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Continuum Model for Decontamination of Chemical Warfare Agent from a Rubbery Polymer using the Maxwell-Stefan Formulation MARK VARADY, STEFAN BRINGUIER, THOMAS PEARL, OptiMetrics, Inc., a DCS Company, SHAWN STEVENSON, BRENT MANTOOTH, RT Directorate, Edgewood Chemical Biological Center — Decontamination of polymers exposed to chemical warfare agents (CWA) often proceeds by application of a liquid solution. Absorption of some decontaminant components proceed concurrently with extraction of the CWA, resulting in multicomponent diffusion in the polymer. In this work, the Maxwell-Stefan equations were used with the Flory-Huggins model of species activity to mathematically describe the transport of two species within a polymer. This model was used to predict the extraction of the nerve agent O-ethyl S-[2(diisopropylamino)ethyl] methylphosphonothioate (VX) from a silicone elastomer into both water and methanol. Comparisons with experimental results show good agreement with minimal fitting of model parameters from pure component uptake data. Reaction of the extracted VX with sodium hydroxide in the liquid-phase was also modeled and used to predict the overall rate of destruction of VX. Although the reaction proceeds more slowly in the methanol-based solution compared to the aqueous solution, the extraction rate is faster due to increasing VX mobility as methanol absorbs into the silicone, resulting in an overall faster rate of VX destruction.

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