

## Direct epoxidation of propene with vapor hydrogen peroxide

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### View abstract data

**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-planck 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  $\text{Na}^+$  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  $\text{OH}^-$  ions to diffuse back and less  $\text{Cl}^-$  ions to diffuse into the membrane.

### Summary/Conclusion

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

[1] R. Krishna, Multicomponent mass transfer, John Wiley and Sons , 1993.

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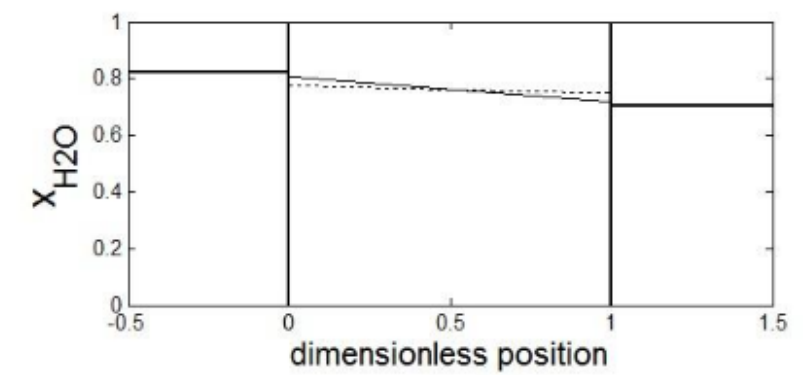
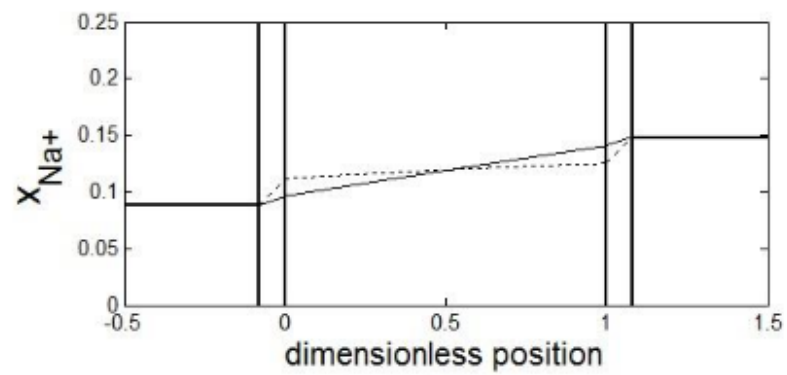
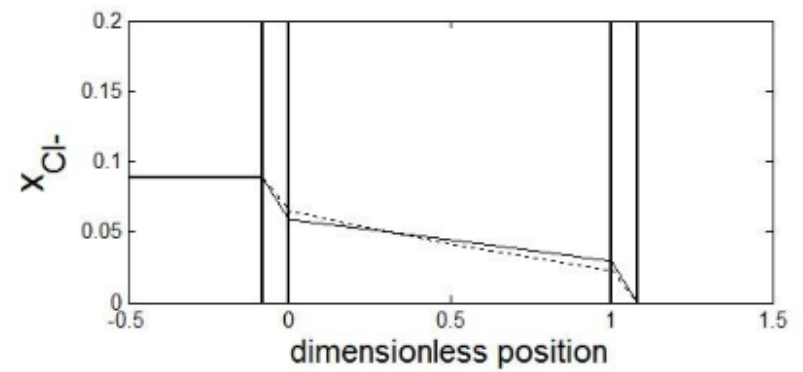
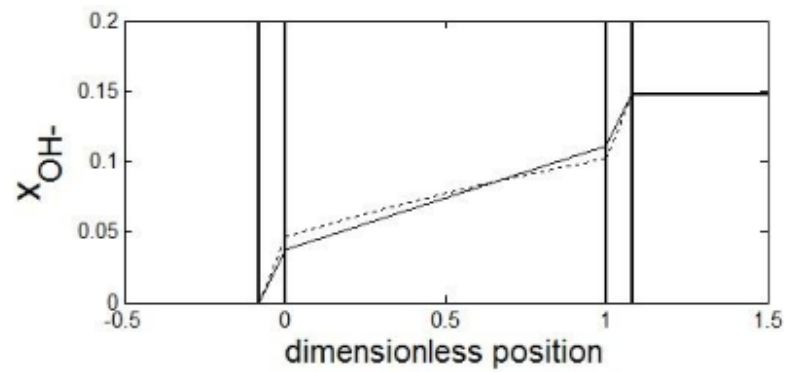


Figure 1. Mole fraction profile of  $Na^+$ ,  $Cl^-$  and  $OH^-$  over anolyte ( $NaCl$ ), membrane and catholyte ( $NaOH$ ) ( $Na^+$  elimination)

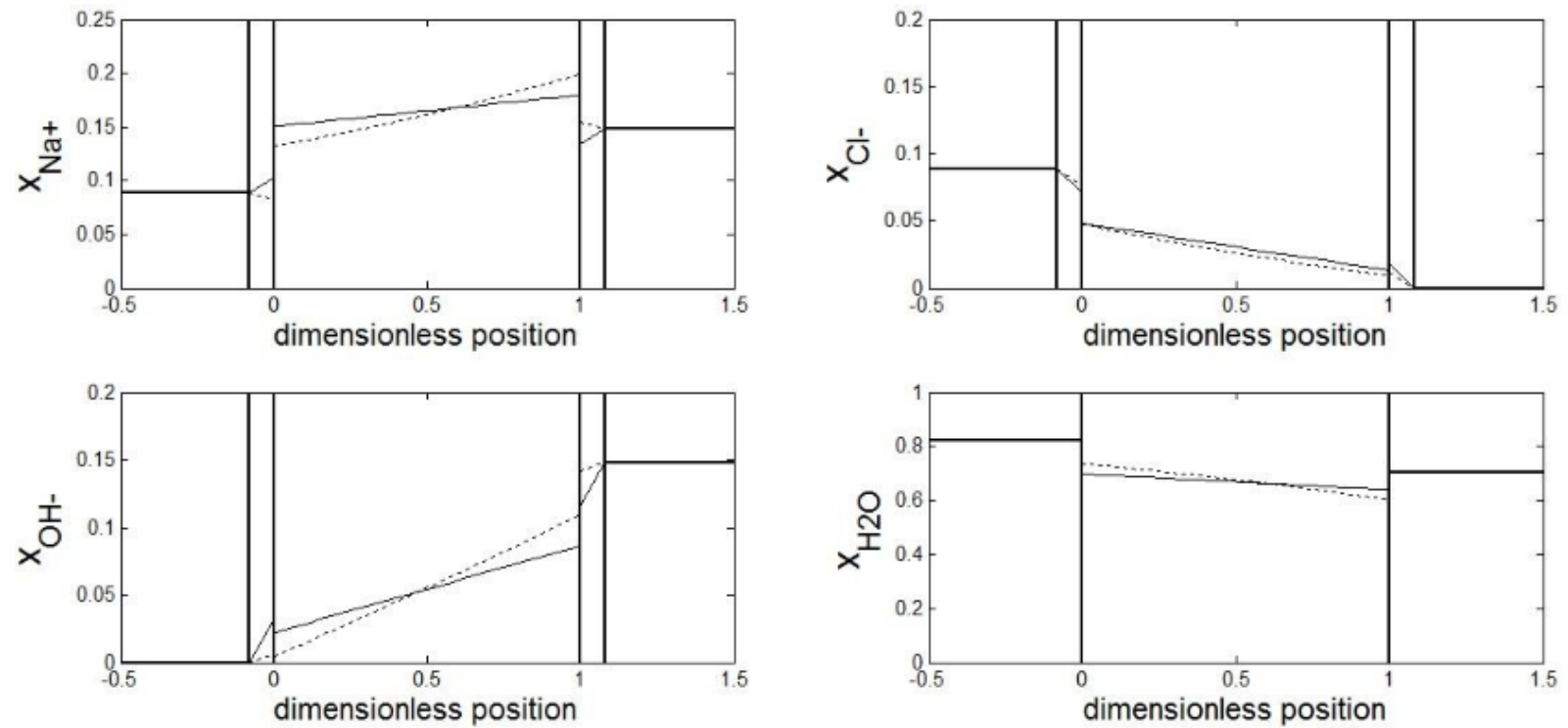


Figure 2. Mole fraction profile of  $Na^+$ ,  $Cl^-$  and  $OH^-$  over anolyte (NaCl), membrane and catholyte (NaOH) ( $OH^-$  elimination)