

Modeling of Electrochemical Cells:
Proton Exchange Membrane Fuel Cells
HYD7007 – 01
Yonsei University

Homework Assignment 02
Spring, 2011

1. The procedure used to describe charge transport in PEMs is described in class as multiscale modeling. This procedure includes several components, such as reactive molecular dynamics, confined random walk theory, and percolation theory. Discuss the level of description of each technique. What information does each technique provide? How is the combined procedure more powerful than the individual parts?
2. Describe a potential application in your own area of research, where you could potentially use multiscale modeling (at least two scales). What information would be required and provided at each scale?
3. Consider a the percolation theory described in the notes of Lecture 06, where the diffusivity of an open pore, D_o , is 1 and the diffusivity of a blocked pore, D_b , is 0. Plot D_{eff} as a function of p_{EMA} for $z=4$ and $z=6$. Explain the behavior as a function of p_{EMA} and z . A percolation threshold is defined as the value of p_{EMA} where D_{eff} goes to zero. Where is the percolation threshold for $z=4$ and $z=6$?