XIV International Congress of the Mexican Hydrogen Society
Cancun, Mexico, 2014

Calculations of Water Uptake and IEC Parameters of Ionic Exchange Membranes with Applications in Fuel Cells

Ernesto López-Chávez[*a], Yesica A. Peña-Castañeda[a], Gerardo González-García[a], Patsi Montserrat Perales-Enciso[b], Fray de Landa Castillo-Alvarado[c], Alberto García-Quiroz[a]

[a]Colegio de Ciencia y Tecnología de la Universidad Autónoma de la Ciudad de México. Av. Fray Servando Teresa de Mier 92. Col. Centro. México. D. F, 06080. México.

[b] Ingeniería en Sistemas de Transporte Urbano de la Universidad Autónoma de la Ciudad de México. Av. Fray Servando Teresa de Mier 92. Col. Centro. México. D. F, 06080. México.

[c] Escuela Superior de Física y Matemáticas del Instituto Politécnico Nacional, Unidad Profesional Adolfo López Mateos. Col. Lindavista. Deleg. Gustavo A. Madero. México, D. F., 07738. México.

ABSTRACT

The water uptake (WU) and ion exchange capacity (IEC) are two important parameters for PEMs, which represent their water retention and the proportion of exchangeable protons in the membrane, respectively. According to the vehicle mechanism of proton transport, an appropriate amount of water content and a suitable value of IEC in PEMs is necessary for achieving high proton conductivity. In this work, studies based on Density Functional Theory (DFT), Molecular Mechanics and Dynamics Simulations were realized in order to develop a theoretical methodology to obtain water uptake and ionic exchange capacity parameters. Unlike other methods, our proposal considers the molecular structure of the monomers of the membrane, the solvation medium and the various interactions between the monomer and water molecules. The methodology is applied to structures of sulfonated poly (ether-imide) (SPEI) with $(-SO_3H)_n$ (n=1,…6) groups. These structures were built and optimized aiming to obtain above properties as a function of the number of sulfonyl groups. The comparative study demonstrates that the SPEI with four sulfonyl groups in its backbone is the polymer having better properties for successful operation in fuel cells.

*Keywords:*water uptake; IEC; PEM.