1100-70-111 **Taylor Farley***, taylor.farley@ttu.edu, and **Mark Vaughn**. *Molecular and mesoscale properties of pores.*

Understanding the mechanisms by which small particles move through pores in a thin substrate is important for rational design of filter and purification media. Controlling water quality is an important application of porous films designed to prevent certain molecules and particulates from passing through pores, while allowing water to pass freely. Improving the quality of highly contaminated water is a challenge.

A realistic model of the filtration process at the atomic scale could assist in designing filters that take advantage of the properties of modern exotic materals. While much is known about macroscale phenomological models of filtration, these models typically are not predictive. We are developing a computational model that can take into account the molecular and mesoscale properties of the pores and the particles. The model allows study of diffusing particles in a pore. The particle is allow to interact with the walls of the pore where it may be absorbed. Finally, to gain insight into the process of diffusion in a pore and to verify assumptions of the model we use video microscopy to observe particles diffusing in narrow glass capillaries. (Received February 04, 2014)