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Theoretical and simulation study of charge distribution and transport in ionomers[1] PHILIP TAYLOR, ELSHAD ALLAHYAROV, Case Western Reserve University, KAYTLIN BRINKER, University of Michigan, ZACHARY TOBIN, Caltech — We have used a combination of analytical theory and simulation to investigate the effect of various material parameters on the proton conductivity of Nafion-like polyelectrolyte membranes. We make use of a cylindrical geometry to model both a hydrophilic channel of small diameter and an ionomer-filled cylindrical pore of larger size. For the water-filled channel we find the proton density distribution as a function of distance from the electrode and from the cylinder axis by means of a combination of a modified Butler-Volmer-Frumkin theory and a lattice-based simulation. For the ionomer-filled pore we study by coarse-grained simulation the proton conductance as a function of sidechain length, with particular attention to the regime where the radius of the cylinder approximates the sidechain length.

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