

PROTECTION - SCIENCE AND TECHNOLOGY ADVANCES FOR CHEMICAL AND BIOLOGICAL PROTECTION

Characterization Of Zirconium Hydroxide And Mof-doped Materials For Cwa Neutralization

Katherine Simpson Arctos Rashelle McDonald Arctos Bruce Salter Arctos Daniel Freedman Army Natick CCDC Natalie Pomerantz Army Natick CCDC Jeffery Owens AFCEC/CXAE

In recent years there has been increased interest in the use of Metal-Organic Frameworks—also known as MOFs—for the mitigation of chemical warfare agents (CWAs) and other harmful substances. MOFs are coveted for their high surface area and sorbent properties, which provide excellent uptake and affinity for CWA compounds. Additionally, zirconium hydroxide $[Zr(OH)_4]$ possesses strong nucleophilic character and serves to promote hydrolysis of CWAs and other threats. Towards the development of a textile for CWA mitigation, an aqueous formulation of $Zr(OH)_4$ and the MOF UiO-66-NH₂ was bound to a cotton textile using tetraethyl orthosilicate (TEOS) and microwave curing. These materials were prepared on a medium-scale industrial microwave textile line, developed in-house at Tyndall AFB. This method ensures scalability of the process and chemistry in the event of a successful candidate requiring technology transition.

Headspace permeation analyses were performed on these fabrics using Gas Chromatography-Mass Spectrometry (GC-MS). The treated textiles were characterized by infrared spectroscopy and X-ray fluorescence and were shown to contain $Zr(OH)_4$. Scanning electron microscopy revealed the presence of micro particles (10–30 μm) bound to the surface and surrounding the cotton fibrils. The wet-weight pickup was also measured in order to determine the scalability and reagent consumption required to produce the treated textile. Some materials were washed in order to test durability, while others were tested without laundering as part of the Uniform Integrated Protective Ensemble (UIPE) criteria. The treated samples effectively reduced the breakthrough of diisopropyl fluorophosphate and bis(2-chloroethyl)sulfide, each tested in separate GC-MS headspace analyses. Breakthrough curves were also obtained for samples against dimethyl methylphosphonate.

The treated materials were also tested for antimicrobial efficacy using the AATCC 147 parallel streak test method. Samples were examined for the presence of a zone of inhibition surrounding the fabric on the petri dish, seeded with a confluent lawn of *Pseudomonas fluorescens* or *Bacillus anthracis*-Sterne strain. No zone of inhibition was visible in the materials, however, it does appear that they are bacteriostatic.

Joe Rossin and Guild Associates, Inc.