THREAT AGENT DEFEAT MODELING AND TESTING

Cbr Defense Technologies And Non-covalent Chemistry Interactions

James Lee NSWCIH

There are questions that have to be answered when designing or modifying products that will sequester or decontaminate chemical warfare agents; (1) will this chemical agent absorb into the surface that needs to be cleaned; (2) will the decontamination solution solubilize this chemical agent; and / or (3) will the sequestering technology (polymer) absorb and trap the chemical agent? One method to answer these questions is to perform live agent testing. However, it is impractical to test all scenarios of interest due to cost and schedule constraints. In addition, testing does not provide the rapid turnaround needed for a new threat encountered in active battle field scenarios. It would be ideal to have a model (software) that predicted agent solubility and polymer absorption (+90% accuracy) in order to provide quick turn-around answers that can be acted upon now; spot checks could still be used to check model predictions later. Consequently, this model would enable first responder or joint force response protocols to be in place much faster. The existing industry models based on heuristics (like Hansen Solubility Parameters) do not work, as we have tested them on products developed in the Navy. Other models (like quantum chemical / Monte Carlo computational methods) are time and resource intensive or only consider very specific interactions like drug receptor sites. We have discovered novel relationships that can be used to predict molecular interaction energies that do not appear in the scientific literature (publications in progress). Preliminary work indicates that these relationships can be used as a basis to begin constructing this ideal model for predicting solubility and polymer absorption.

Approved for public release; distribution is unlimited.