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Analytical model describes ion conduction in fuel cell membranes[1] DANIEL HERBST, STEVE TSE, THOMAS WITTEN, University of Chicago — Many fuel cell designs employ polyelectrolyte membranes, but little is known about how to tune the parameters (water level, morphology, etc.) to maximize ion conductivity. We came up with a simple model based on a random, discrete water distribution and ion confinement due to neighboring polymer. The results quantitatively agree with molecular dynamics (MD) simulations and explain experimental observations. We find that when the ratio of water volume to polymer volume, V_w/V_p, is small, the predicted ion self-diffusion coefficient scales roughly as $D_w(T)\sqrt{V_w/V_p}\exp(-\cdots V_p/V_w)$, where $D_w(T)$ is the limiting value in pure water at temperature T. At high water levels the model also agrees with MD simulation, plateauing to $D_w(T)$. The model predicts a maximum conductivity at a water level higher than is typically used, and that it would be beneficial to increase water retention even at the expense of lower ion concentration. Also, membranes would conduct better if they phase-separated into water-rich and polymer-rich regions.

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