Molecular Dynamics Modeling of Conductive Transport in Proton-Exchange Membrane (PEM) Fuel Cells.


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With the current interest on proton exchange membrane fuel cells there is a renewed interest in understanding the mechanism of proton conduction. This is of special significance in view of recent efforts to extend the operating temperatures to above 100°C, for its associated advantages of better system integration, CO tolerance, cathode electrode kinetics and water and thermal management. For this, however a detailed and fundamental understanding of proton conduction and fully and partly hydrated proton exchange membranes is essential. At the present moment most attempts to model such systems have met with limited success.

The principal factor that strongly influences the proton conductivity in the membrane is determined by the water content [7]. The amount of water present is affected by a number of parameters such as cation form, ion exchange capacity of the membrane and equivalent weight (EW) [8, 9, 10]. In the presence of water, as well as other polar solvents, the sulfonic acid groups dissociate protonating the solvent molecules and forming a hydrophilic phase including the solvated -SO₃⁻ ions tethered to the hydrophobic backbone through the side chain [11].

The model presented, based on the findings of Elliot et al [12], provides a novel approach to modeling proton conduction in PEMs. Rather than a fully connected polymer, the PEM is represented as formed by the association of different species. Such a technique will ensure that the model undergoes all the possible and significant structural changes and rearrangements during the course of the calculation. The theoretical approach adopted can be summarized in two main points: (i) focus on charge transfer processes (CT, intermolecular H⁺ transfer) that have been neglected in previous studies, which demonstrate proton conduction by cation translational diffusion. (ii) Elevating the complexity of the calculation to an ab-initio level allows one to have a better insight on the effect of relative humidity (≈50-60%), operational temperature and structural changes in the polymer.

This approach will enhance the comprehension of chain-bending forces as well as charge transfer between ions, because of the different configuration of the model vs. the real and fully connected polymeric chain.

In conclusion, an improved SCRF model is utilized to provide a realistic description of the shape of the dielectric cavity and increased accuracy in the estimation of the free energy of solvation shell; producing a detailed picture for proton conduction in PEM.

References: