Ion transport Modeling in a Bipolar Membrane

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1. Introduction

The COL(Carbonate-based Oxidative Leaching) process is an environmentally-friendly technique for collecting only uranium from spent fuel with oxidation-leaching/precipitation of carbonate solution. The bipolar membrane used for the electrolyte circulation of the salt used in the COL process is a special form of ion exchange membrane which combines CEM(cation exchange membrane) and AEM(anion exchange membrane). After arranging positive ion exchange layer toward negative terminal and positive ion exchange layer toward positive terminal, then supply electricity, water molecules are decomposed into protons and hydroxyl ions by a strong electric field in the transition region inside bipolar membrane.[1)]

In this study, a theoretical approach to increase the efficiency of Na^+ and $NO3^-$ ion collecting device using bipolar membrane was taken and simulating using the COMSOL program was tried. The details of results are also discussed.

2. Modeling

2.1 Theoretical model

The bipolar membrane is an ion exchange membrane which has the structure of both anion exchange layer and cation exchange layer attached to each other. As shown in Figure 1, reaction $H_20 \rightarrow H^+ + OH^-$ occurs when an electric current is applied to dissociate water into H^+ and OH^-.[2)]

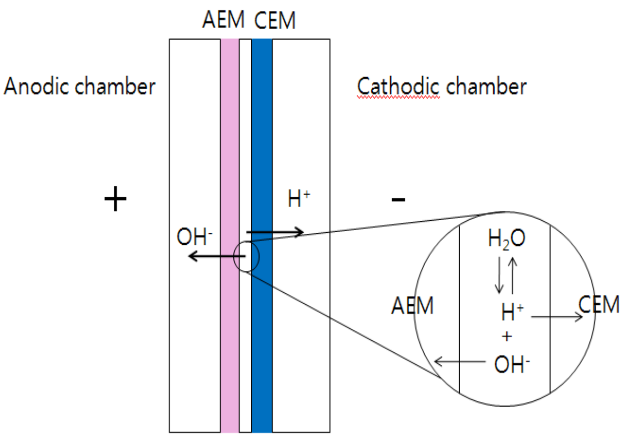

Fig 1. Bipolar electrodialysis configuration

Based on the conservation of mass of each of the species, we formulated the following theoretical model. The mass balance equations in the diffusion layers are given by,

$$\nabla \cdot \overrightarrow{N_i} = R_i$$

where the fluxes, $\overrightarrow{N_i}$, are given by the Nernst-Planck equation,

$$\overrightarrow{N_i} = -D_i \nabla c_i - z_i u_{m,i} F c_i \nabla \phi + c_i u$$

Furthermore, it is assumed that the electrolyte in the diffusion layers are stagnant, i.e., u=0[3)]

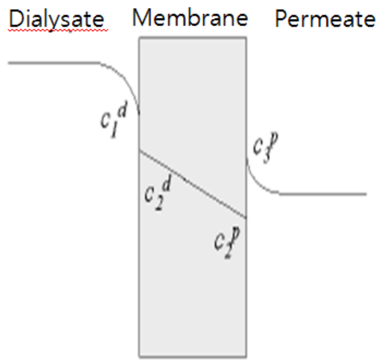

Fig 2. Diagram of the concentration profile across the membrane

There are discontinuities in the concentration profile at the boundaries between liquid and membrane phase. So to get continuous flux over the phase boundaries, apply a special type of boundary condition using the stiff-spring method.

$$(-D\nabla c_1 - zu_m F c_1 \nabla\phi + c_1 u)\cdot n = M(c_2 - Kc_1) \quad \text{at boundary}^{d/m}$$

$$(-D\nabla c_2 - zu_m F c_2 \nabla\phi)\cdot n = M(Kc_1 - c_2) \quad \text{at boundary}^{m/d}$$

$$(-D\nabla c_2 - zu_m F c_2 \nabla\phi)\cdot n = M(Kc_3 - c_2) \quad \text{at boundary}^{m/p}$$

$$(-D\nabla c_3 - zu_m F c_3 \nabla\phi + c_3 u)\cdot n = M(c_2 - Kc_3) \quad \text{at boundary}^{p/m}$$

Here M is a (nonphysical) velocity large enough to let the concentration differences in the brackets approach zero. These boundary conditions also give a continuous flux across the interfaces provided that M is sufficiently large.

2.2 COMSOL

The COMSOL is a modeling package software capable of simulating physical phenomenon. The software can implement interdependent equation by selecting physical phenomena of different characteristics. The program is also capable of creating PDE the user needs and linking it to another physical phenomenon.

3. Calculation Results

The surface plot in figure 3 and 4 visualizes the OH^- and H^+ concentration distribution throughout the model domains – The anodic chamber(Ⅰ) and the cathodic chamber(Ⅱ). The middle region is a dialysate region. The AEM and CEM thicknesses are 0.07mm and the dialysate region thickness is 0.02mm. The length of model is 3mm. The H^+ and OH^- ion's velocity were 10^{-3}m/s^2 in the dialysate region.

The concentration of the dialysate decreases markedly over the first 0.5mm form the inlet. The figure further shows the developing diffusion layers on both sides of the wall. The concentration jump that arises at the boundary between the dialysate and the membrane are also observed.

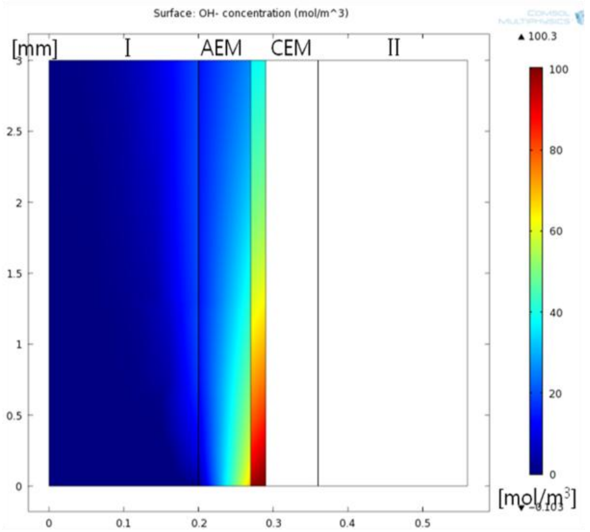

Fig 3. OH^- concentration in the domain

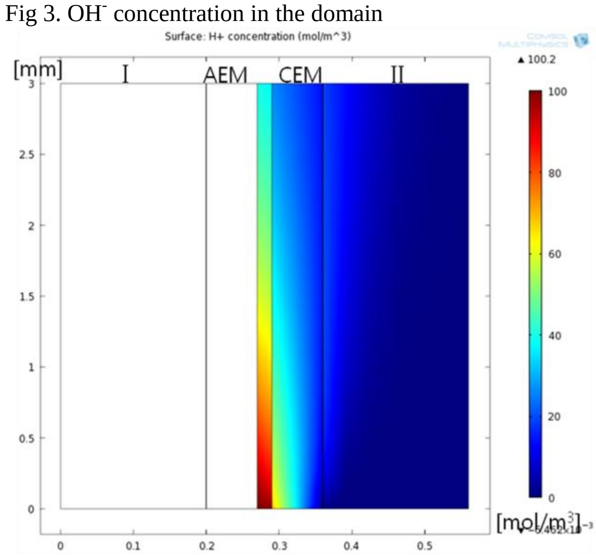

Fig 4. H^+ concentration in the domain

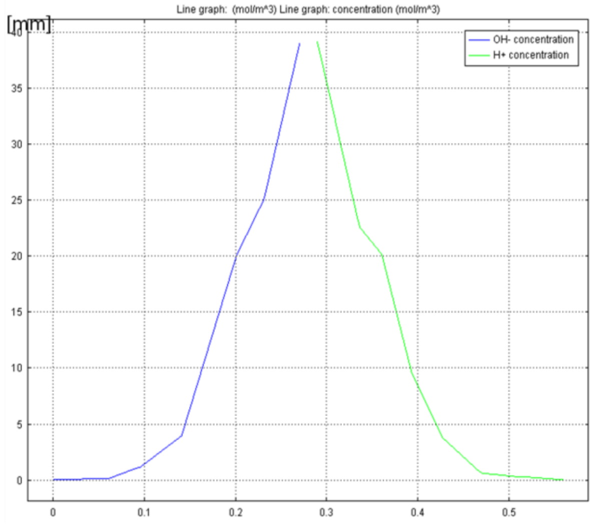

Fig 4. The line graphs of the H^+, OH^- concentration

4. Conclusions

In the study, concentration changes in the ions H^+ and OH^- passing through bipolar membrane consisting of CEM and AEM were simulated. Changes in concentration of each ion as it passed through the membrane were obtained. Further studies will be pursued to compare actual experimental values with theoretical values to establish an optimized system.

REFERENCES

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