the electronetrality condition. Also, the back migration of OH^- is decreasing when current is applied to the system. In case of OH^- elimination the transport of ions is as expected but increasing the current density can limit the transport of sodium ions.

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[4] H. Strathmann, Ion-exchange membrane separation processes, firts ed., Elsevier, 2004.

[5]M. Higa, et al, Simulation of the transport of ions against their concentration gradient across charged membrane, J. Mem. Sci. 37 (1987) 251-266.

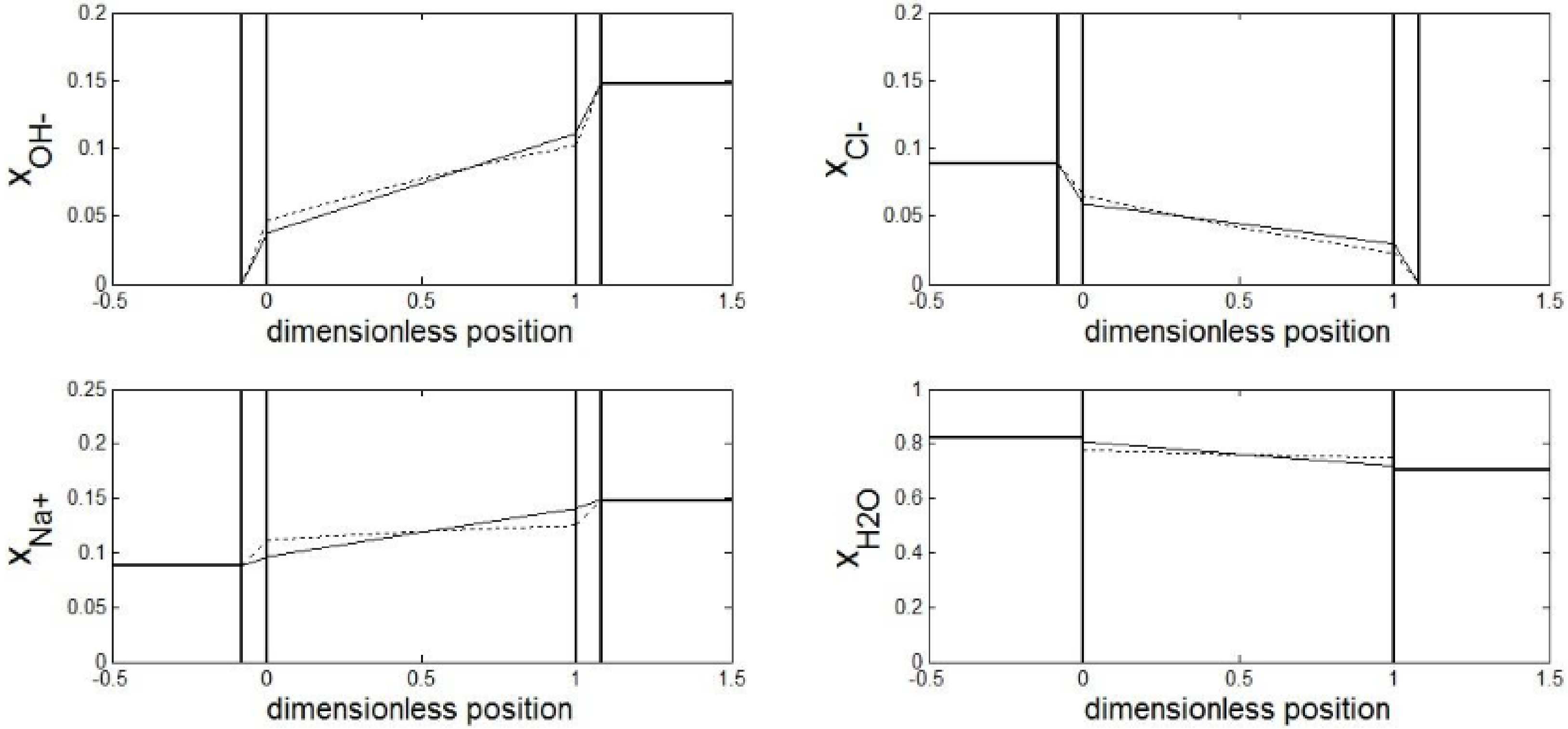

Figure 1. Mole fraction profile of Na+, Cl- and OH- over anolyte (NaCl), membrane and catholyte (NaOH) (Na+ elimination)

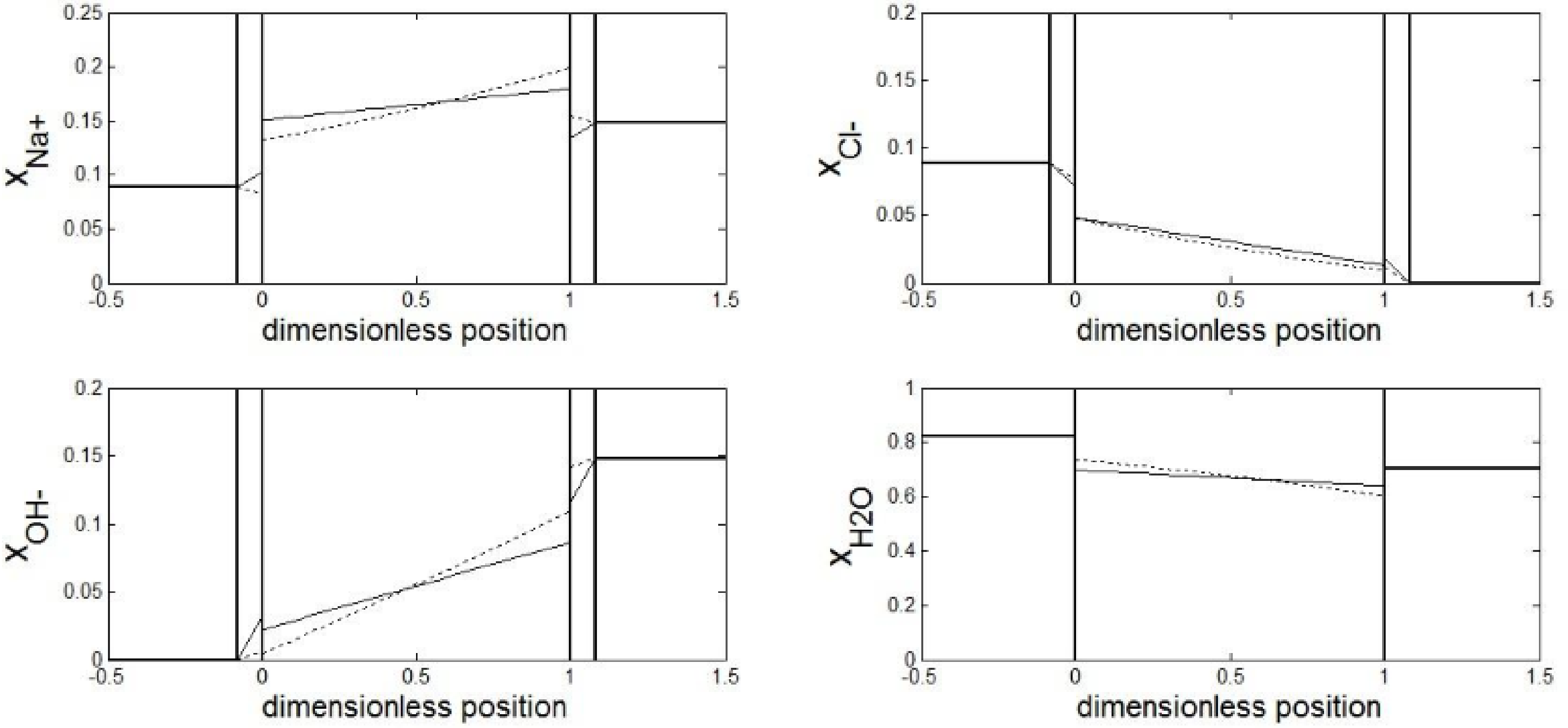

Figure 2. Mole fraction profile of Na+, Cl- and OH- over anolyte (NaCl), membrane and catholyte (NaOH) (OH- elimination)