

Abstract Submitted  
for the MAR13 Meeting of  
The American Physical Society

**States of Water in Non-Equilibrium Glassy Polymers** ERIC DAVIS, YOSSEF ELABD, Chemical and Biological Engineering Department, Drexel University — For many applications (e.g., packaging, medical devices) a deeper fundamental understanding of the molecular nature of water in glassy polymer coatings is of significant interest. In this study, the sorption and diffusion of water in two glassy polymers, poly(methyl methacrylate) (PMMA) and poly(styrene) (PS), were measured with both quartz crystal microbalance (QCM) and time-resolved Fourier transform infrared-attenuated total reflectance (FTIR-ATR) spectroscopy. Non-Fickian diffusion was observed in both PMMA and PS using both experimental techniques due to the non-equilibrium state of the polymers. The specific states of water were observed with FTIR-ATR spectroscopy, where dimers exist in PMMA below a critical concentration and larger clusters were observed above this concentration. Contrastingly, water only exists in PS as larger clusters over the entire sorption isotherm. A correlation between the states of water and the diffusive activation energy of water was observed. Additionally, the pseudo-equilibrium water sorption isotherms in PMMA and PS were accurately predicted with the non-equilibrium statistical associating fluid theory (NE-SAFT). We predict that the combination of time-resolved FTIR-ATR spectroscopy and NE-SAFT can be used on other water-glassy polymer systems to provide a molecular understanding of non-equilibrium sorption and diffusion.

Eric Davis  
Chemical and Biological Engineering Department, Drexel University

Date submitted: 17 Nov 2012

Electronic form version 1.4