

Suwalee Martkumchan 2009: Molecular Dynamics Simulation of Ion Conduction in Chitosan Membrane for PEM Fuel Cell. Master of Engineering (Chemical Engineering), Major Field: Chemical Engineering, Department of Chemical Engineering. Thesis Advisor: Associate Professor Thongchai Srinophakun, Ph.D. 81 pages.

The propose of this research was to study the ion conductivity mechanism of chitosan membrane at the molecular level. Chitosan materials were formulated by molecular dynamics simulation named Materials Studio 4.3 using COMPASS force field. The systems contained chitosan, hydronium ions and various amounts of water, 10, 20, 30 and 40 wt% of water. The molecular dynamics simulation was used to estimate the diffusion coefficient, the ion conductivity and the coordinations between particles. The system containing 40 % of water by weight was suitable as a conducting material, which had an ion conductivity value of 10^{-2} S/cm. The results were compared with reference reported experimental data. Such material was studied in the temperature range of 298 – 360 K. The resulting conductivity followed Arrhenius behavior. Chitosan 70, 80 and 90 degree of deacetylation were studied at constant 40 % of water by weight. As a result, the ion conductivities were similar to the 40 % of water system. The coordination was studied to evaluate the location of particles in the system to understand the transport mechanism of the ions. Conductivity was appropriate in the systems in which the eigen ion and water clusters formed.

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Thesis Advisor's signature

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