Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Multicomponent Diffusion of Penetrant Mixtures in Rubbery Polymers: A Molecular Dynamics Study STEFAN BRINGUIER, MARK VARADY, OptiMetrics, Inc. a DCS Company, CRAIG KNOX, Leidos, Inc., JERRY CABALO, R&T Directorate, Edgewood Chemical Biological Center, THOMAS PEARL, OptiMetrics, Inc. a DCS Company, BRENT MANTOOTH, R&T Directorate, Edgewood Chemical Biological Center — The importance of understanding transport of chemical species across liquid-solid boundaries is of particular interest in the decontamination of harmful chemicals absorbed within polymeric materials. To characterize processes associated with liquid-phase extraction of absorbed species from polymers, it is necessary to determine an appropriate physical description of species transport in multicomponent systems. The Maxwell-Stefan (M-S) formulation is a rigorous description of mass transport in multicomponent solutions, in which, mutual diffusivities determine the degree of relative motion between interacting molecules in response to a chemical potential gradient. The work presented focuses on the determination of M-S diffusivities from molecular dynamics (MD) simulations of nerve agent O-ethyl S-[2(diisopropylamino)ethyl] methylphosphonothioate (VX), water, and methanol mixtures within a poly(dimethylsiloxane) matrix. We investigate the composition dependence of M-S diffusivities and compare the results to values predicted using empirical relations for binary and ternary mixtures. Finally, we highlight the pertinent differences in molecular mechanisms associated with species transport and employ non-equilibrium MD to probe transport across the mixture-polymer interface.

Stefan Bringuier
OptiMetrics, Inc. a DCS Company

Date submitted: 05 Nov 2015 Electronic form version 1.4