Environmental Fate of Low Volatility Agents on Operational Surfaces Using New Hazard Prediction Tools

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Hazard prediction modeling requires a clear understanding of the physicochemical interactions and environmental processes governing the fate of chemical threats in the environment. The primary objective of agent fate modeling is to provide operational tools to mitigate vapor and contact hazards of chemical threats. By implementing best practices of known estimation models, the prediction of the secondary evaporation and environmental fate of a multicomponent chemical threat droplet dispersed on operational substrates in an outdoor environment over time is attainable. Chemical warfare agents (CWAs) and Toxic Industrial Chemicals (TICs) that have low vapor pressures can persist in the environment for a substantial time and can penetrate into porous and permeable substrates causing potential exposures to personnel on the ground. SRC, Inc has continued to work with DTRA to develop and expand the capabilities of the secondary evaporation model known as the Droplet Reaction and Evaporation of Agents Model (DREAM). DREAM's objective is to simulate and predict the environmental fate of a single sessile, multicomponent chemical threat droplet on a substrate in an outdoor environment over time. Specifically, DREAM predicts the time dependent evaporation rate, degradation reactions, and mass of a remaining of a chemical threat droplet on a variety of outdoor surfaces. This information can be analyzed independently in a standalone application or in conjunction with atmospheric transport and dispersion (AT&D) models such as the Second-order Closure Integrated Puff, (SCIPUFF) model deployed in the Hazard Prediction Assessment Capability (HPAC) and Joint Effects Model (JEM) to inform the persistence of chemical threats released in the environment. Utilizing experimentally measured wind tunnel and droplet geometry data, in addition to quantum chemical computational data developed in collaboration with CCDC CBC, ENSCO, and Avarint, SRC expanded the model's applicability to include 13 new CWAs and TICs, an increase of 59 agent substrate combinations. Some of the key features allowing this expansion are the addition of temperature and pH dependent parameters such as base catalyzed reaction kinetics and development of a fragment based Quantitative Structure Property Relationship (QSPR) for determination of molar volume, and integration of measured droplet geometry parameters such as contact angle. These adaptations and several algorithm refinements resulted in much better agreement between experimental droplet evaporation data and modeled output of DREAM. In addition, progress towards the environmental adaptation of DREAM has resulted in preliminary equations to support the environmental fate of agents on soil and plants that will capitalize on the ongoing agent fate research in measuring sorption and partition coefficients. Using the methodologies developed under this effort, SRC will continue to add new agents and environmental parameters in future releases of DREAM to create a more relevant and operationally useful secondary evaporation model.