Modeling Of Chemical Warfare Agent Decontamination Dynamics Of Protective Military Coatings

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Abstract

Chemical warfare agent (CWA) decontamination is a critical operation for safely returning contaminated military assets to service. Development of effective decontamination procedures for full-scale assets is highly scenario dependent and presents a difficult task because experiments are extremely dangerous and expensive. Field-deployable computational tools that can accurately model the transport and reaction of CWA on military assets and capture scenario-dependent variables could enable cost-effective operational decontamination procedures.

Most military assets utilize polymer-based protective coatings comprising a large fraction of their exposed surface and thus are most susceptible in a CWA exposure. This work develops COMSOL models of (1) liquid-phase CWA spreading and sorption in polymer-based coatings, (2) extraction into a decontamination solution and reaction, and (3) post decontamination vapor emission and contact transfer. The chemical diffusion model is implemented using the General Form PDE module, which enables the use of the generalized Maxwell-Stefan model with the viscoelastic response of the polymer included in the chemical potential of the system. The models are incorporated into a single computational tool that uses the LiveLink for MATLAB functionality to take user inputs, construct the COMSOL models, and postprocess results.

Results for selected case studies are presented and demonstrate optimizing the timing of the CWA decontamination process, addressing logistical challenges, and guiding the product development process.

Reference

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Figures used in the abstract

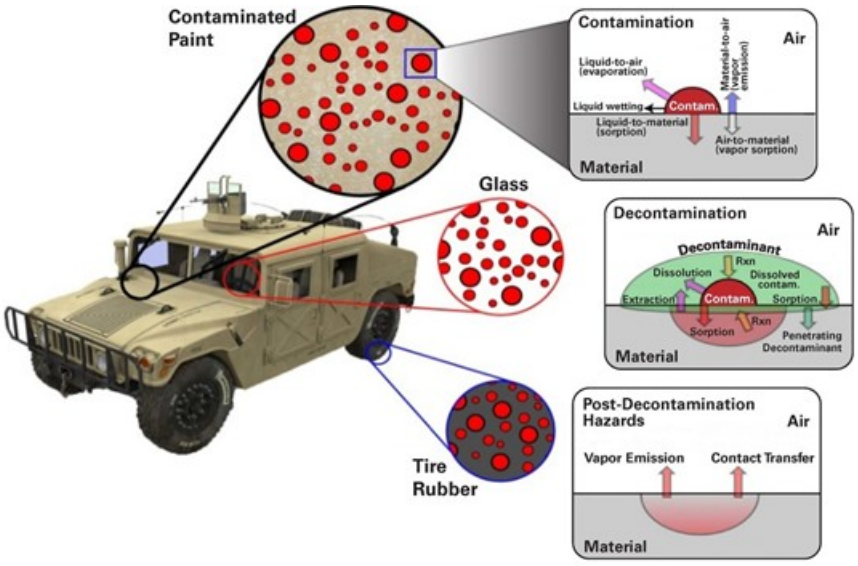

Figure 1 : Schematic of transport and reaction processes occurring for chemical warfare agent (CWA) droplets on a military asset