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A Resistance Chemical Vapor Deposition Model Extended To Tics, Tims, And CWAs: Model Sensitivity Insights

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Hazardous chemicals are used in industry, commerce, and by warfighters and their adversaries. During an airborne release of chemicals to the environment, ground deposition and re-aerosolization represent both real-time and delayed hazards to ground personnel. When modeling airborne releases of hazardous material, we at the Defense Threat Reduction Agency (DTRA) Reachback office use the Hazard Prediction and Assessment Capability (HPAC) software, which incorporates a rudimentary representation of the deposition velocity parameter. Ultimately, a material's deposition velocity determines how quickly it is deposited on the ground or canopy, and the temporal geospatial extent of the hazard plume. Unfortunately, experimental values are sorely lacking in the literature for operational use and model validation. We have incorporated a more robust representation of ground deposition in the context of Wesely's resistance model, which accounts for both vegetative canopy and meteorological contributions to uptake of gaseous material into the environment. This advanced deposition model has been used in atmospheric sciences for several decades for use with a select set of atmospherically relevant hazardous materials. Wesely's model incorporates chemical-specific parameters accounting for reactivity, aqueous solubility, and gas-phase diffusivity. Releases of chemical warfare agents (CWAs) and many toxic industrial chemicals (TICs) fall outside of the validated set of materials traditionally used with the Wesely model. As such, we performed a multivariate sensitivity analysis to determine the variables' magnitude-of-effect on the computed deposition velocity and correlations between the variables for materials available in the HPAC software suite. The results highlight a greater need for experiments incorporating vegetative uptake measurements, as the physicochemical interaction between the material and the type of land cover has the strongest influence on the deposition velocity.