Reactions on Zorflex Activated Carbon Cloth with CW Agents Measured Using NMR, GC, and MS Techniques

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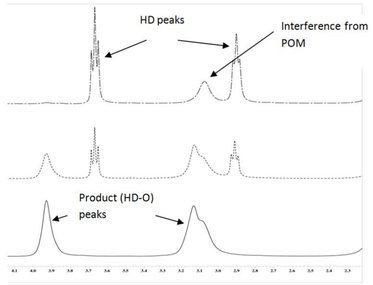
Introduction

Integrated Protective Fabric System (IPFS) Program materials are being studied for garment systems that will provide improved water and thermal transport while also providing improved protection for the warfighter against chemical weapons agent (CWA) and biological agent permeation. Zorflex® activated carbon cloth (Calgon Carbon, Pittsburgh, PA) is a woven cloth that allows water and air permeation but has high absorption and surface area to absorb organic molecules. Performance is improved by adding reactive components to the cloth that will react with CWA to cause decontamination. Studies of cloth treated with several reactive compounds were done against the agents HD, GD, and VX, and the simulant CEES. Determining the reactivity on cloth requires a number of complementary methods since the strong absorption on the cloth can prevent analysis of analytes. The reactivity was studied by using solids and liquids nuclear magnetic resonance (NMR). Studies of permeation of CWA through the fabric were studied with a novel headspace GC method using a vial in a vial. Samples of fabric were also solvent extracted to determine residual CWA and to identify reaction products using GC/MS and LC/MS. Reactions of reagents in solution were done to determine kinetics in a homogeneous system. Reactions were also studied in the presence of common battlefield contaminants, in particular JP8 fuel, which can saturate the carbon cloth.

Nuclear Magnetic Resonance (NMR) Methods:

- Solids NMR using a high-speed rotor is used to study reaction of neat CW agent on solid materials.
- CWA can also be deposited on solid and solvent extracted, and then run by liquids NMR to perform quantitation of starting reagents and products.
- Reactivity of reagents was studied in solution to determine kinetics.
- Extracts are also run by GC/MS and LC/MS.

Reaction of HD with POM:



Kinetics can be determined from multiple NMR runs on the same sample.
Reaction was observed even when the fabric was saturated with JP8 fuel.

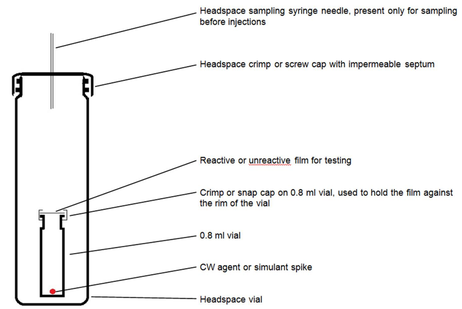
Polyoxometalates (POM) on activated carbon cloth: Calgon Zorflex™ carbon film was received from Natick Soldier Research, Development, and Engineering Center (SRDEC), Natick, MA. Polyoxometalate (POM) compounds were obtained from Prof. Craig Hill and Dr. Zhen Luo, Emory University, Atlanta, GA. POM was applied to the Zorflex fabric at Natick.

Nanoparticles on ACC: Metal oxide nanoparticles were deposited and tested for reactivity.

Technical reports with more details about methods and results are in preparation.

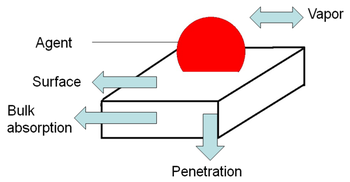
GC Methods:

The Headspace vial-in-vial method has been developed for determining permeation through a film of reactive material. CWA is placed in the inner vial, and permeates through the film into the outer vial. It is sampled and analyzed by Headspace GC.



Conclusion:

A large number of fabric systems have been tested to determine performance with CWA in ways that give consistent results. Multiple analytical methods are needed to study reactions on solid materials. The CWA can be distributed in multiple locations.



Vapor and penetration are the main immediate hazards to the wearer. But the bulk absorption and reactions raise questions about long-term safety. More alternate spectroscopic methods are needed to determine 100% mass balance and fate of the agent. High throughput, operando methods are under development to obtain more information about the distribution of the CWA throughout the material under different environmental and operational conditions. Methods will be developed for acceptance testing and QC of the materials.

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