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Reactive decontamination of absorbing thin film polymer coatings: model development and parameter determination MARK VARADY, OptiMetrics, Inc. a DCS Company, Abingdon, MD, 21009, BRENT MANTOOTH, Edgewood Chemical Biological Center, APG, MD 21010, THOMAS PEARL, OptiMetrics, Inc. a DCS Company, Abingdon, MD, 21009, MATTHEW WILLIS, Edgewood Chemical Biological Center, APG, MD 21010 — A continuum model of reactive decontamination in absorbing polymeric thin film substrates exposed to the chemical warfare agent O-ethyl S-[2-(diisopropylamino)ethyl] methylphosphonothioate (known as VX) was developed to assess the performance of various decontaminants. Experiments were performed in conjunction with an inverse analysis method to obtain the necessary model parameters. The experiments involved contaminating a substrate with a fixed VX exposure, applying a decontaminant, followed by a time-resolved, liquid phase extraction of the absorbing substrate to measure the residual contaminant by chromatography. Decontamination model parameters were uniquely determined using the Levenberg-Marquardt nonlinear least squares fitting technique to best fit the experimental time evolution of extracted mass. The model was implemented numerically in both a 2D axisymmetric finite element program and a 1D finite difference code, and it was found that the more computationally efficient 1D implementation was sufficiently accurate. The resulting decontamination model provides an accurate quantification of contaminant concentration profile in the material, which is necessary to assess exposure hazards.

Mark Varady
OptiMetrics, Inc. a DCS Company, 100 Walter Ward Boulevard,
Suite 100, Abingdon, MD, 21009

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