Simulation of ion transport in a perfluorinated bi-layer membrane for Chlor-alkali electrolysis process

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[Abstract]

In order to study transport behavior of ions in the membrane for chlor-alkali process, we developed the simulation model based on the Maxwell-Stefan theory. In this study, we considered the distribution of water uptake across the thickness of the membrane and tried to explain the peculiar aspects of high ion-selectivity of Na ion seen in the actual chlor-alkali cell operation.

Flemion ®, a perfluorinated bi-layer membrane, was used for an electrolysis test as shown in Fig.1, and its molecular structure is given as a general formula shown in Fig. 2. Activity of the electrolytes in the membranes was obtained by the absorption experiments in which the concentrations of NaOHaq and NaClaq were changed 5-40wt% and 1-5N respectively, and estimated the key parameters for Pitzer model, which correlates activity with osmotic coefficients for multi-components electrolyte system. According to Maxwell-Stefan theory the interactive parameters of diffusivity are determined in consideration of interactions between fixed ions and cations and anions and water existed in the membrane. In this study the interactive diffusivity between ions and water was given from the published data and both the diffusivity between functional group (COO^-) and cation(Na^+) and one between functional group (COO^-) and anion (OH^-) were obtained from the measurements of membrane resistance and static transport number done in the various concentrations of NaOHaq and NaClaq. Fig.3 shows the relationship between the interactive diffusivities of Na ion (DNa-mem) and OH ion (DOH-mem) plotted against water uptake. Since the interactive diffusivity between the functional groups and water was not given from the above experiments, we estimated them by assuming that the flux of water across the membrane was constant in steady state condition.

The numerical model is one-dimensional one, and as boundary conditions for calculation the concentrations of all species at both surfaces of the membrane were determined so as to satisfy the Donnan equilibrium at the both surfaces. Numerical calculation was carried out on the assumption of steady state condition.

This numerical model gave interesting results. When the electrical current is applied, water uptake at everyplace inside of the membrane increases, and the amount of the flux of electro-osmotic water influences on ion-selectivity of membrane. The proposed numerical model explains well the relationship between electrochemical properties of the membrane and electrolytic performance.

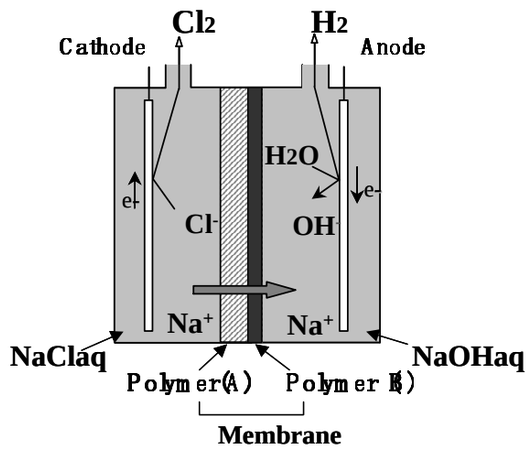

Fig.1.Schematic figure of a membrane cell

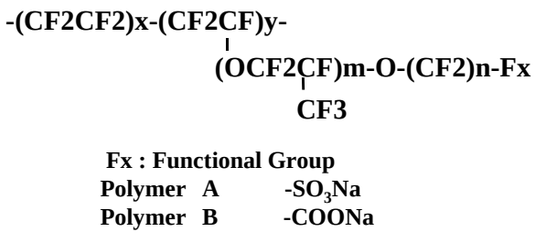

Fig.2 Molecular structure of Flemion ®

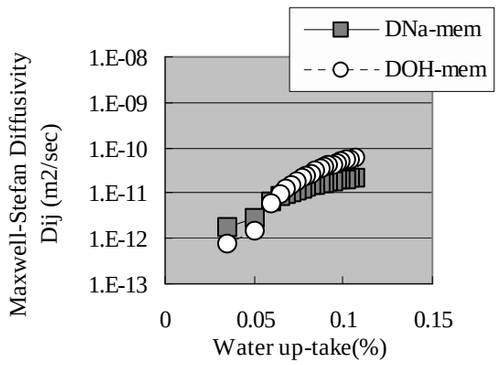

Fig.3 Relationship between Maxwell-Stefan Diffusivity of polymer B and water uptake