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Modeling the transport of chemical warfare agents and simulants in polymeric substrates for reactive decontamination THOMAS PEARL, OptiMetrics Inc., a DCS company, Abingdon, MD 21009, BRENT MANTOOTH, Edgewood Chemical Biological Center, APG, MD 21010, MARK VARADY, OptiMetrics Inc., a DCS company, Abingdon, MD 21009, MATTHEW WILLIS, Edgewood Chemical Biological Center, APG, MD 21010 — Chemical warfare agent simulants are often used for environmental testing in place of highly toxic agents. This work sets the foundation for modeling decontamination of absorbing polymeric materials with the focus on determining relationships between agents and simulants. The correlations of agents to simulants must consider the three way interactions in the chemical-material-decontaminant system where transport and reaction occur in polymer materials. To this end, diffusion modeling of the subsurface transport of simulants and live chemical warfare agents was conducted for various polymer systems (e.g., paint coatings) with and without reaction pathways with applied decontamination. The models utilized 1D and 2D finite difference diffusion and reaction models to simulate absorption and reaction in the polymers, and subsequent flux of the chemicals out of the polymers. Experimental data including vapor flux measurements and dynamic contact angle measurements were used to determine model input parameters. Through modeling, an understanding of the relationship of simulant to live chemical warfare agent was established, focusing on vapor emission of agents and simulants from materials.

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